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Supporting Information

Rapid and Quantitative Detection of the Inflammatory Marker Neopterin Based on a Visible Luminescent Zn(II)-Eu(III) Nanocluster

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Concents

1. General Procedures

All chemical materials and solvents were purchased from commercial sources. IR spectra were determined on a FTIR-650 spectrometer. The thermogravimetric analyses were carried out on a Perking Elmer Diamond TG-DTA spectrum GX. The sample is under a N_2 flow of 200 mL min^{-1}, and heated from room temperature to 800 °C with a heating rate of 5°C min^{-1}. NMR spectra were recorded on an AVANCE III AV500 at 298 K. Dynamic light scattering (DLS) measurement was carried out on a Malvern Zetasizer Nano ZS. Scanning electron microscopy (SEM) and elemental mapping images were obtained from a Nova NanoSEM 200 microscope. Transmission electron microscopy (TEM) images were recorded on a JEOL JEM-2100F transmission electron microscope with the sample after dried from the CH_3CN solution. The UV-vis absorbance spectra were measured on an UV-3600 spectrophotometer. Visible emission spectra were recorded on a FLS 980 fluorimeter. The light source for the spectra was a 450 W xenon arc lamp with continuous spectral distribution from 190 to 2600 nm. The luminescence detection to the analyte was carried out in fetal calf serum (FCS), and simulated urine containing Na_2SO_4, NH_4Cl, NaCl, KCl, creatinine, creatine, glucose, glycine and urea. The color of emission light of the complex with the addition of the analyte was checked using a ZF-20D UV lamp. The test papers used to detect the analyte were prepared by soaking the strip-type filter papers in the CH_3CN solution of the complex for 10 mins, and then dried in oven at 110 °C overnight.

The analysis of frontier molecular orbitals. The energy levels of frontier molecular orbitals of the Schiff base ligand were calculated using density functional theory (DFT) in the Gaussian16 package.[1] The input structure was derived from the cif file. Optimizations are carried out in gas phase using the B3LYP functional.[2] All the optimizations are carried out with 6-311++G** and Stuttgart effective core-potential (ECP).[3]

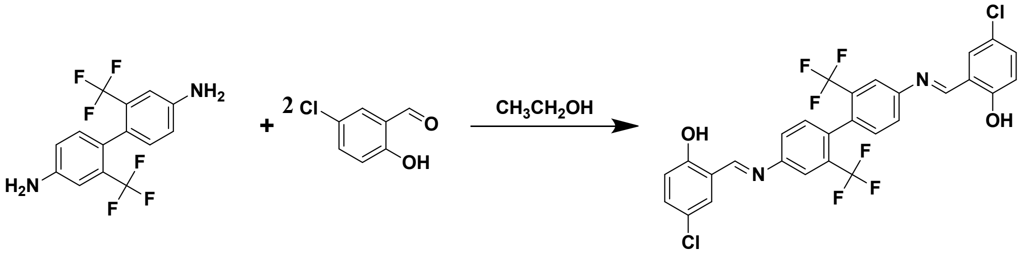
[1] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.;

Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A.; Peralta, Jr., J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16*, *Revision C.01*, *Gaussian*, *Inc.*, *Wallingford CT*, **2019**.

[2] (a) Becke, A. D. *J. Chem .Phys.* **1993**, *98*, 5648-5652; (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785-789; (c) Vosko, S. H.; Wilk, L.; Nusair, M.; *Can. J. Phys.* **1980**, *58*, 1200-1211; (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623-11627.

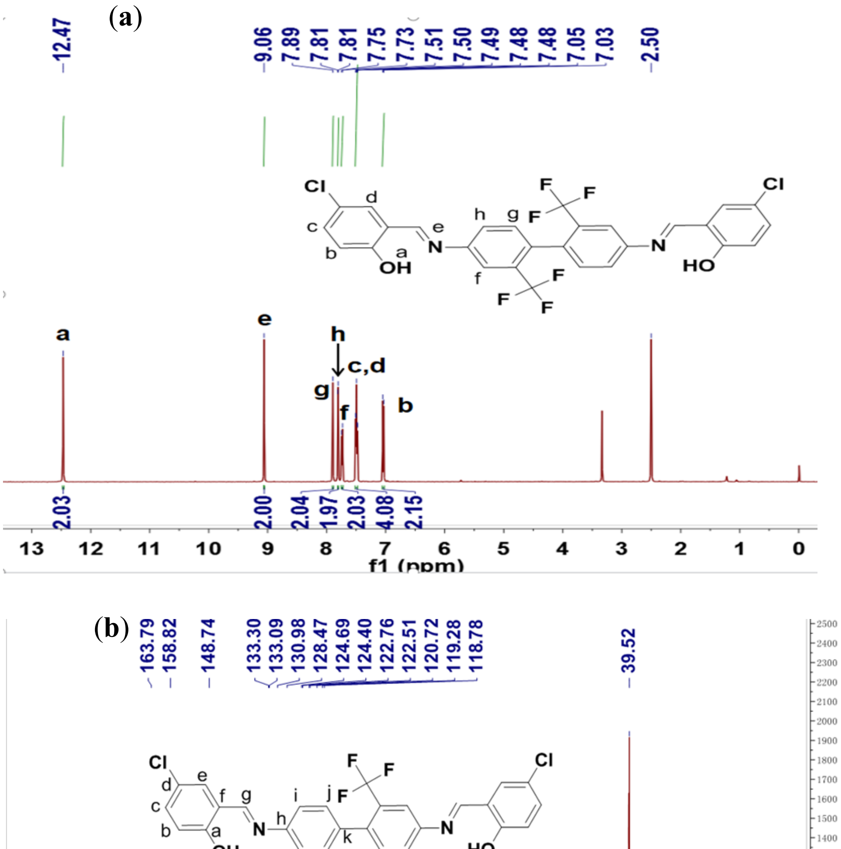
[3] (a) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1987**, *86*, 866-872; (b) Dolg, M.; Stoll, H.; Preuss, H. *J. Chem. Phys.* **1989**, *90*, 1730-1734.

2. Synthesis of H_2L, 1 and the Gd(III) analogue



Scheme S1. The synthetic route of H_2L.

Synthesis of H_2L. A 10 mL EtOH solution of 2,2'-bis(trifluoromethyl)benzidine (1.5 mmol, 0.48 g) was added drop by drop to a 10 mL EtOH solution of 5-chlorosalicylaldehyde (3.0 mmol, 0.47 g). The resulting solution was stirred and heated at 100°C for 3 hrs to give light yellow solid of H_2L. The product was obtained by vacuum filtration, and washed three times using EtOH (3 × 5 mL). Yield: 0.86 g (96%). ^1H NMR (500 MHz, DMSO, δ): 12.47 (s, 2H), 9.06 (s, 2H), 7.89 (s, 2H), 7.81 (d, J = 2.5 Hz, 2H), 7.75 (d, J = 8.1 Hz, 2H), 7.50–7.48 (m, 4H), 7.05 (d, J = 8.7 Hz, 2H). ^{13}C NMR (500 MHz, DMSO, δ): 163.8, 158.8, 148.7, 134.6, 133.3, 133.1, 131.0, 128.5, 124.4, 123.6, 122.8, 120.7, 119.3, 118.8. IR (KBr, cm^{-1}): 3874 (m), 3385 (s), 1571 (s), 1426 (s), 1260 (w), 1165 (m), 1129 (w), 952 (w), 689 (s), 619 (m).



^{13}C NMR (500 MHz, DMSO) δ 163.8(g), 158.8(d), 148.7(h), 134.6(c), 133.3(l), 133.1(b), 131.0(j), 128.5(k), 124.4(i), 123.6(m), 122.8(a), 120.7(n), 119.3(f), 118.8(e).

Figure S1. ^{1}H NMR (**a**) and ^{13}C NMR (**b**) spectra of the ligand H_2L.

Synthesis of the nanocluster 1. $Eu(OAc)_3 \cdot 6H_2O$ (0.20 mmol, 0.065g), $Zn(CF_3SO_3)_2 \cdot 4H_2O$ (0.20 mmol, 0.073 g), H_2L (0.20 mmol, 0.12 g) were dissolved in a mixed solutioin of EtOH (6 mL), MeOH (4 mL) and DMF (1mL), and then triethylamine in 1 mL of MeOH (1.0 mol/L) was added. The resulting solution was heated to reflux with stirring in the air for 30 mins, and then left to cool at room temperature. The yellow crystalline product of **1** was formed after one month by slow vapor diffusion of diethyl ether into the solution. Yield (based on $Eu(OAc)_3 \cdot 4H_2O$): 0.0130g (15%). IR (KBr, cm^{-1}): 3867 (s), 3658 (s), 3390 (m), 1562 (s), 1420 (s), 1253 (w), 1168 (m), 1036 (m), 945 (w), 838 (w), 672 (m), 628 (m). m. p. > 236 ^{o}C (decomposed).

Synthesis of the Gd(III) analogue: The synthetic procedure was the same as that for **1** using $Gd(OAc)_3 \cdot 6H_2O$ (0.20 mmol, 0.088 g), $Zn(CF_3SO_3)_2 \cdot 4H_2O$ (0.2 mmol, 0.087 g), H_2L (0.20 mmol, 0.12 g). The yellow crystalline product of the Gd(III) analogue was obtained after one month by slow vapor diffusion of diethyl ether into the solution. Yield (based on $Gd(OAc)_3 \cdot 6H_2O$): 0.0123 g (12%). IR (KBr, cm^{-1}): 3857 (s), 3654 (s), 3395 (m), 1572 (s), 1410 (s), 1248 (w), 1170 (m), 1030 (m), 943 (w), 835 (w), 682(m), 613 (m). m. p. > 239 ^{o}C (decompose).

3. IR spectra of H_2L and 1

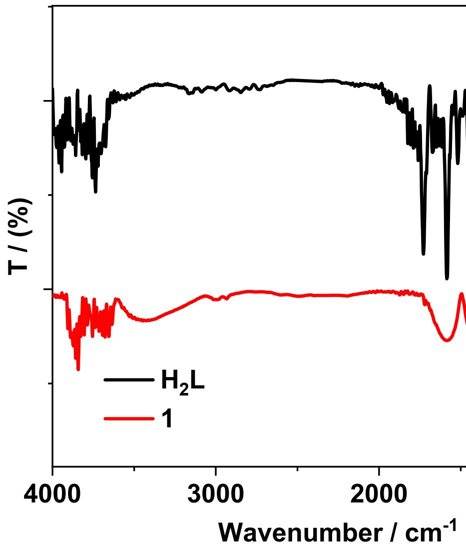


Figure S2. IR spectra of the ligand H_2L and **1**.

4. The PXRD spectrum of 1

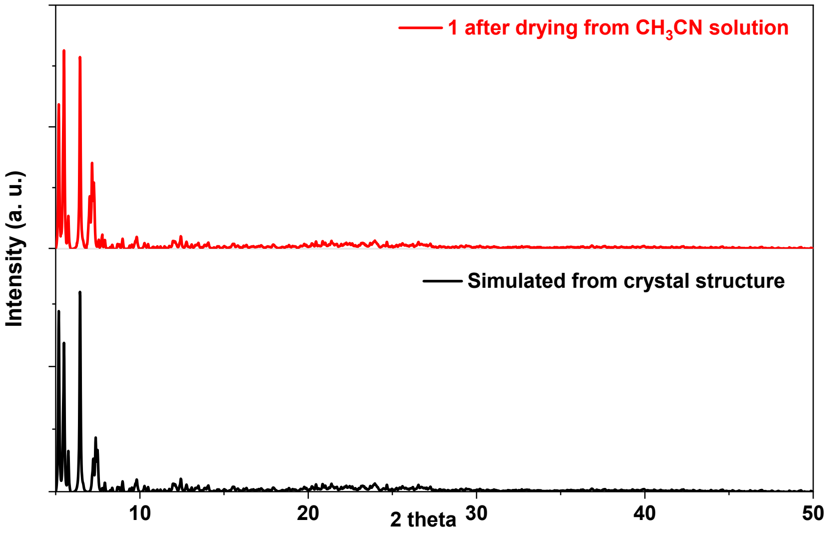


Figure S3. The PXRD spectrum of the solid sample of **1** (red).

5. The thermogravimetric analysis of 1

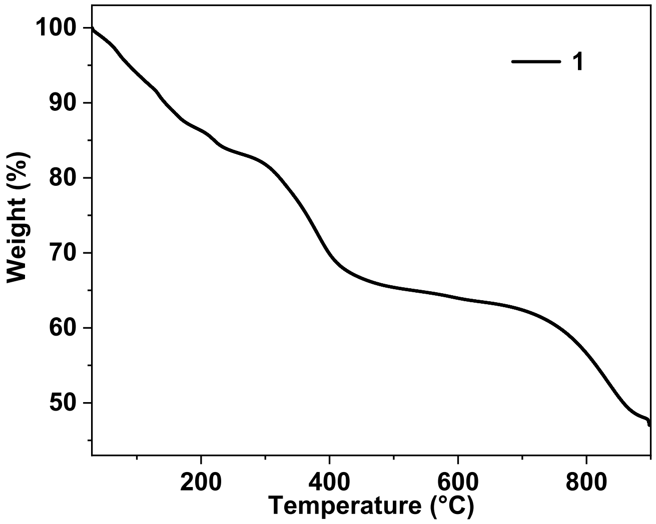


Figure S4. The thermogravimetric analysis of **1**.

6. UV-vis absorption spectra of H_2L, 1 and Neo

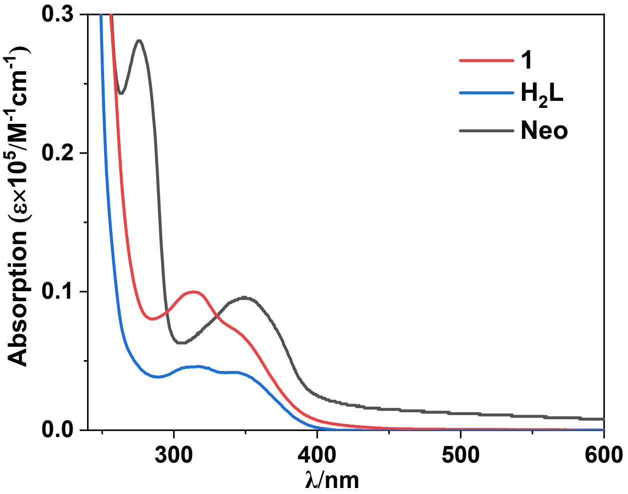
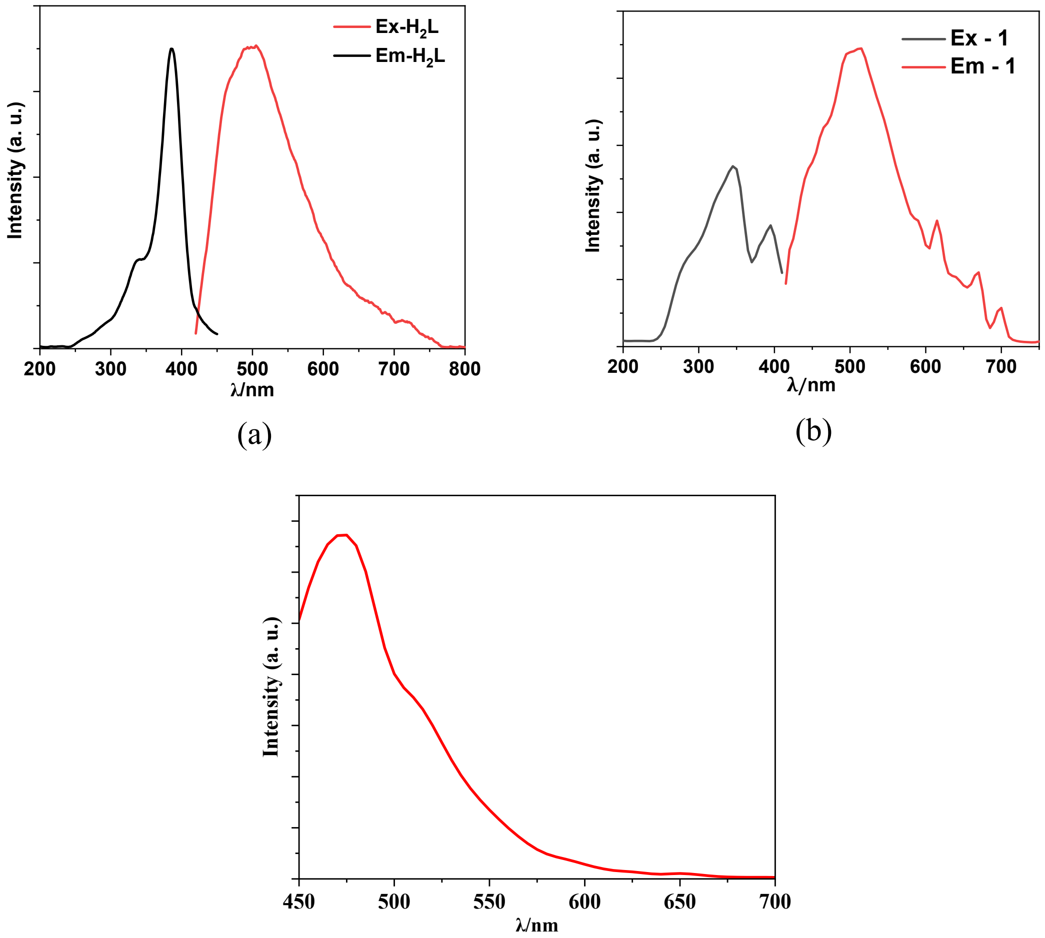


Figure S5. UV-vis absorption spectra of H_2L, **1** and Neo in CH_3CN ($c = 10\ \mu M$).

7. The excitation and emission spectra of H_2L, 1 and Neo



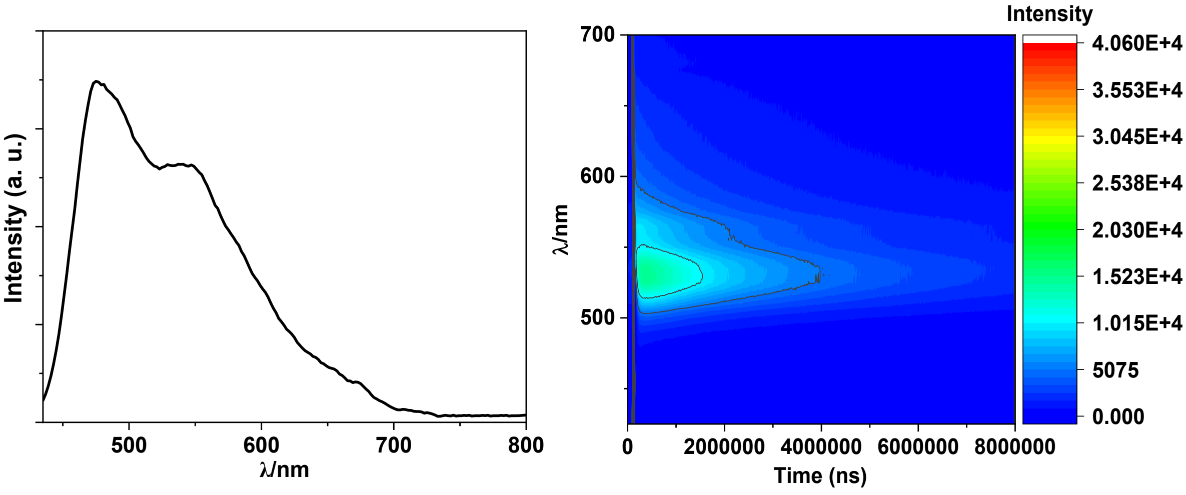
(a)

(b)

(c)

Figure S6. (a) The excitation (λ_{em} = 510 nm) and emission (λ_{ex} = 395 nm) spectra of free ligand H_2L (10 μM) in CH_3CN at room temperature. (b) The excitation (λ_{em} = 616 nm) and emission (λ_{ex} = 395 nm) spectra of **1** (10 μM) in CH_3CN. (c) The emission spectrum of Neo (20 μM) in CH_3CN (λ_{ex} = 395 nm).

8. The emission spectra of the Gd(III) analogue at 77 K



(**a**) (**b**)

Figure S7. The 2-D (**a**) and 3-D (**b**) emission spectra of the Gd(III) analogue (10 μM) in CH_3CN at 77 K. ($\lambda_{ex} = 395$ nm)

9. The emission spectra of 1 with the addition of Neo in 24 hrs in CH_3CN

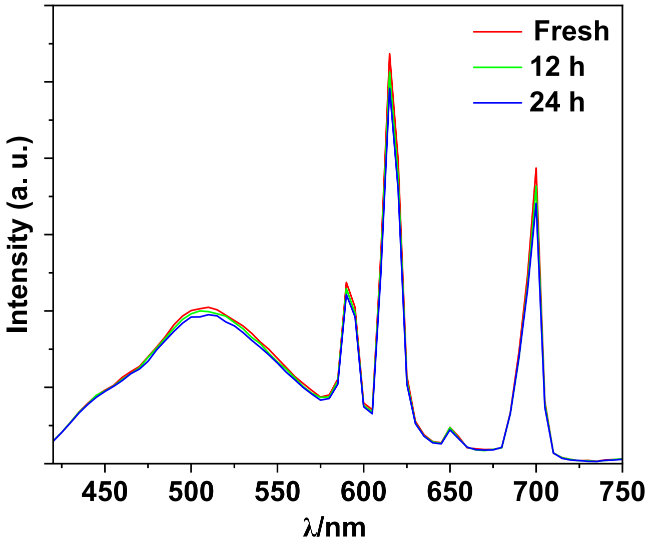
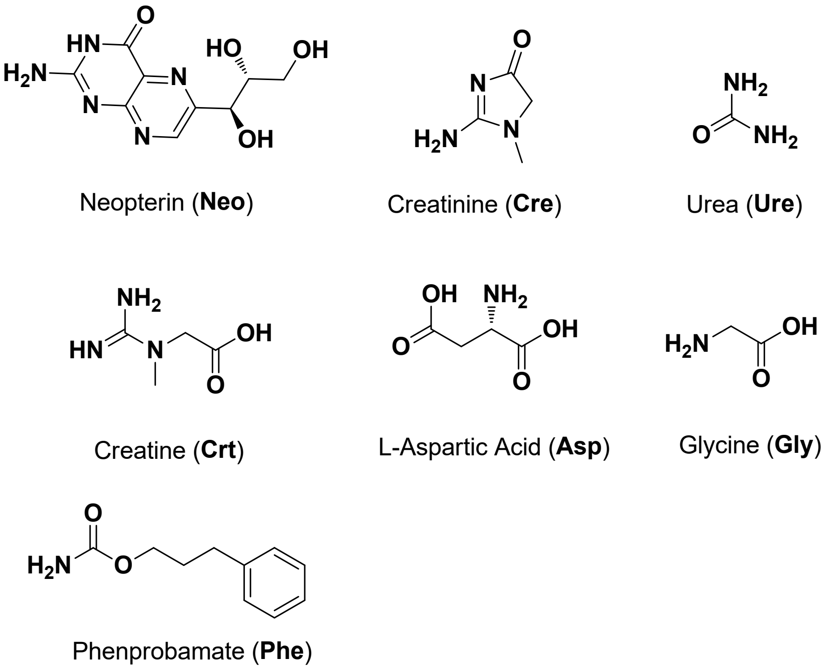


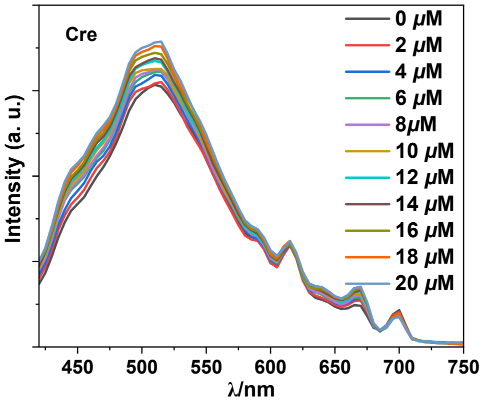
Figure S8. The emission spectra of **1** (10 μM) with the addition of Neo (10 μM) in 24 hrs.

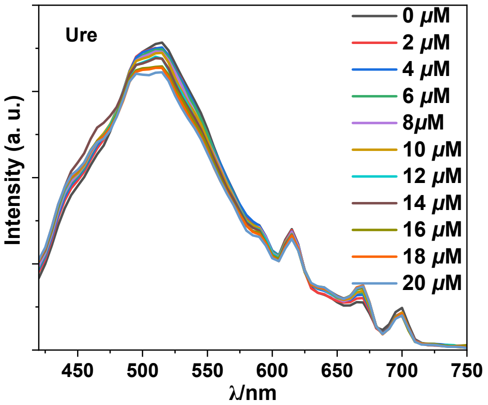
10. Chemical structures of Neo and interferents

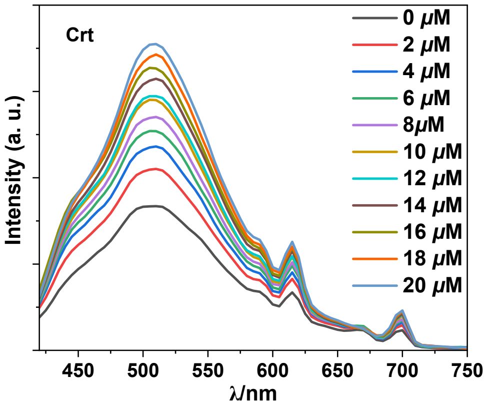


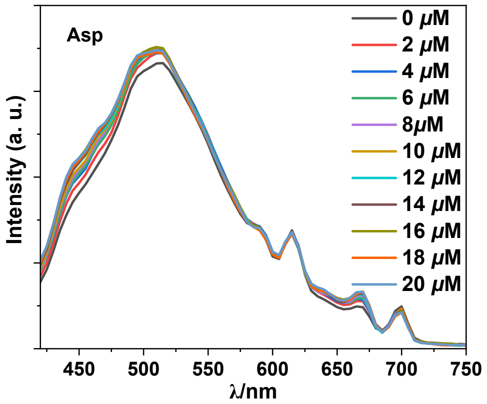
Scheme S2. Chemical structures of Neo and interferents.

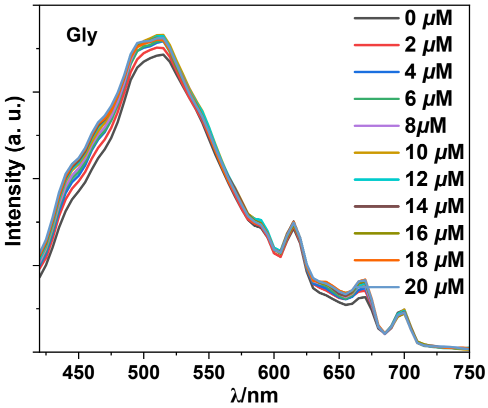
11. The emission spectra of 1 with the addition of interferents in CH_3CN

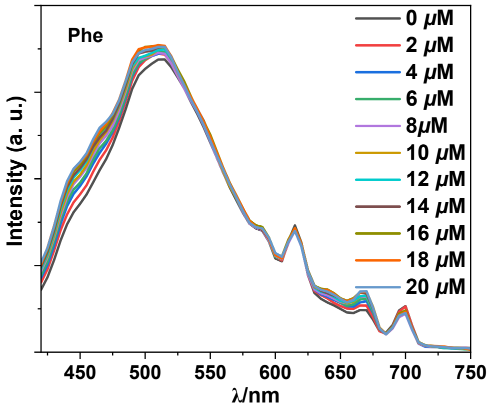

Cre
Intensity (a. u.)
λ/nm
450
500
550
600
650
700
750
0 µM
2 µM
4 µM
6 µM
8µM
10 µM
12 µM
14 µM
16 µM
18 µM
20 µM

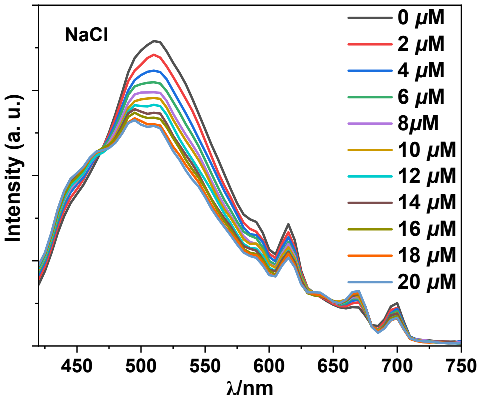

Ure
Intensity (a. u.)
λ/nm
450
500
550
600
650
700
750
0 µM
2 µM
4 µM
6 µM
8µM
10 µM
12 µM
14 µM
16 µM
18 µM
20 µM

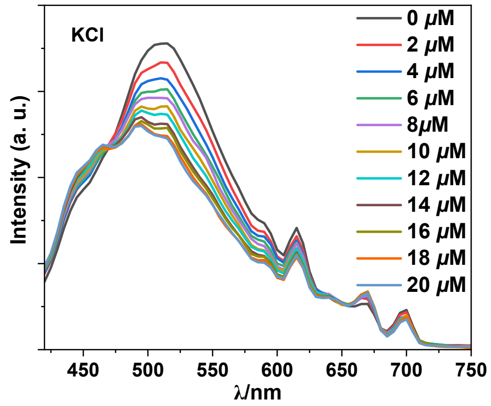

Crt
Intensity (a. u.)
λ/nm
450
500
550
600
650
700
750
0 µM
2 µM
4 µM
6 µM
8µM
10 µM
12 µM
14 µM
16 µM
18 µM
20 µM


Asp
Intensity (a. u.)
λ/nm
450
500
550
600
650
700
750
0 µM
2 µM
4 µM
6 µM
8µM
10 µM
12 µM
14 µM
16 µM
18 µM
20 µM


Gly
Intensity (a. u.)
λ/nm
450
500
550
600
650
700
750
0 µM
2 µM
4 µM
6 µM
8µM
10 µM
12 µM
14 µM
16 µM
18 µM
20 µM


Phe
Intensity (a. u.)
λ/nm
450
500
550
600
650
700
750
0 µM
2 µM
4 µM
6 µM
8µM
10 µM
12 µM
14 µM
16 µM
18 µM
20 µM


NaCl
Intensity (a. u.)
λ/nm
450
500
550
600
650
700
750
0 µM
2 µM
4 µM
6 µM
8µM
10 µM
12 µM
14 µM
16 µM
18 µM
20 µM


KCl
Intensity (a. u.)
λ/nm
450
500
550
600
650
700
750
0 µM
2 µM
4 µM
6 µM
8µM
10 µM
12 µM
14 µM
16 µM
18 µM
20 µM

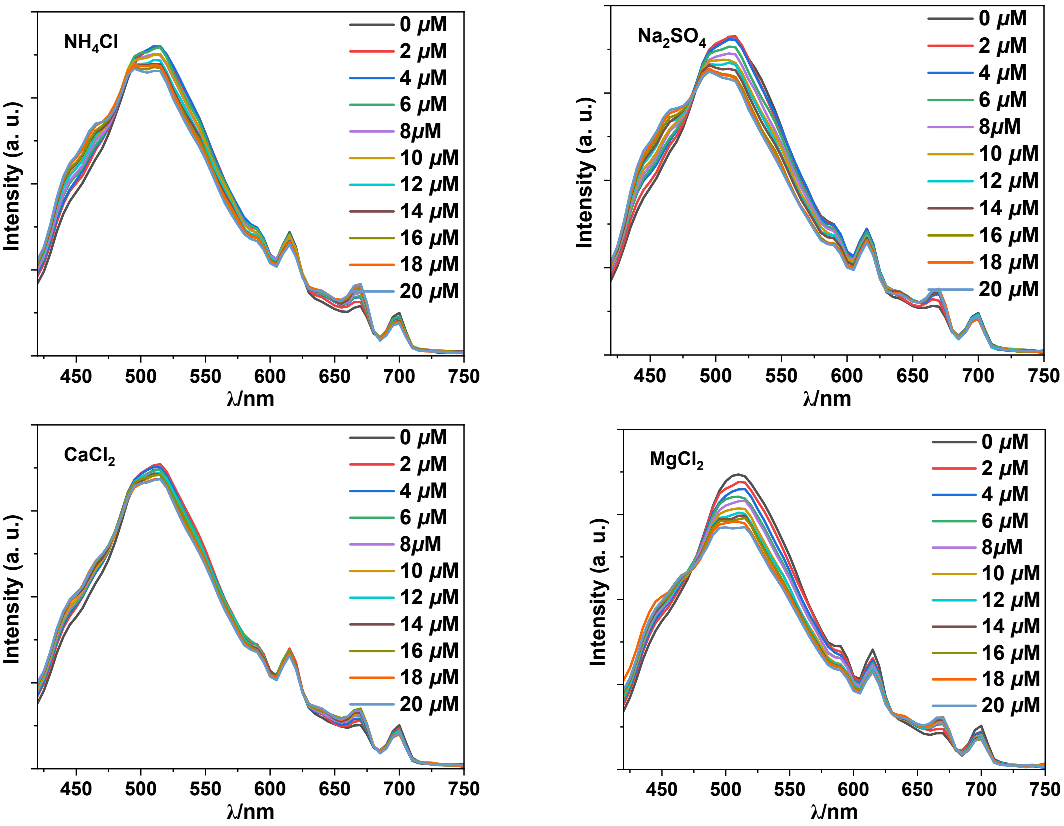
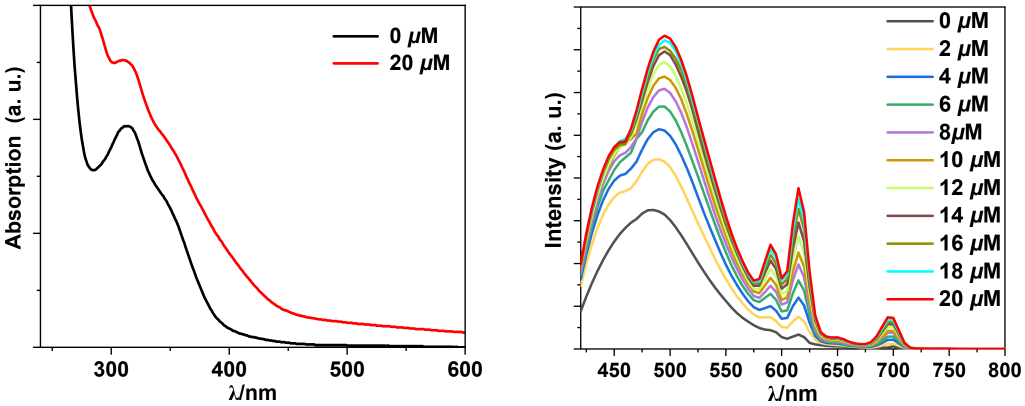


Figure S9. The emission spectra of **1** (10 μM) with the addition of interferents in CH_3CN. (λ_{ex} = 395 nm)

12. UV-vis and emission spectra of 1 with the addition of Neo in H_2O



(a) (b)

Figure S10. UV-vis spectra (a) and emission spectra (b) of **1** (10 μM) with the addition of Neo in H_2O. (λ_{ex} = 395 nm)

13. UV-vis titration of 1 with the addition of Neo in CH_3CN

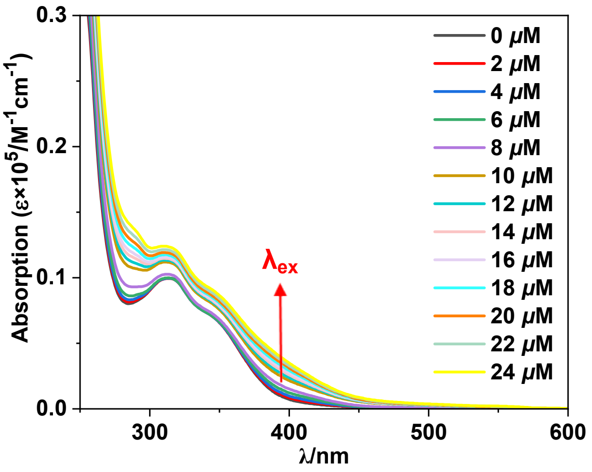


Figure S11. UV-vis titration of **1** (10 μM) with the addition of Neo in CH_3CN.

14. The excitation and emission spectra of Neo

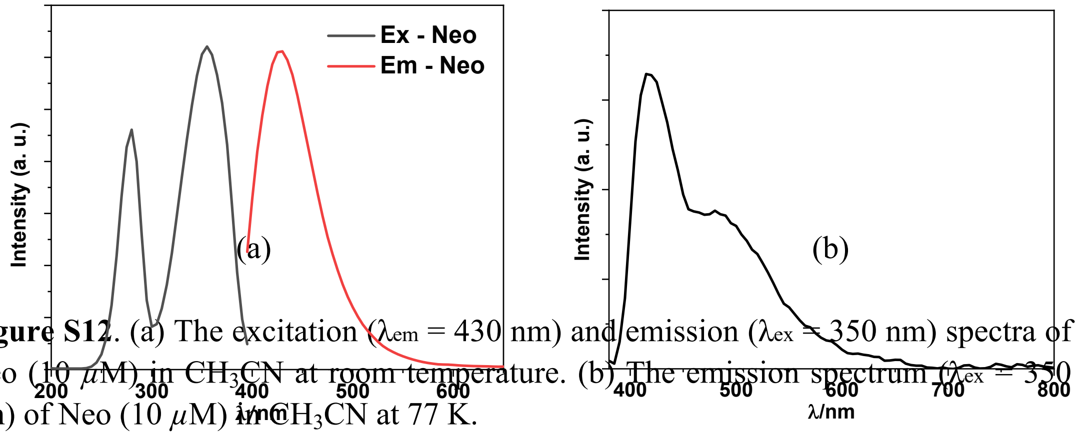


Figure S12. (a) The excitation (λ_{em} = 430 nm) and emission (λ_{ex} = 350 nm) spectra of Neo (10 μM) in CH_3CN at room temperature. (b) The emission spectrum (λ_{ex} = 350 nm) of Neo (10 μM) in CH_3CN at 77 K.

15. X-Ray Crystallography

Data were collected on a Smart APEX CCD diffractometer with graphite monochromated Mo-K*α* radiation (λ = 0.71073 Å) at 233 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 structure was solved by Olex2 program. 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.[2] Some uncoordinated solvent molecules such as H_2O were found to be badly disordered. Attempts to model the disorder were unsatisfactory. The contributions to the scattering factors due to these solvent molecules were removed by use of the utility SQUEEZE (Sluis and Spek, 1990) in PLATON98 (Spek, 1998). PLATON98 was used as incorporated in WinGX (Farrugia, 1999). Crystallographic data for **1** (CCDC reference number 2222896) are presented in Table S1 and selected bond lengths and angles are given in Table S2. See http://www.rsc.org/suppdata/cc/ for crystallographic data in CIF format.

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

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

Table S1. Crystal data and structure refinement for **1**.

	1
Formula	$C_{190}H_{296}Cl_4Eu_{26}F_{18}N_4O_{204}S_2Zn_{22}$
Fw	11837.21
Crystal system	Triclinic

Space group	P-1
a [Å]	19.8012(12)
b [Å]	22.2405(13)
c [Å]	25.7774(15)
α [deg]	85.1870(10)
β [deg]	85.3070(10)
γ [deg]	72.3620(10)
V / [Å^3]	10761.2(11)
d / [g/cm^3]	1.810
Z	1
T [K]	233(1)
F(000)	5596
μ, mm^{-1}	5.045
θ rang, deg	0.96-25.00
reflns meads	37557
reflns used	37557
params	2053
R1^a, wR2^a [$I > 2\sigma(I)$]	0.0667, 0.1725
R1, wR2 (all data)	0.1193, 0.1924
Quality of fit	1.014

[a] $R1 = \Sigma|F_o| - |F_c|\Sigma|F_o|$. $wR2 = [\Sigma w[(F_o^2 - F_c^2)^2]/\Sigma|[w(F_o^2)^2]]^{1/2}$. $w=1/[\sigma^2(F_o^2)+(0.075P)^2]$, where $P = [\max(F_o^2,0)+2F_c^2]/3$.

Table S2. Selected Bond Lengths (Å) and angles (◦) for **1**

Eu(1)-O(3)	2.264(10)	Eu(1)-O(31)	2.284(9)
Eu(1)-O(5)	2.271(14)	Eu(1)-O(36)	2.356(10)
Eu(1)-O(9)	2.251(10)	Eu(2)-O(13)	2.339(9)
Eu(1)-O(11)	2.412(12)	Eu(2)-O(14)	2.321(9)
Eu(1)-O(13)	2.990(10)	Eu(2)-O(31)	2.287(9)
Eu(1)-O(20)	2.272(10)	Eu(2)-O(32)	2.378(9)

Eu(2)-O(35)	2.357(9)	Eu(7)-O(87)	2.278(10)
Eu(2)-O(36)	2.357(10)	Eu(8)-O(35)	2.357(9)
Eu(2)-O(40)	2.289(8)	Eu(8)-O(37)	2.265(9)
Eu(2)-O(43)	2.447(9)	Eu(8)-O(39)	2.335(9)
Eu(3)-O(20)	2.255(9)	Eu(8)-O(40)	2.332(9)
Eu(3)-O(23)	2.323(9)	Eu(8)-O(43)	2.444(9)
Eu(3)-O(30)	2.300(10)	Eu(8)-O(60)	2.297(9)
Eu(3)-O(31)	2.384(9)	Eu(8)-O(75)	2.333(9)
Eu(3)-O(32)	2.332(10)	Eu(8)-O(91)	2.356(9)
Eu(3)-O(41)	2.337(9)	Eu(9)-O(63)	2.350(9)
Eu(3)-O(70)	2.372(9)	Eu(9)-O(64)	2.260(10)
Eu(3)-O(92)	2.302(10)	Eu(9)-O(71)	2.291(10)
Eu(4)-O(19)	2.296(11)	Eu(9)-O(75)	2.296(9)
Eu(4)-O(21)	2.313(11)	Eu(9)-O(76)	2.268(11)
Eu(4)-O(23)	2.323(9)	Eu(9)-O(87)	3.065(11)
Eu(4)-O(25)	2.333(12)	Eu(9)-O(88)	2.290(10)
Eu(4)-O(26)	2.269(13)	Eu(9)-O(91)	2.300(9)
Eu(4)-O(70)	2.475(10)	Eu(10)-O(42)	2.338(8)
Eu(4)-O(92)	2.318(9)	Eu(10)-O(53)	2.300(9)
Eu(4)-O(96)	2.348(9)	Eu(10)-O(54)	2.292(8)
Eu(5)-O(17)	2.420(10)	Eu(10)-O(55)	2.408(9)
Eu(5)-O(41)	2.445(9)	Eu(10)-O(60)	2.379(9)
Eu(5)-O(42)	2.435(8)	Eu(10)-O(63)	2.279(8)
Eu(5)-O(44)	2.429(10)	Eu(10)-O(67)	2.296(10)
Eu(5)-O(45)	2.450(10)	Eu(10)-O(91)	2.327(9)
Eu(5)-O(48)	2.288(9)	Eu(11)-O(16)	2.281(10)
Eu(5)-O(53)	2.280(8)	Eu(11)-O(39)	2.927(10)
Eu(5)-O(92)	2.318(9)	Eu(11)-O(60)	2.263(8)
Eu(5)-O(96)	2.300(9)	Eu(11)-O(61)	2.249(11)
Eu(6)-O(12)	2.271(12)	Eu(11)-O(63)	2.311(9)
Eu(6)-O(14)	2.268(10)	Eu(11)-O(73)	2.353(11)
Eu(6)-O(35)	2.303(9)	Eu(11)-O(75)	2.331(9)
Eu(6)-O(37)	2.324(9)	Eu(11)-O(93)	2.270(11)
Eu(6)-O(38)	2.263(12)	Eu(12)-O(46)	2.270(11)
Eu(6)-O(68)	2.312(13)	Eu(12)-O(48)	2.344(9)
Eu(6)-O(80)	2.488(14)	Eu(12)-O(52)	2.305(10)
Eu(6)-O(98)	2.361(12)	Eu(12)-O(53)	2.365(9)
Eu(7)-O(14)	2.357(9)	Eu(12)-O(54)	2.335(9)
Eu(7)-O(37)	2.357(10)	Eu(12)-O(55)	2.478(9)
Eu(7)-O(40)	2.246(9)	Eu(12)-O(56)	2.285(10)
Eu(7)-O(69)	2.178(12)	Eu(12)-O(59)	2.346(11)
Eu(7)-O(78)	2.582(11)	Eu(13)-O(7)	2.267(11)
Eu(7)-O(79)	2.342(11)	Eu(13)-O(20)	2.372(10)
Eu(7)-O(85)	2.306(12)	Eu(13)-O(29)	2.303(12)

Eu(13)-O(32)	2.275(9)
Eu(13)-O(36)	2.274(10)
Eu(13)-O(83)	2.278(12)
Eu(13)-O(86)	2.290(13)
Zn(1)-N(1)	2.097(14)
Zn(1)-O(1)	2.049(11)
Zn(1)-O(3)	2.080(10)
Zn(1)-O(8)	1.991(13)
Zn(1)-O(10)	2.005(13)
Zn(2)-O(1)	2.006(12)
Zn(2)-O(3)	1.957(10)
Zn(2)-O(4)	1.946(16)
Zn(2)-O(6)	1.913(14)
Zn(3)-O(18)	1.993(14)
Zn(3)-O(24)	1.987(14)
Zn(3)-O(70)	1.940(9)
Zn(3)-O(97)	1.984(14)
Zn(4)-O(27)	1.917(12)
Zn(4)-O(28)	1.998(10)
Zn(4)-O(44)	1.993(10)
Zn(4)-O(47)	1.943(12)
Zn(5)-O(15)	2.005(10)
Zn(5)-O(77)	1.962(11)
Zn(5)-O(78)	1.944(12)
Zn(5)-O(84)	1.938(11)
Zn(6)-N(2)	2.123(13)
Zn(6)-O(2)	2.037(11)
Zn(6)-O(16)	2.053(10)
Zn(6)-O(74)	1.968(11)
Zn(6)-O(94)	2.003(14)
Zn(7)-O(2)	2.000(12)
Zn(7)-O(16)	1.958(10)
Zn(7)-O(62)	1.921(14)
Zn(7)-O(72)	1.945(13)
Zn(8)-O(33)	1.989(11)
Zn(8)-O(49)	2.012(10)
Zn(8)-O(89)	2.286(10)
Zn(8)-O(90)#1	2.179(9)
Zn(8)-O(90)	2.160(10)
Zn(8)-O(95)	2.113(9)
Zn(9)-O(22)	2.083(10)
Zn(9)-O(23)	2.027(9)
Zn(9)-O(34)	2.028(11)
Zn(9)-O(95)	2.068(9)
Zn(9)-O(96)	2.053(9)
Zn(10)-O(48)	2.058(9)
Zn(10)-O(50)	2.050(10)
Zn(10)-O(51)	2.067(10)
Zn(10)-O(54)	2.060(8)
Zn(10)-O(95)	2.071(8)
Zn(11)-O(55)	1.933(9)
Zn(11)-O(57)	1.950(14)
Zn(11)-O(58)	1.945(15)
Zn(11)-O(66)	1.921(13)
O(3)-Eu(1)-O(5)	78.7(4)
O(3)-Eu(1)-O(11)	76.9(4)
O(3)-Eu(1)-O(13)	154.9(4)
O(3)-Eu(1)-O(20)	79.1(3)
O(3)-Eu(1)-O(31)	144.7(4)
O(3)-Eu(1)-O(36)	115.6(4)
O(5)-Eu(1)-O(11)	143.2(4)
O(5)-Eu(1)-O(13)	76.7(4)
O(5)-Eu(1)-O(20)	123.2(4)
O(5)-Eu(1)-O(31)	134.0(4)
O(5)-Eu(1)-O(36)	72.9(4)
O(9)-Eu(1)-O(3)	88.0(4)
O(9)-Eu(1)-O(5)	75.5(5)
O(9)-Eu(1)-O(11)	76.5(4)
O(9)-Eu(1)-O(13)	81.7(3)
O(9)-Eu(1)-O(20)	153.7(4)
O(9)-Eu(1)-O(31)	110.5(4)
O(9)-Eu(1)-O(36)	135.1(4)
O(11)-Eu(1)-O(13)	122.0(3)
O(20)-Eu(1)-O(11)	78.3(4)
O(20)-Eu(1)-O(13)	118.6(3)
O(20)-Eu(1)-O(31)	71.3(3)
O(20)-Eu(1)-O(36)	71.1(3)
O(31)-Eu(1)-O(11)	78.6(3)
O(31)-Eu(1)-O(13)	60.2(3)
O(31)-Eu(1)-O(36)	72.6(3)
O(36)-Eu(1)-O(11)	143.2(4)
O(36)-Eu(1)-O(13)	60.6(3)
O(13)-Eu(2)-O(32)	132.5(3)
O(13)-Eu(2)-O(35)	81.6(3)
O(13)-Eu(2)-O(36)	71.7(4)
O(13)-Eu(2)-O(43)	122.2(4)
O(14)-Eu(2)-O(13)	83.0(4)
O(14)-Eu(2)-O(32)	119.1(3)

O(14)-Eu(2)-O(35)	69.8(3)	O(70)-Eu(3)-O(31)	121.3(3)
O(14)-Eu(2)-O(36)	85.7(3)	O(92)-Eu(3)-O(23)	75.6(3)
O(14)-Eu(2)-O(43)	122.7(3)	O(92)-Eu(3)-O(31)	141.8(3)
O(31)-Eu(2)-O(13)	71.8(3)	O(92)-Eu(3)-O(32)	121.7(3)
O(31)-Eu(2)-O(14)	150.6(3)	O(92)-Eu(3)-O(41)	69.7(3)
O(31)-Eu(2)-O(32)	71.6(3)	O(92)-Eu(3)-O(70)	72.8(3)
O(31)-Eu(2)-O(35)	119.3(3)	O(19)-Eu(4)-O(21)	71.9(4)
O(31)-Eu(2)-O(36)	72.5(3)	O(19)-Eu(4)-O(23)	110.3(4)
O(31)-Eu(2)-O(40)	137.6(3)	O(19)-Eu(4)-O(25)	81.1(4)
O(31)-Eu(2)-O(43)	84.3(3)	O(19)-Eu(4)-O(70)	75.3(4)
O(32)-Eu(2)-O(43)	82.7(3)	O(19)-Eu(4)-O(92)	139.4(4)
O(35)-Eu(2)-O(32)	143.8(3)	O(19)-Eu(4)-O(96)	152.5(4)
O(35)-Eu(2)-O(36)	145.8(3)	O(21)-Eu(4)-O(23)	77.6(3)
O(35)-Eu(2)-O(43)	65.6(3)	O(21)-Eu(4)-O(25)	140.6(4)
O(36)-Eu(2)-O(32)	69.1(3)	O(21)-Eu(4)-O(70)	117.5(4)
O(36)-Eu(2)-O(43)	147.8(3)	O(21)-Eu(4)-O(92)	144.6(3)
O(40)-Eu(2)-O(13)	149.8(4)	O(21)-Eu(4)-O(96)	81.2(3)
O(40)-Eu(2)-O(14)	70.1(3)	O(23)-Eu(4)-O(25)	140.0(4)
O(40)-Eu(2)-O(32)	74.8(3)	O(23)-Eu(4)-O(70)	66.2(3)
O(40)-Eu(2)-O(35)	76.6(3)	O(23)-Eu(4)-O(96)	68.0(3)
O(40)-Eu(2)-O(36)	118.0(3)	O(25)-Eu(4)-O(70)	81.1(4)
O(40)-Eu(2)-O(43)	66.2(3)	O(25)-Eu(4)-O(96)	118.7(4)
O(20)-Eu(3)-O(23)	110.5(3)	O(26)-Eu(4)-O(19)	91.0(5)
O(20)-Eu(3)-O(30)	82.9(4)	O(26)-Eu(4)-O(21)	77.7(4)
O(20)-Eu(3)-O(31)	69.8(3)	O(26)-Eu(4)-O(23)	140.1(4)
O(20)-Eu(3)-O(32)	72.7(3)	O(26)-Eu(4)-O(25)	74.6(4)
O(20)-Eu(3)-O(41)	144.1(3)	O(26)-Eu(4)-O(70)	153.7(4)
O(20)-Eu(3)-O(70)	79.0(3)	O(26)-Eu(4)-O(92)	110.3(4)
O(20)-Eu(3)-O(92)	146.3(3)	O(26)-Eu(4)-O(96)	77.6(4)
O(23)-Eu(3)-O(31)	78.3(3)	O(92)-Eu(4)-O(23)	75.2(3)
O(23)-Eu(3)-O(32)	145.6(3)	O(92)-Eu(4)-O(25)	72.5(4)
O(23)-Eu(3)-O(41)	69.4(3)	O(92)-Eu(4)-O(70)	70.7(3)
O(23)-Eu(3)-O(70)	67.9(3)	O(92)-Eu(4)-O(96)	67.9(3)
O(30)-Eu(3)-O(23)	137.7(4)	O(96)-Eu(4)-O(70)	124.0(3)
O(30)-Eu(3)-O(31)	142.0(4)	O(17)-Eu(5)-O(41)	71.2(3)
O(30)-Eu(3)-O(32)	76.3(4)	O(17)-Eu(5)-O(42)	70.4(3)
O(30)-Eu(3)-O(41)	122.5(3)	O(17)-Eu(5)-O(44)	131.1(3)
O(30)-Eu(3)-O(70)	76.2(4)	O(17)-Eu(5)-O(45)	77.4(4)
O(30)-Eu(3)-O(92)	72.9(4)	O(41)-Eu(5)-O(45)	137.3(3)
O(32)-Eu(3)-O(31)	70.7(3)	O(42)-Eu(5)-O(41)	53.4(3)
O(32)-Eu(3)-O(41)	88.1(3)	O(42)-Eu(5)-O(45)	138.0(3)
O(32)-Eu(3)-O(70)	142.5(3)	O(44)-Eu(5)-O(41)	146.1(3)
O(41)-Eu(3)-O(31)	75.3(3)	O(44)-Eu(5)-O(42)	148.7(3)
O(41)-Eu(3)-O(70)	128.4(3)	O(44)-Eu(5)-O(45)	53.7(4)

O(48)-Eu(5)-O(17)	136.6(3)
O(48)-Eu(5)-O(41)	105.4(3)
O(48)-Eu(5)-O(42)	73.8(3)
O(48)-Eu(5)-O(44)	76.0(3)
O(48)-Eu(5)-O(45)	117.2(3)
O(48)-Eu(5)-O(92)	144.9(3)
O(48)-Eu(5)-O(96)	76.3(3)
O(53)-Eu(5)-O(17)	75.5(3)
O(53)-Eu(5)-O(41)	118.8(3)
O(53)-Eu(5)-O(42)	67.6(3)
O(53)-Eu(5)-O(44)	93.7(3)
O(53)-Eu(5)-O(45)	78.8(3)
O(53)-Eu(5)-O(48)	68.8(3)
O(53)-Eu(5)-O(92)	145.8(3)
O(53)-Eu(5)-O(96)	145.0(3)
O(92)-Eu(5)-O(17)	75.7(3)
O(92)-Eu(5)-O(41)	67.5(3)
O(92)-Eu(5)-O(42)	118.2(3)
O(92)-Eu(5)-O(44)	91.5(3)
O(92)-Eu(5)-O(45)	77.3(3)
O(96)-Eu(5)-O(17)	136.5(4)
O(96)-Eu(5)-O(41)	72.5(3)
O(96)-Eu(5)-O(42)	105.3(3)
O(96)-Eu(5)-O(44)	75.1(3)
O(96)-Eu(5)-O(45)	116.6(3)
O(96)-Eu(5)-O(92)	68.7(3)
O(12)-Eu(6)-O(35)	77.7(4)
O(12)-Eu(6)-O(37)	143.9(4)
O(12)-Eu(6)-O(68)	136.4(4)
O(12)-Eu(6)-O(80)	71.7(5)
O(12)-Eu(6)-O(98)	75.5(5)
O(14)-Eu(6)-O(12)	83.4(4)
O(14)-Eu(6)-O(35)	71.7(3)
O(14)-Eu(6)-O(37)	72.0(3)
O(14)-Eu(6)-O(68)	100.8(4)
O(14)-Eu(6)-O(80)	74.6(4)
O(14)-Eu(6)-O(98)	144.4(4)
O(35)-Eu(6)-O(37)	69.8(3)
O(35)-Eu(6)-O(68)	145.2(4)
O(35)-Eu(6)-O(80)	136.4(4)
O(35)-Eu(6)-O(98)	129.1(4)
O(37)-Eu(6)-O(80)	123.7(4)
O(37)-Eu(6)-O(98)	138.3(4)
O(38)-Eu(6)-O(12)	111.0(4)
O(38)-Eu(6)-O(14)	143.7(4)
O(38)-Eu(6)-O(35)	79.0(4)
O(38)-Eu(6)-O(37)	78.2(4)
O(38)-Eu(6)-O(68)	91.1(5)
O(38)-Eu(6)-O(80)	140.9(5)
O(38)-Eu(6)-O(98)	71.6(4)
O(68)-Eu(6)-O(37)	75.5(4)
O(68)-Eu(6)-O(80)	67.9(5)
O(68)-Eu(6)-O(98)	76.9(5)
O(98)-Eu(6)-O(80)	71.7(5)
O(14)-Eu(7)-O(78)	132.2(3)
O(37)-Eu(7)-O(14)	69.9(3)
O(37)-Eu(7)-O(78)	134.5(3)
O(40)-Eu(7)-O(14)	70.2(3)
O(40)-Eu(7)-O(37)	70.2(3)
O(40)-Eu(7)-O(78)	81.2(3)
O(40)-Eu(7)-O(79)	134.7(4)
O(40)-Eu(7)-O(85)	88.2(4)
O(40)-Eu(7)-O(87)	87.3(3)
O(69)-Eu(7)-O(14)	85.6(4)
O(69)-Eu(7)-O(37)	80.2(4)
O(69)-Eu(7)-O(40)	146.7(4)
O(69)-Eu(7)-O(78)	131.8(4)
O(69)-Eu(7)-O(79)	78.5(5)
O(69)-Eu(7)-O(85)	105.3(5)
O(69)-Eu(7)-O(87)	98.5(4)
O(79)-Eu(7)-O(14)	138.2(4)
O(79)-Eu(7)-O(37)	142.2(4)
O(79)-Eu(7)-O(78)	53.5(4)
O(85)-Eu(7)-O(14)	70.2(4)
O(85)-Eu(7)-O(37)	139.1(4)
O(85)-Eu(7)-O(78)	71.4(4)
O(85)-Eu(7)-O(79)	77.1(4)
O(87)-Eu(7)-O(14)	140.9(3)
O(87)-Eu(7)-O(37)	72.5(3)
O(87)-Eu(7)-O(78)	71.3(4)
O(87)-Eu(7)-O(79)	80.1(4)
O(87)-Eu(7)-O(85)	142.8(4)
O(35)-Eu(8)-O(43)	65.6(3)
O(37)-Eu(8)-O(35)	69.8(3)
O(37)-Eu(8)-O(39)	82.4(4)
O(37)-Eu(8)-O(40)	70.4(3)
O(37)-Eu(8)-O(43)	122.9(3)
O(37)-Eu(8)-O(60)	149.9(3)

O(37)-Eu(8)-O(75)	85.1(3)
O(37)-Eu(8)-O(91)	120.2(3)
O(39)-Eu(8)-O(35)	81.3(3)
O(39)-Eu(8)-O(43)	122.4(3)
O(39)-Eu(8)-O(91)	132.7(3)
O(40)-Eu(8)-O(35)	75.8(3)
O(40)-Eu(8)-O(39)	149.1(3)
O(40)-Eu(8)-O(43)	65.6(3)
O(40)-Eu(8)-O(75)	119.3(3)
O(40)-Eu(8)-O(91)	75.8(3)
O(60)-Eu(8)-O(35)	119.0(3)
O(60)-Eu(8)-O(39)	71.5(3)
O(60)-Eu(8)-O(40)	138.3(3)
O(60)-Eu(8)-O(43)	84.7(3)
O(60)-Eu(8)-O(75)	72.5(3)
O(60)-Eu(8)-O(91)	71.4(3)
O(75)-Eu(8)-O(35)	144.9(3)
O(75)-Eu(8)-O(39)	71.0(3)
O(75)-Eu(8)-O(43)	148.5(3)
O(75)-Eu(8)-O(91)	70.5(3)
O(91)-Eu(8)-O(35)	143.4(3)
O(91)-Eu(8)-O(43)	81.9(3)
O(63)-Eu(9)-O(87)	137.9(3)
O(64)-Eu(9)-O(63)	75.6(3)
O(64)-Eu(9)-O(71)	82.0(4)
O(64)-Eu(9)-O(75)	146.5(4)
O(64)-Eu(9)-O(76)	73.7(4)
O(64)-Eu(9)-O(87)	141.7(3)
O(64)-Eu(9)-O(88)	119.9(4)
O(64)-Eu(9)-O(91)	100.1(4)
O(71)-Eu(9)-O(63)	77.4(3)
O(71)-Eu(9)-O(75)	88.3(4)
O(71)-Eu(9)-O(87)	117.7(3)
O(71)-Eu(9)-O(91)	148.1(3)
O(75)-Eu(9)-O(63)	71.0(3)
O(75)-Eu(9)-O(87)	70.5(3)
O(75)-Eu(9)-O(91)	72.2(3)
O(76)-Eu(9)-O(63)	134.0(4)
O(76)-Eu(9)-O(71)	129.9(4)
O(76)-Eu(9)-O(75)	133.8(4)
O(76)-Eu(9)-O(87)	68.6(3)
O(76)-Eu(9)-O(88)	78.7(4)
O(76)-Eu(9)-O(91)	80.2(4)
O(88)-Eu(9)-O(63)	147.1(4)
O(88)-Eu(9)-O(71)	76.6(4)
O(88)-Eu(9)-O(75)	88.4(4)
O(88)-Eu(9)-O(87)	46.2(3)
O(88)-Eu(9)-O(91)	126.3(3)
O(91)-Eu(9)-O(63)	72.4(3)
O(91)-Eu(9)-O(87)	80.0(3)
C(71)-Eu(9)-O(87)	23.9(3)
O(42)-Eu(10)-O(55)	129.4(3)
O(42)-Eu(10)-O(60)	75.3(3)
O(53)-Eu(10)-O(42)	69.0(3)
O(53)-Eu(10)-O(55)	74.3(3)
O(53)-Eu(10)-O(60)	141.3(3)
O(53)-Eu(10)-O(91)	119.9(3)
O(54)-Eu(10)-O(42)	70.9(3)
O(54)-Eu(10)-O(53)	76.5(3)
O(54)-Eu(10)-O(55)	67.4(3)
O(54)-Eu(10)-O(60)	78.1(3)
O(54)-Eu(10)-O(67)	136.8(3)
O(54)-Eu(10)-O(91)	144.7(3)
O(60)-Eu(10)-O(55)	120.9(3)
O(63)-Eu(10)-O(42)	144.1(3)
O(63)-Eu(10)-O(53)	146.9(3)
O(63)-Eu(10)-O(54)	111.2(3)
O(63)-Eu(10)-O(55)	79.2(3)
O(63)-Eu(10)-O(60)	70.4(3)
O(63)-Eu(10)-O(67)	82.3(4)
O(63)-Eu(10)-O(91)	73.2(3)
O(67)-Eu(10)-O(42)	121.8(3)
O(67)-Eu(10)-O(53)	72.2(3)
O(67)-Eu(10)-O(55)	75.8(4)
O(67)-Eu(10)-O(60)	143.0(3)
O(67)-Eu(10)-O(91)	78.0(3)
O(91)-Eu(10)-O(42)	85.6(3)
O(91)-Eu(10)-O(55)	144.1(3)
O(91)-Eu(10)-O(60)	70.5(3)
O(16)-Eu(11)-O(39)	155.5(3)
O(16)-Eu(11)-O(63)	77.8(4)
O(16)-Eu(11)-O(73)	76.3(4)
O(16)-Eu(11)-O(75)	116.2(3)
O(60)-Eu(11)-O(16)	143.1(4)
O(60)-Eu(11)-O(39)	61.3(3)
O(60)-Eu(11)-O(63)	72.0(3)
O(60)-Eu(11)-O(73)	77.5(3)
O(60)-Eu(11)-O(75)	73.2(3)

O(60)-Eu(11)-O(93)	109.0(3)	O(56)-Eu(12)-O(59)	81.1(4)
O(61)-Eu(11)-O(16)	79.1(4)	O(59)-Eu(12)-O(53)	71.7(4)
O(61)-Eu(11)-O(39)	76.9(4)	O(59)-Eu(12)-O(55)	80.3(4)
O(61)-Eu(11)-O(60)	135.3(4)	O(7)-Eu(13)-O(20)	78.2(4)
O(61)-Eu(11)-O(63)	121.9(4)	O(7)-Eu(13)-O(29)	83.9(5)
O(61)-Eu(11)-O(73)	143.3(4)	O(7)-Eu(13)-O(32)	147.5(4)
O(61)-Eu(11)-O(75)	73.0(4)	O(7)-Eu(13)-O(36)	87.0(4)
O(61)-Eu(11)-O(93)	77.1(4)	O(7)-Eu(13)-O(83)	130.4(4)
O(63)-Eu(11)-O(39)	119.7(3)	O(7)-Eu(13)-O(86)	76.3(4)
O(63)-Eu(11)-O(73)	78.8(3)	O(29)-Eu(13)-O(20)	75.5(4)
O(63)-Eu(11)-O(75)	71.1(3)	O(32)-Eu(13)-O(20)	71.5(3)
O(73)-Eu(11)-O(39)	121.7(3)	O(32)-Eu(13)-O(29)	99.2(4)
O(75)-Eu(11)-O(39)	60.8(3)	O(32)-Eu(13)-O(83)	80.9(4)
O(75)-Eu(11)-O(73)	143.0(3)	O(32)-Eu(13)-O(86)	124.2(4)
O(93)-Eu(11)-O(16)	88.9(4)	O(36)-Eu(13)-O(20)	70.8(4)
O(93)-Eu(11)-O(39)	80.9(3)	O(36)-Eu(13)-O(29)	146.2(4)
O(93)-Eu(11)-O(63)	153.3(4)	O(36)-Eu(13)-O(32)	72.4(3)
O(93)-Eu(11)-O(73)	75.5(4)	O(36)-Eu(13)-O(83)	132.8(4)
O(93)-Eu(11)-O(75)	135.5(4)	O(36)-Eu(13)-O(86)	83.8(4)
O(46)-Eu(12)-O(48)	77.2(4)	O(83)-Eu(13)-O(20)	135.3(4)
O(46)-Eu(12)-O(52)	77.9(4)	O(83)-Eu(13)-O(29)	75.1(4)
O(46)-Eu(12)-O(53)	108.7(3)	O(83)-Eu(13)-O(86)	80.1(5)
O(46)-Eu(12)-O(54)	141.3(3)	O(86)-Eu(13)-O(20)	144.6(4)
O(46)-Eu(12)-O(55)	153.0(3)	O(86)-Eu(13)-O(29)	125.0(4)
O(46)-Eu(12)-O(56)	89.7(4)	O(1)-Zn(1)-N(1)	87.3(5)
O(46)-Eu(12)-O(59)	74.7(4)	O(1)-Zn(1)-O(3)	79.1(4)
O(48)-Eu(12)-O(53)	66.5(3)	O(3)-Zn(1)-N(1)	157.1(5)
O(48)-Eu(12)-O(55)	124.4(3)	O(8)-Zn(1)-N(1)	98.5(5)
O(48)-Eu(12)-O(59)	117.4(4)	O(8)-Zn(1)-O(1)	105.4(6)
O(52)-Eu(12)-O(48)	81.8(3)	O(8)-Zn(1)-O(3)	102.8(5)
O(52)-Eu(12)-O(53)	144.3(3)	O(8)-Zn(1)-O(10)	100.1(6)
O(52)-Eu(12)-O(54)	79.4(3)	O(10)-Zn(1)-N(1)	92.7(5)
O(52)-Eu(12)-O(55)	118.1(3)	O(10)-Zn(1)-O(1)	154.2(6)
O(52)-Eu(12)-O(59)	141.2(4)	O(10)-Zn(1)-O(3)	91.7(5)
O(53)-Eu(12)-O(55)	71.9(3)	O(3)-Zn(2)-O(1)	83.1(4)
O(54)-Eu(12)-O(48)	68.9(3)	O(4)-Zn(2)-O(1)	104.1(6)
O(54)-Eu(12)-O(53)	74.4(3)	O(4)-Zn(2)-O(3)	116.8(6)
O(54)-Eu(12)-O(55)	65.6(3)	O(6)-Zn(2)-O(1)	121.8(5)
O(54)-Eu(12)-O(59)	137.7(3)	O(6)-Zn(2)-O(3)	123.8(6)
O(56)-Eu(12)-O(48)	152.5(4)	O(6)-Zn(2)-O(4)	105.2(7)
O(56)-Eu(12)-O(52)	71.8(4)	O(24)-Zn(3)-O(18)	112.3(6)
O(56)-Eu(12)-O(53)	141.0(3)	O(70)-Zn(3)-O(18)	103.0(5)
O(56)-Eu(12)-O(54)	112.2(4)	O(70)-Zn(3)-O(24)	111.3(5)
O(56)-Eu(12)-O(55)	76.5(3)	O(70)-Zn(3)-O(97)	118.0(6)

O(97)-Zn(3)-O(18)	103.8(6)
O(97)-Zn(3)-O(24)	108.2(7)
O(27)-Zn(4)-O(28)	117.3(5)
O(27)-Zn(4)-O(44)	111.1(5)
O(27)-Zn(4)-O(47)	105.0(6)
O(44)-Zn(4)-O(28)	99.4(4)
O(47)-Zn(4)-O(28)	117.7(5)
O(47)-Zn(4)-O(44)	105.7(5)
O(77)-Zn(5)-O(15)	118.3(5)
O(78)-Zn(5)-O(15)	105.7(4)
O(78)-Zn(5)-O(77)	107.7(5)
O(84)-Zn(5)-O(15)	115.3(5)
O(84)-Zn(5)-O(77)	100.2(5)
O(84)-Zn(5)-O(78)	109.3(5)
O(2)-Zn(6)-N(2)	87.9(5)
O(2)-Zn(6)-O(16)	78.2(4)
O(16)-Zn(6)-N(2)	160.9(5)
O(74)-Zn(6)-N(2)	95.6(5)
O(74)-Zn(6)-O(2)	160.2(6)
O(74)-Zn(6)-O(16)	93.2(4)
O(74)-Zn(6)-O(94)	96.5(5)
O(94)-Zn(6)-N(2)	95.7(5)
O(94)-Zn(6)-O(2)	102.6(6)
O(94)-Zn(6)-O(16)	100.0(5)
O(16)-Zn(7)-O(2)	81.4(4)
O(62)-Zn(7)-O(2)	103.7(6)
O(62)-Zn(7)-O(16)	115.5(5)
O(62)-Zn(7)-O(72)	108.5(6)
O(72)-Zn(7)-O(2)	118.8(5)
O(72)-Zn(7)-O(16)	125.0(5)
O(33)-Zn(8)-O(49)	97.0(5)
O(33)-Zn(8)-O(89)	87.8(4)
O(33)-Zn(8)-O(90)	166.1(4)
O(33)-Zn(8)-O(90)#1	93.0(4)
O(33)-Zn(8)-O(95)	101.0(4)
O(49)-Zn(8)-O(89)	88.0(4)
O(49)-Zn(8)-O(90)#1	164.3(4)
O(49)-Zn(8)-O(90)	91.4(4)
O(49)-Zn(8)-O(95)	100.6(4)
O(90)#1-Zn(8)-O(89)	80.3(3)
O(90)-Zn(8)-O(89)	81.4(4)
O(90)-Zn(8)-O(90)#1	76.6(4)
O(95)-Zn(8)-O(89)	166.7(4)
O(95)-Zn(8)-O(90)	88.2(4)
O(95)-Zn(8)-O(90)#1	89.3(3)
O(23)-Zn(9)-O(22)	94.9(4)
O(23)-Zn(9)-O(34)	89.7(4)
O(23)-Zn(9)-O(95)	169.8(3)
O(23)-Zn(9)-O(96)	79.7(4)
O(34)-Zn(9)-O(22)	99.7(4)
O(34)-Zn(9)-O(95)	93.7(4)
O(34)-Zn(9)-O(96)	159.4(4)
O(95)-Zn(9)-O(22)	94.0(4)
O(96)-Zn(9)-O(22)	98.8(4)
O(96)-Zn(9)-O(95)	94.1(4)
O(48)-Zn(10)-O(51)	98.1(4)
O(48)-Zn(10)-O(54)	80.0(3)
O(48)-Zn(10)-O(95)	94.9(3)
O(50)-Zn(10)-O(48)	158.5(4)
O(50)-Zn(10)-O(51)	100.8(4)
O(50)-Zn(10)-O(54)	87.7(4)
O(50)-Zn(10)-O(95)	94.2(4)
O(51)-Zn(10)-O(95)	93.3(4)
O(54)-Zn(10)-O(51)	96.4(4)
O(54)-Zn(10)-O(95)	169.6(4)
O(55)-Zn(11)-O(57)	105.6(5)
O(55)-Zn(11)-O(58)	114.1(6)
O(58)-Zn(11)-O(57)	109.7(7)
O(66)-Zn(11)-O(55)	120.2(5)
O(66)-Zn(11)-O(57)	103.9(6)
O(66)-Zn(11)-O(58)	102.7(6)