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Supporting Information

Large Ln_{42} coordination nanorings: NIR luminescent sensing of metal ions and nitro explosives

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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: NMR: AVANCE III AV500. 500 spectrometer (^{1}H, 500 MHz) at 298 K; Powder XRD: D8ADVANCE; HRMS(ESI) analysis: MicroOTOF-QII; IR: Nicolet IS10 spectrometer. Melting points were obtained in sealed glass capillaries under dinitrogen and are uncorrected. The thermogravimetric analyses were carried out on a TA Instruments Q600. Elemental analyses (C, H, N) were carried out on a EURO EA3000 elemental analysis. Conductivity measurement was carried out with a DDS-11 conductivity bridge for 10^{-4} M solution in CH_3CN. Dynamic light scattering (DLS) measurement was carried out on a Malvern Zetasizer Nano ZS for 10^{-5} M solution in CH_3CN. Field emission scanning electron microscopy (FESEM) images were recorded on a Nova NanoSEM 200 scanning electron microscope. Absorption spectra were obtained on a UV-3600 spectrophotometer, and excitation and emission spectra on a FLS 980 fluorimeter.

Photophysical Studies Visible and NIR luminescence 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. Liquid nitrogen cooled Ge PIN diode detector was used to detect the NIR emissions from 800 nm to 1700 nm. The temporal decay curves of the fluorescence signals were stored by using the attached storage digital oscilloscope. The quantum yields (Φ_{em}) were obtained by using an integrating sphere, according to eqn $\Phi_{em} = N_{em} / N_{abs}$, where N_{em} and N_{abs} are the numbers of emitted and absorbed photons, respectively. Systematic errors have been deducted through the standard instrument corrections. All the measurements were carried out at room temperature.

2. Synthesis of 1 and 2

$[Nd_{42}(L)_{14}(OH)_{28}(OAc)_{84}]$ (1) $Nd(OAc)_3$ (0.40 mmol, 0.1285 g) and HL (2-Hydroxy-3-methoxybenzaldehyde)(0.30 mmol, 0.0456 g) were dissolved in 30 mL EtOH at room temperature, and a solution of Triethylamine in EtOH (1.0 mol/L, 1 ml) was then added. The resulting solution was stirred and heated under reflux for 30 mins. It was allowed to cool and was then filtered. Diethyl ether was allowed to diffuse slowly into the filtrate at room temperature and pale yellow crystals were obtained after one week. The crystals were filtered off and washed with EtOH (3×5 ml). Yield (based on $Nd(OAc)_3$): 0.0479 g (37 %). m. p. > 203 ^oC (dec.). Elemental analysis (after dried in the oven at 120°C for two hours): Found: C, 24.65; H, 2.53 %. Calc. for $C_{280}H_{378}Nd_{42}O_{238}$: C, 24.71; H, 2.80 %. IR (KBr, cm^{-1}): 1650 (s), 1570 (s), 1410 (m), 1310 (w), 1310 (w), 1240 (s), 1210 (s), 1170 (w), 1074 (s), 1030 (s), 954 (s), 854 (s), 785 (w), 747 (m), 725 (m), 667 (m), 612 (w).

$[La_{42}(L)_{14}(OH)_{28}(OAc)_{84}]$ (2) $La(OAc)_3 \cdot 1.5H_2O$ (0.40 mmol, 0.1372 g) and HL (2-Hydroxy-3-methoxybenzaldehyde) (0.30 mmol, 0.0456 g) were dissolved in 30 mL EtOH at room temperature, and a solution of Triethylamine in EtOH (1.0 mol/L, 1 ml) was then added. The resulting solution was stirred and heated under reflux for 30 mins. It was allowed to cool and was then filtered. Diethyl ether was allowed to diffuse slowly into the filtrate at room temperature and pale yellow crystals were obtained after one week. The crystals were filtered off and washed with EtOH (3×5 ml). Yield (based on $La(OAc)_3 \cdot 1.5H_2O$): 0.0534 g (42 %). m. p. > 201^oC (dec.). Elemental analysis (after dried in the oven at 120°C for two hours): Found: C, 24.96; H, 2.78 %. Calc. for $C_{280}H_{378}La_{42}O_{238}$: C, 25.12; H, 2.85 %. IR (KBr, cm^{-1}): 1652 (s), 1559 (s), 1410 (m), 1350 (w), 1310 (w), 1250 (m), 1213 (s), 1170 (w), 1070 (w), 1050 (w), 1030 (m), 957 (m), 946 (s), 859 (m), 784 (m), 727 (m), 678 (m), 646 (w).

3. IR spectra of free ligand HL and clusters 1 and 2.

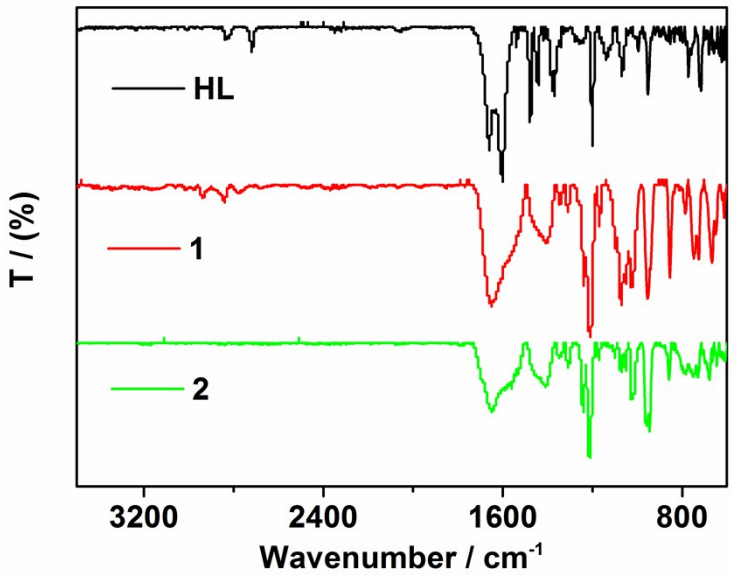


Figure S1. IR spectra of free ligand HL and clusters **1** and **2**.

4. The thermogravimetric analyses of 1

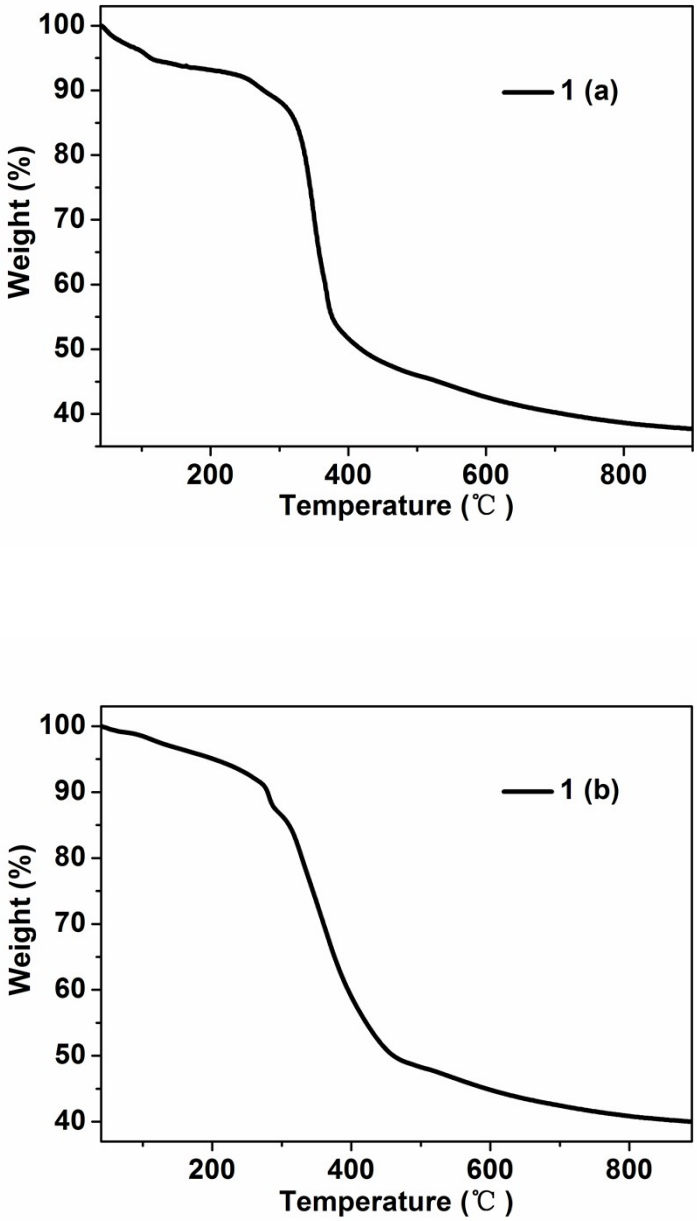
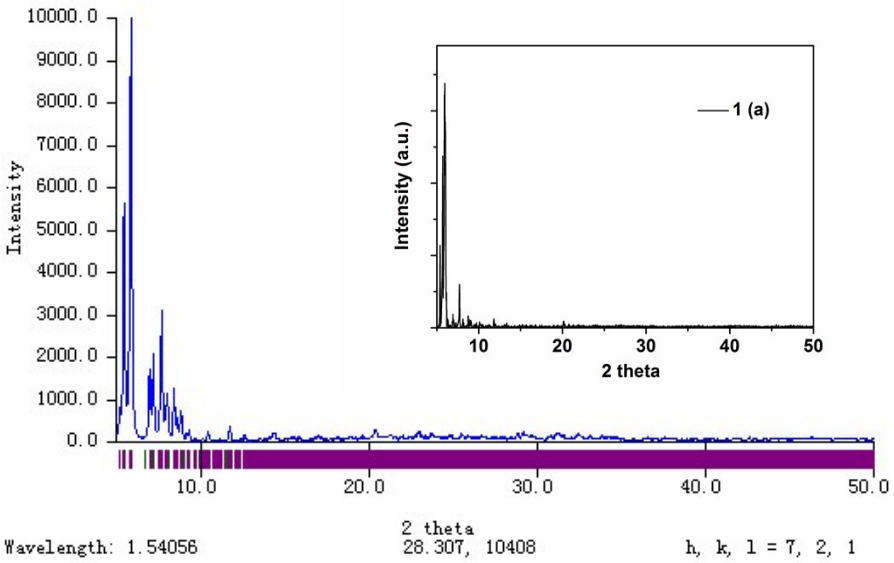
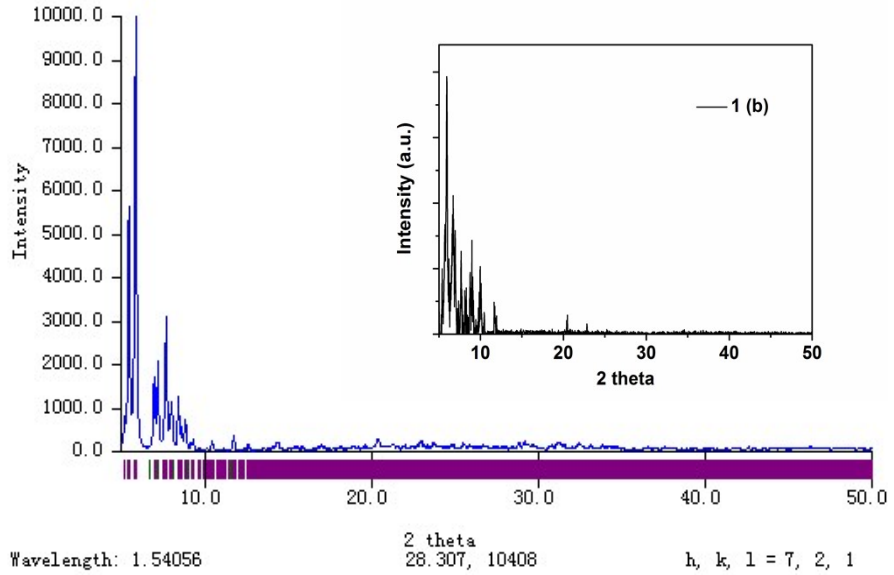


Figure S2. The thermogravimetric analyses of **1** before (a) and after (b) dried in the oven at 120°C for two hours.

5. Powder XRD patterns of 1 and 2





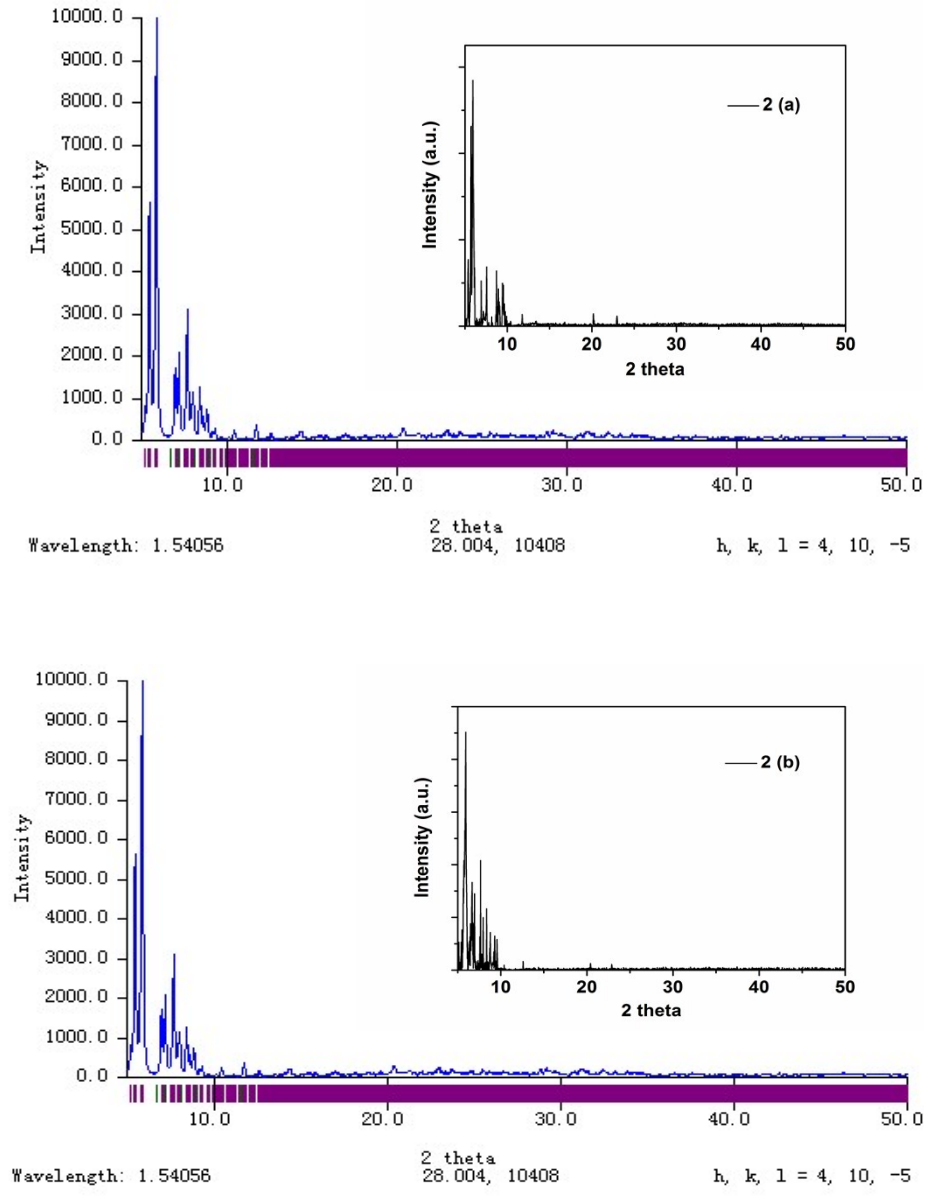


Figure S3. Powder XRD patterns of **1** and **2** before (a) and after (b) dried in the oven at 120°C for two hours.

6. Dynamic light scattering (DLS) measurements of 1

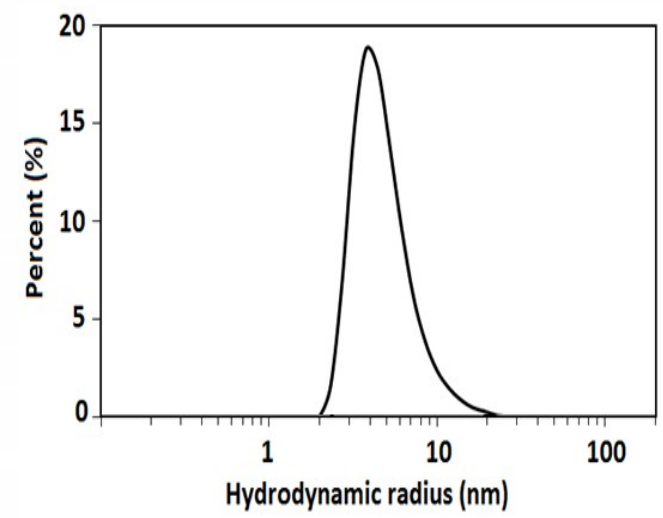


Figure S4. Dynamic light scattering (DLS) measurements of **1** in CH_3CN.

7. ^{1}H NMR spectrum of 1

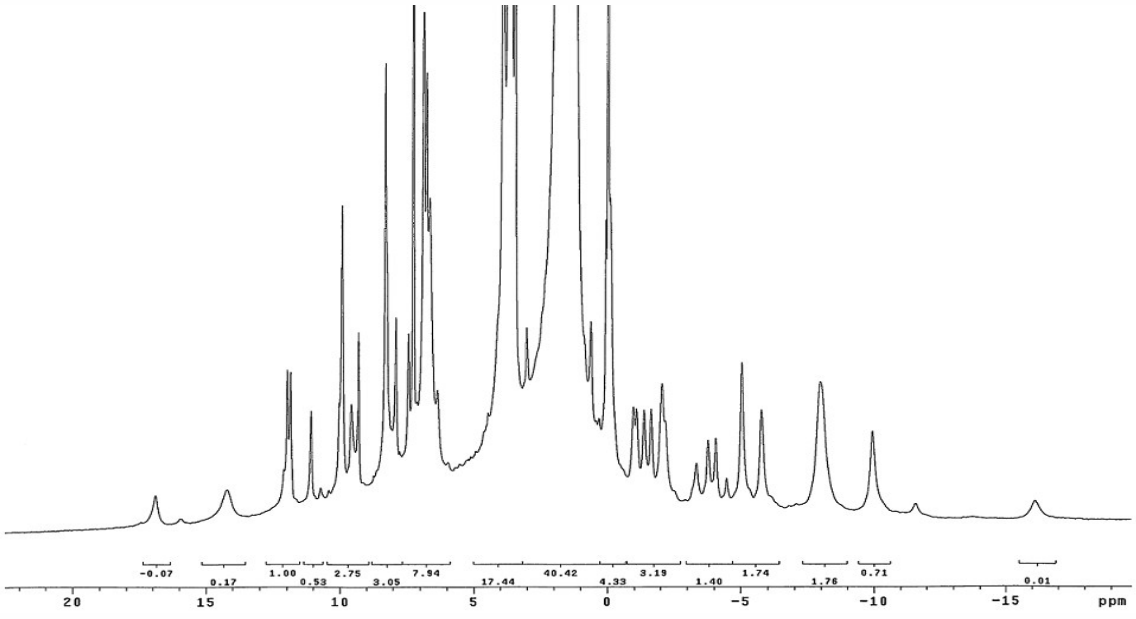


Figure S5. ^{1}H NMR spectrum of **1** in CD_3CN.

8. Photophysical properties of 1 and 2

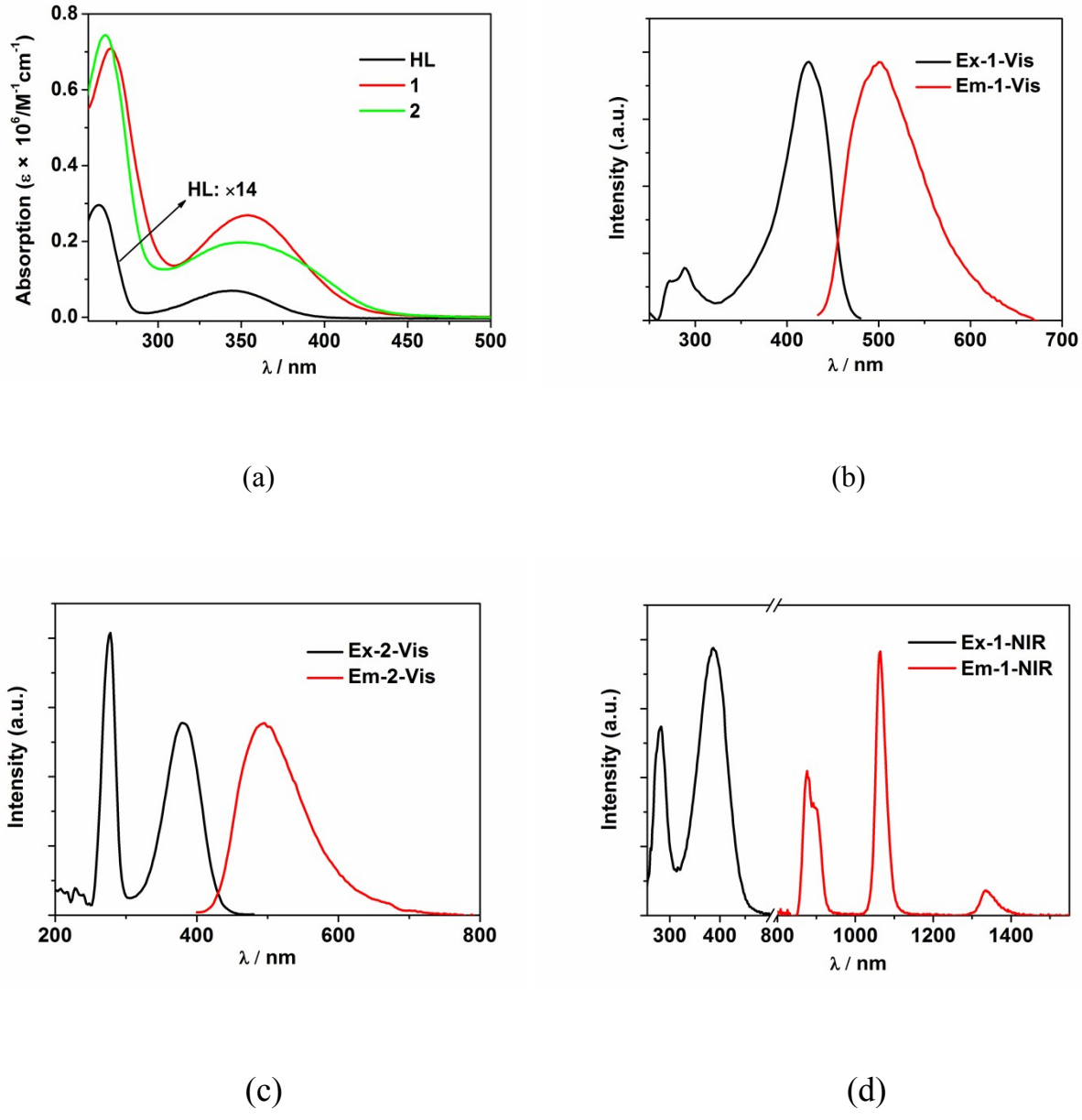


Figure S6. (a) UV-vis absorption spectra of the free ligand HL and clusters **1** and **2** in CH_3CN; (b) The excitation and visible emission spectra of **1** in CH_3CN; (c) The excitation and visible emission spectra of **2** in CH_3CN; (d) The excitation and NIR emission spectra of **1** in CH_3CN. (The solid samples of **1** and **2** used for the preparation of solutions are solvent free with dried in the oven at 120°C for two hours)

9. The NIR emission lifetime of 1

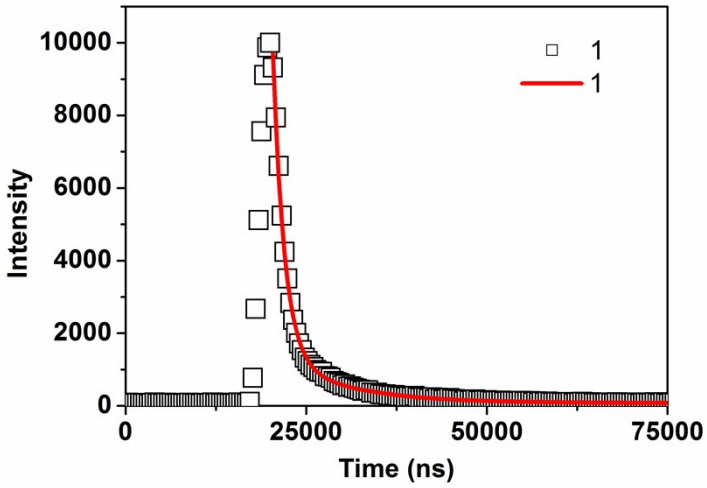


Figure S7. The NIR emission lifetime of **1** in CH_3CN.

10. Chemical structures of nitro explosives

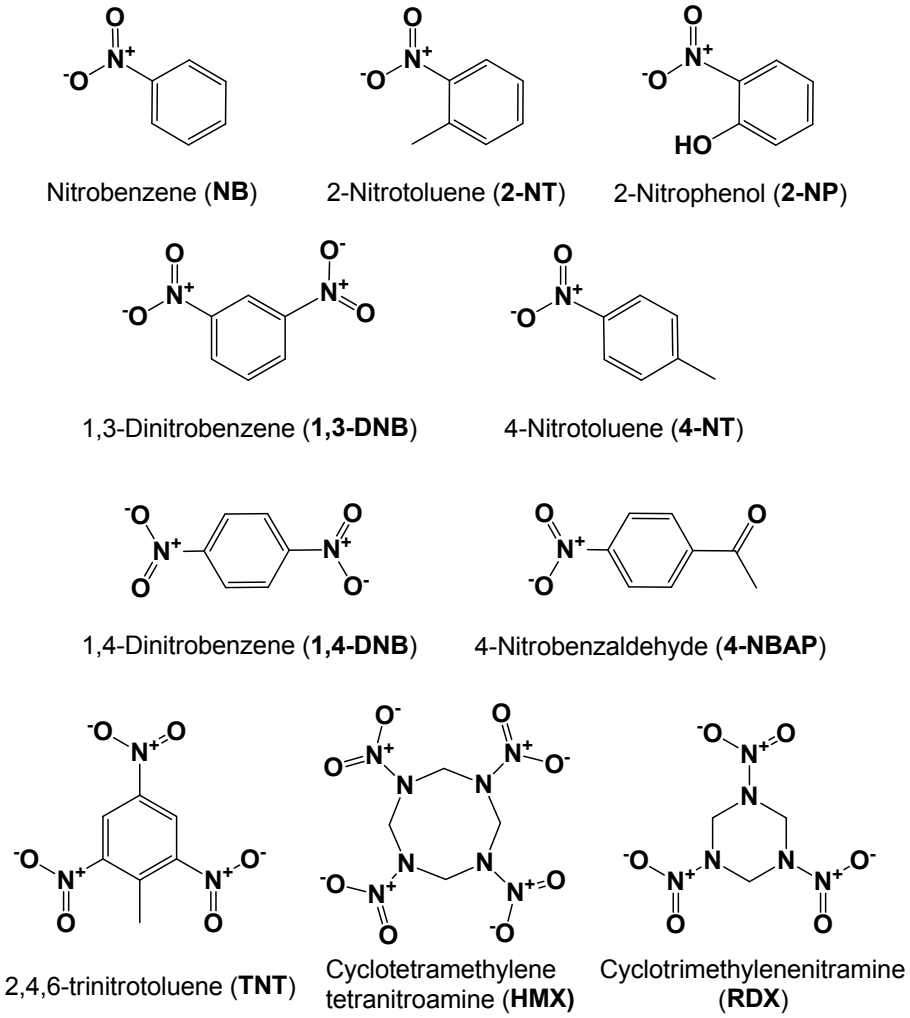
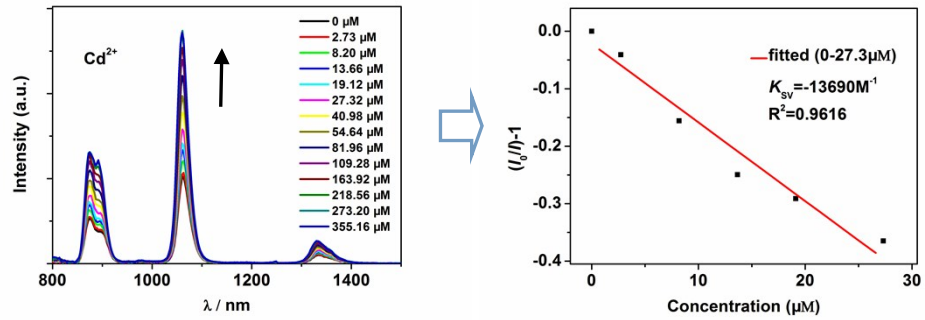
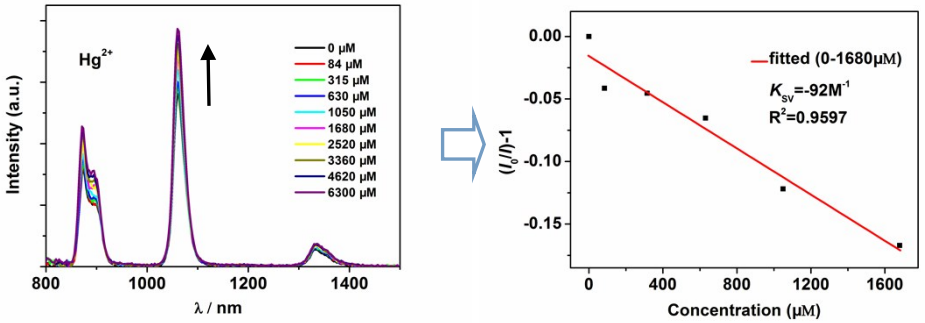
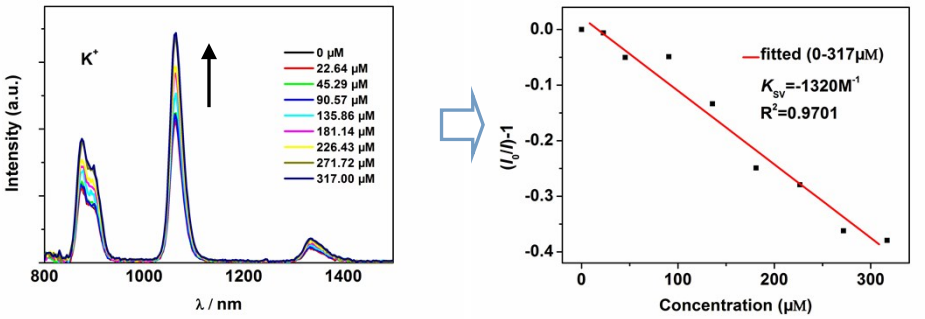


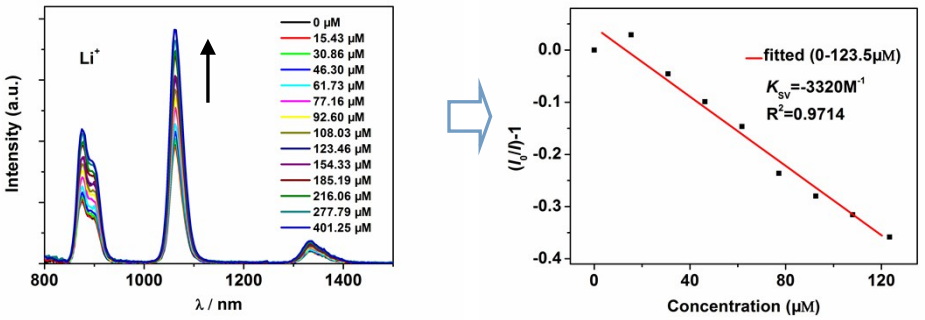
Figure S8. Chemical structures of nitro explosives.

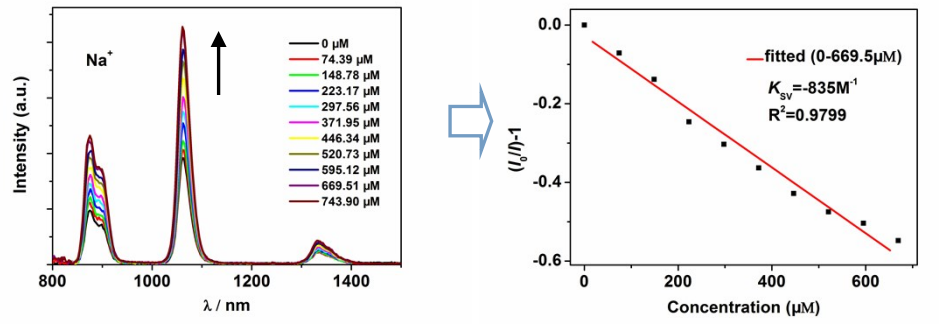
11. NIR luminescent sensing of 1 to metal ions

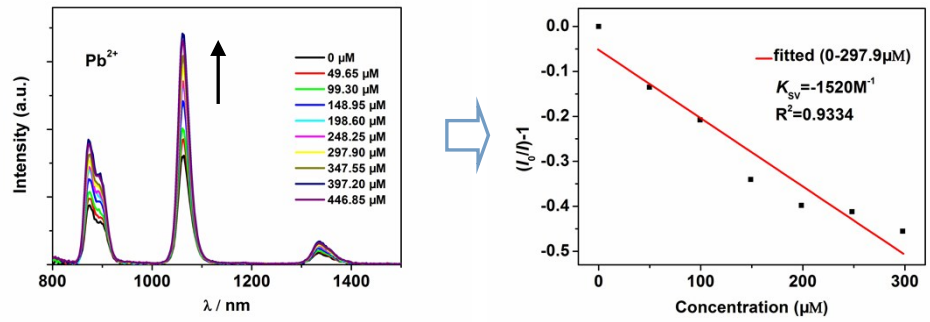


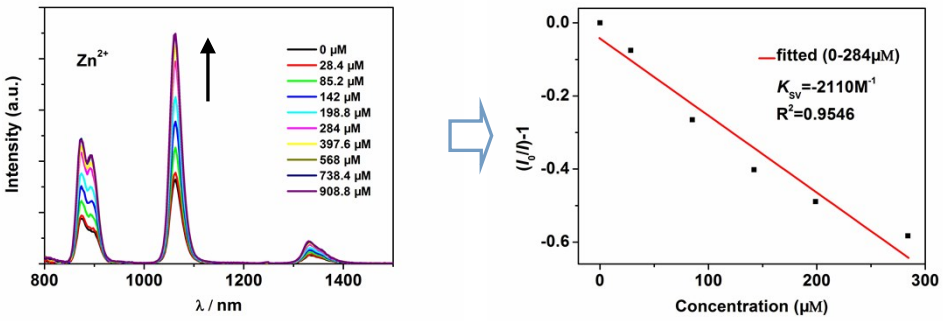


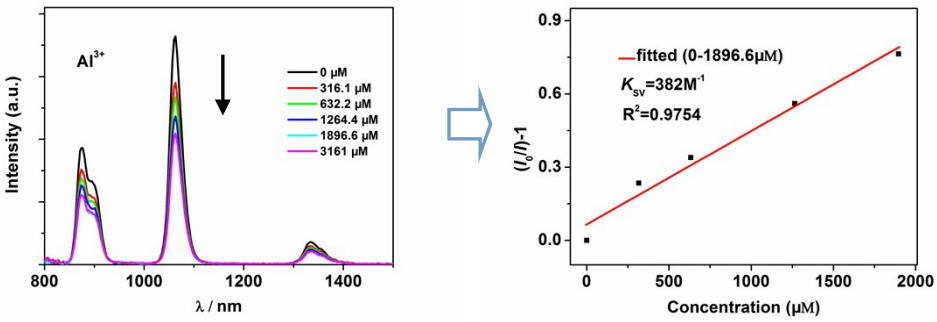


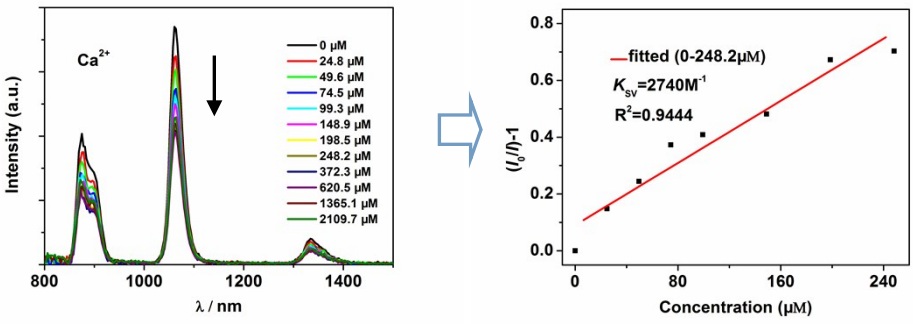


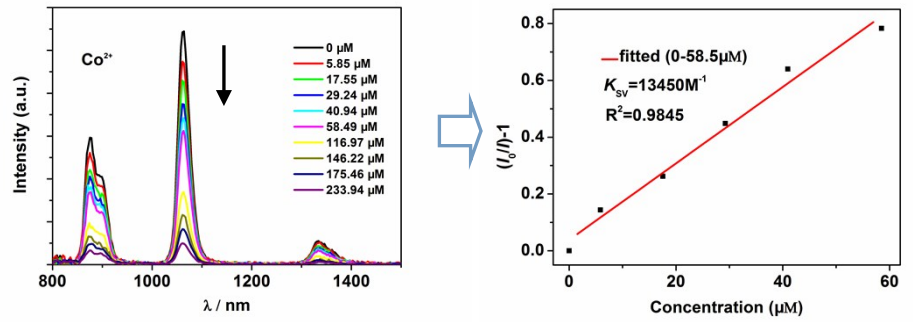

Na+
0 μM
74.39 μM
148.78 μM
223.17 μM
297.56 μM
371.95 μM
446.34 μM
520.73 μM
595.12 μM
669.51 μM
743.90 μM
Intensity (a.u.)
λ / nm
fitted (0-669.5μM)
Ksv=-835M-1
R2=0.9799
(I0/I)-1
Concentration (μM)

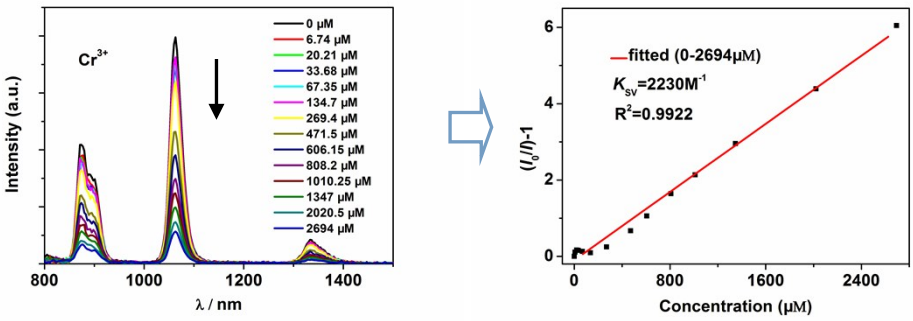

Pb2+
0 μM
49.65 μM
99.30 μM
148.95 μM
198.60 μM
248.25 μM
297.90 μM
347.55 μM
397.20 μM
446.85 μM
Intensity (a.u.)
λ / nm
fitted (0-297.9μM)
Ksv=-1520M-1
R2=0.9334
(I0/I)-1
Concentration (μM)

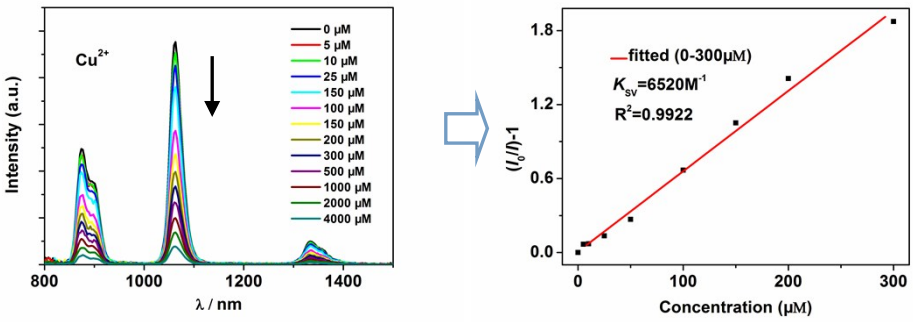

Zn2+
0 μM
28.4 μM
85.2 μM
142 μM
198.8 μM
284 μM
397.6 μM
568 μM
738.4 μM
908.8 μM
Intensity (a.u.)
λ / nm
fitted (0-284μM)
Ksv=-2110M-1
R2=0.9546
(I0/I)-1
Concentration (μM)


Al3+
0 μM
316.1 μM
632.2 μM
1264.4 μM
1896.6 μM
3161 μM
Intensity (a.u.)
λ / nm
fitted (0-1896.6μM)
Ksv=382M-1
R2=0.9754
(I0/I)-1
Concentration (μM)


Ca2+
0 μM
24.8 μM
49.6 μM
74.5 μM
99.3 μM
148.9 μM
198.5 μM
248.2 μM
372.3 μM
620.5 μM
1365.1 μM
2109.7 μM
Intensity (a.u.)
λ / nm
fitted (0-248.2μM)
KSV=2740M-1
R2=0.9444
(I0/I)-1
Concentration (μM)


Co2+
0 μM
5.85 μM
17.55 μM
29.24 μM
40.94 μM
58.49 μM
116.97 μM
146.22 μM
175.46 μM
233.94 μM
Intensity (a.u.)
λ / nm
fitted (0-58.5μM)
KSV=13450M-1
R2=0.9845
(I0/I)-1
Concentration (μM)


Cr3+
0 μM
6.74 μM
20.21 μM
33.68 μM
67.35 μM
134.7 μM
269.4 μM
471.5 μM
606.15 μM
808.2 μM
1010.25 μM
1347 μM
2020.5 μM
2694 μM
Intensity (a.u.)
λ / nm
fitted (0-2694μM)
KSV=2230M-1
R2=0.9922
(I0/I)-1
Concentration (μM)


Cu2+
0 μM
5 μM
10 μM
25 μM
150 μM
100 μM
150 μM
200 μM
300 μM
500 μM
1000 μM
2000 μM
4000 μM
Intensity (a.u.)
λ / nm
fitted (0-300μM)
KSV=6520M-1
R2=0.9922
(I0/I)-1
Concentration (μM)

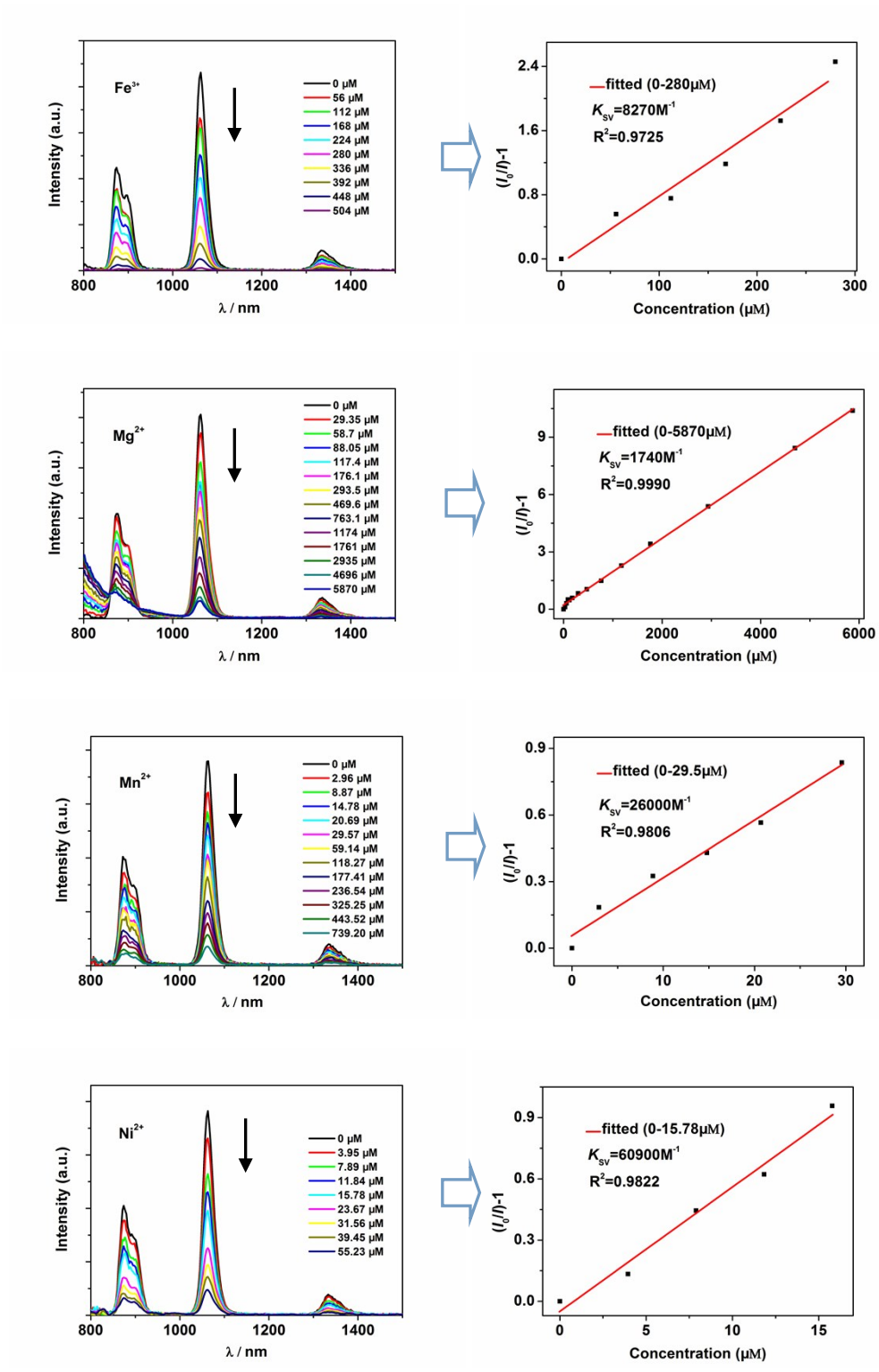
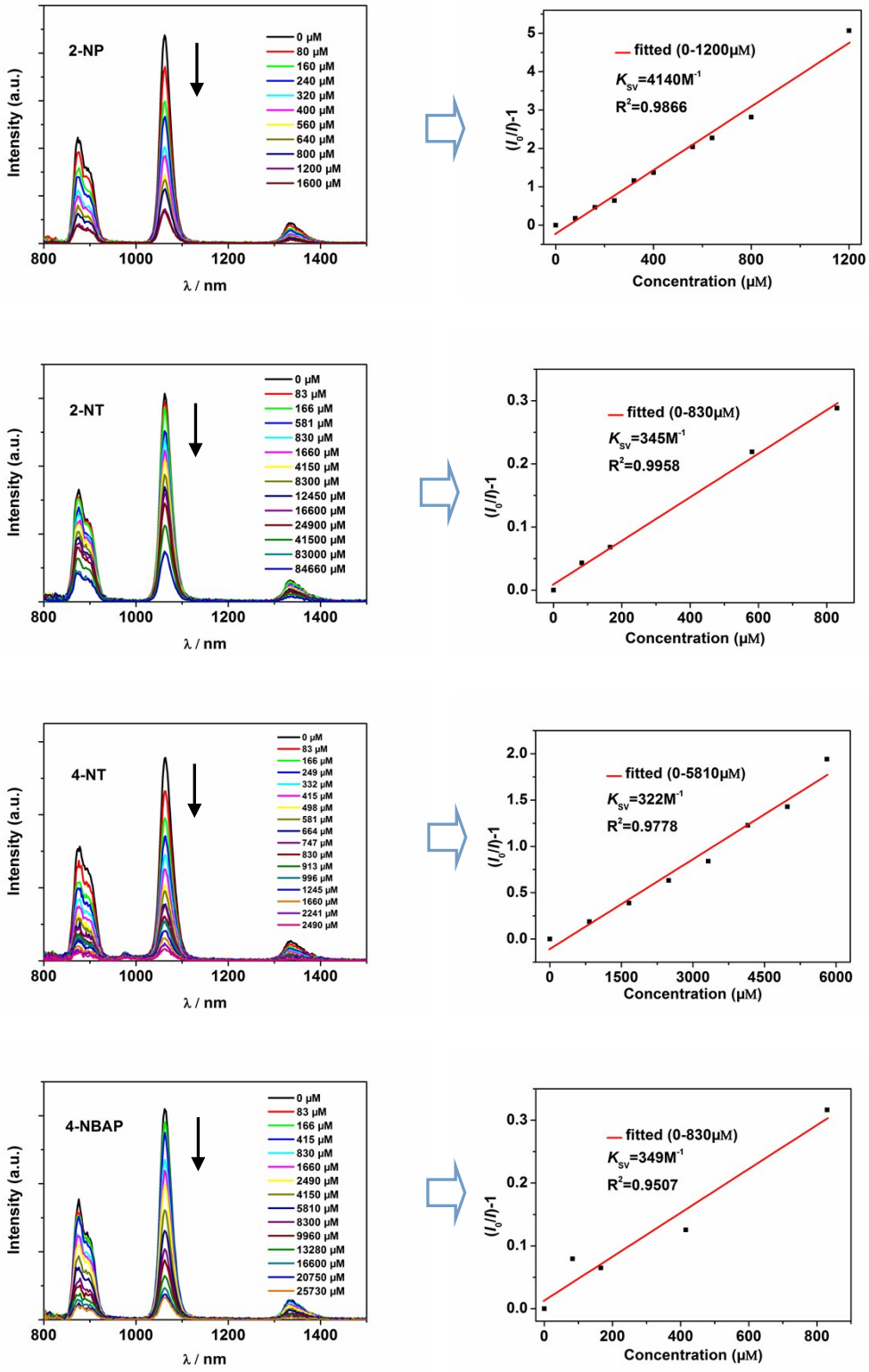
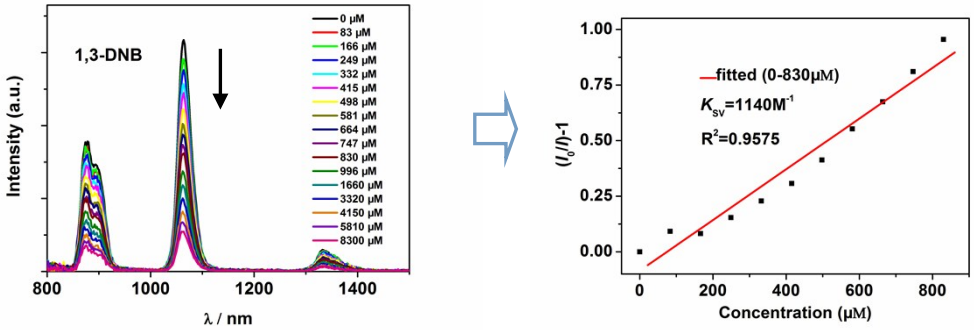
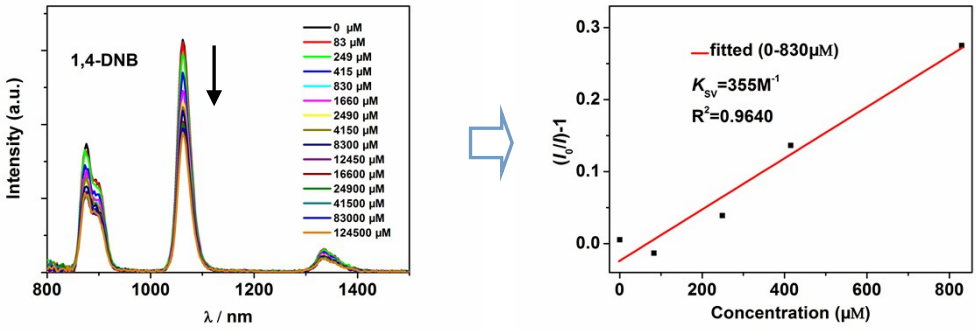


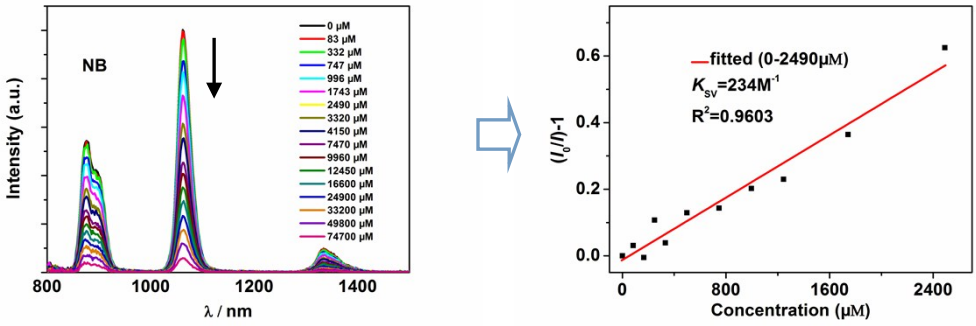
Figure S9. NIR luminescent sensing of **1** (15 μM) to metal ions in CH_3CN (λ_{ex} = 388 nm).

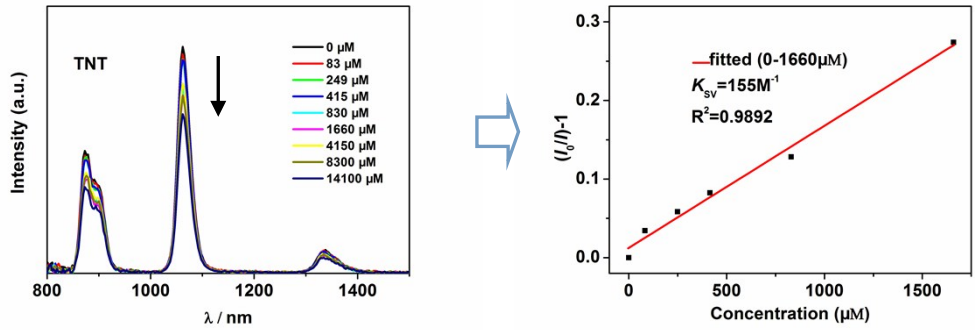
12. NIR luminescent sensing of 1 to nitro explosives




1,3-DNB
Intensity (a.u.)
λ / nm
0 μM
83 μM
166 μM
249 μM
332 μM
415 μM
498 μM
581 μM
664 μM
747 μM
830 μM
996 μM
1660 μM
3320 μM
4150 μM
5810 μM
8300 μM
fitted (0-830μM)
K_{sv}=1140M^{-1}
R^2=0.9575
(I_0/I)-1
Concentration (μM)


1,4-DNB
Intensity (a.u.)
λ / nm
0 μM
83 μM
249 μM
415 μM
830 μM
1660 μM
2490 μM
4150 μM
8300 μM
12450 μM
16600 μM
24900 μM
41500 μM
83000 μM
124500 μM
fitted (0-830μM)
K_{sv}=355M^{-1}
R^2=0.9640
(I_0/I)-1
Concentration (μM)


NB
Intensity (a.u.)
λ / nm
0 μM
83 μM
332 μM
747 μM
996 μM
1743 μM
2490 μM
3320 μM
4150 μM
7470 μM
9960 μM
12450 μM
16600 μM
24900 μM
33200 μM
49800 μM
74700 μM
fitted (0-2490μM)
K_{sv}=234M^{-1}
R^2=0.9603
(I_0/I)-1
Concentration (μM)


TNT
Intensity (a.u.)
λ / nm
0 μM
83 μM
249 μM
415 μM
830 μM
1660 μM
4150 μM
8300 μM
14100 μM
fitted (0-1660μM)
K_{sv}=155M^{-1}
R^2=0.9892
(I_0/I)-1
Concentration (μM)

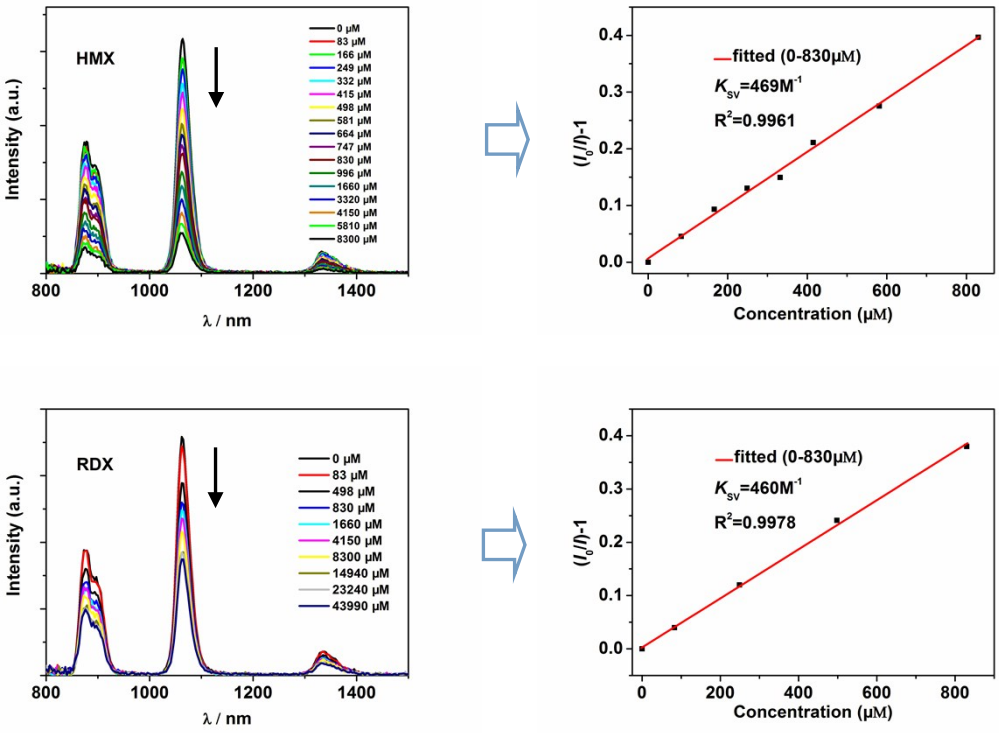


Figure S10. NIR luminescent sensing of **1** (15 μM) to nitro explosives in CH_3CN (λ_{ex} = 388 nm).

13. UV-Vis spectra of 1 with the addition of Cd^{2+}

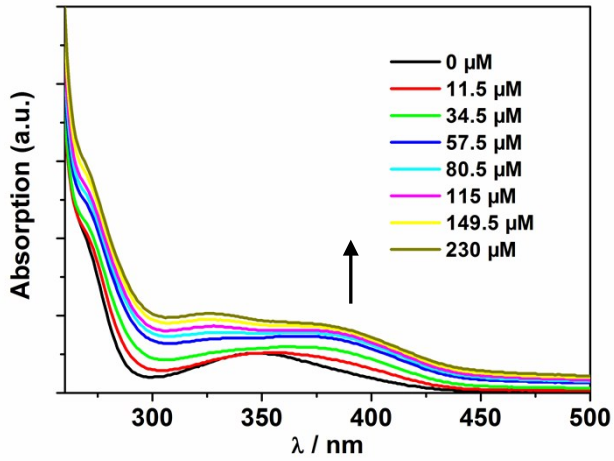


Figure S11. UV-Vis spectra of **1** with the addition of different concentrations of Cd^{2+} in CH_3CN.

14. UV-Vis absorption spectra of explosives in CH_3CN

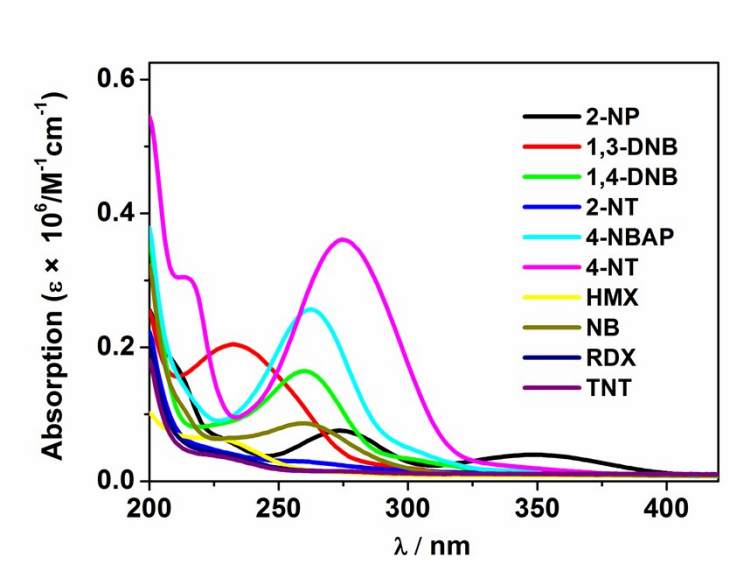


Figure S12. UV-Vis absorption spectra of explosives in CH_3CN.

15. 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]

For the crystal structures of **1** and **2**, some uncoordinated solvent molecules such as C_2H_5OH, $C_2H_5OC_2H_5$ and H_2O molecules 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** and **2** (CCDC reference numbers 1943243-1943244) are presented in Table S1 and selected bond lengths are given in Tables S2 and S3. 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) G. H. Sheldrick, SHELX 97, *A software package for the solution and refinement of X-ray data*; University of Göttingen: Göttingen, Germany, **1997**.

(3) 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** and **2**.

	1	**2**
Formula	$C_{280}H_{378}Nd_{42}O_{238}$	$C_{280}H_{378}La_{42}O_{238}$
Fw	13609.90	13386.04
Crystal system	Monoclinic	Monoclinic
Space group	P2(1)/c	P2(1)/c
a [Å]	24.556(5)	24.689(5)
b [Å]	39.353(8)	39.712(8)
c [Å]	34.244(7)	34.537(7)
α [deg]	90	90
β [deg]	110.06(3)	109.93(3)
γ [deg]	90	90
V / [Å^3]	31084(11)	31833(11)
d / [g/cm^3]	1.454	1.397
Z	2	2
T [K]	190(1)	190(1)
F(000)	12964	12712
μ, mm^{-1}	3.504	2.815
θ rang, deg	3.00-25.00	3.00-25.00
reflns meads	54284	54890
reflns used	54284	54890
params	2521	2521
R1[a], wR2[a] [$I > 2\sigma(I)$]	0.0667, 0.1696	0.0626, 0.1496
R1, wR2 (all data)	0.1132, 0.1925	0.1048, 0.1651
Quality of fit	0.983	0.961

[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) for **1**.

Nd(1)-O(12)	2.371(9)	Nd(7)-O(103)	2.309(8)
Nd(1)-O(79)	2.401(8)	Nd(7)-O(92)	2.347(9)
Nd(1)-O(76)	2.413(8)	Nd(7)-O(95)	2.355(8)
Nd(1)-O(68)	2.413(8)	Nd(7)-O(97)	2.370(8)
Nd(1)-O(71)	2.414(8)	Nd(7)-O(89)	2.407(8)
Nd(1)-O(11)	2.426(8)	Nd(7)-O(91)	2.423(8)
Nd(1)-O(74)	2.427(9)	Nd(7)-O(17)	2.424(8)
Nd(1)-O(72)	2.448(8)	Nd(7)-O(16)	2.549(9)
Nd(1)-O(75)	2.532(8)	Nd(8)-O(119)	2.348(8)
Nd(2)-O(90)	2.333(9)	Nd(8)-O(52)	2.389(9)
Nd(2)-O(75)	2.358(8)	Nd(8)-O(53)	2.435(8)
Nd(2)-O(78)	2.359(9)	Nd(8)-O(56)	2.446(9)
Nd(2)-O(86)	2.361(7)	Nd(8)-O(59)	2.465(8)
Nd(2)-O(84)	2.365(8)	Nd(8)-O(61)	2.473(9)
Nd(2)-O(14)	2.409(9)	Nd(8)-O(58)	2.486(8)
Nd(2)-O(79)	2.452(8)	Nd(8)-O(57)	2.499(10)
Nd(2)-O(13)	2.497(9)	Nd(8)-O(60)	2.541(9)
Nd(3)-O(90)	2.356(8)	Nd(9)-O(70)	2.340(9)
Nd(3)-O(69)	2.376(8)	Nd(9)-O(68)	2.349(9)
Nd(3)-O(91)	2.449(8)	Nd(9)-O(66)	2.353(7)
Nd(3)-O(85)	2.454(8)	Nd(9)-O(63)	2.366(8)
Nd(3)-O(88)	2.469(9)	Nd(9)-O(56)	2.383(9)
Nd(3)-O(84)	2.477(8)	Nd(9)-O(11)	2.408(8)
Nd(3)-O(89)	2.481(8)	Nd(9)-O(53)	2.435(8)
Nd(3)-O(81)	2.490(9)	Nd(9)-O(10)	2.525(8)
Nd(3)-O(80)	2.506(9)	Nd(10)-O(64)	2.352(10)
Nd(4)-O(28)	2.395(8)	Nd(10)-O(68)	2.362(8)
Nd(4)-O(3)	2.402(9)	Nd(10)-O(79)	2.414(8)
Nd(4)-O(31)	2.438(7)	Nd(10)-O(73)	2.440(10)
Nd(4)-O(32)	2.439(8)	Nd(10)-O(67)	2.468(9)
Nd(4)-O(27)	2.442(10)	Nd(10)-O(66)	2.474(8)
Nd(4)-O(26)	2.455(9)	Nd(10)-O(77)	2.476(9)
Nd(4)-O(2)	2.456(8)	Nd(10)-O(78)	2.491(8)
Nd(4)-O(29)	2.493(8)	Nd(10)-O(74)	2.532(8)
Nd(4)-O(30)	2.525(8)	Nd(11)-O(87)	2.340(9)
Nd(5)-O(28)	2.349(8)	Nd(11)-O(97)	2.358(7)
Nd(5)-O(25)	2.378(8)	Nd(11)-O(105)	2.440(8)
Nd(5)-O(31)	2.442(7)	Nd(11)-O(94)	2.466(9)
Nd(5)-O(33)	2.455(9)	Nd(11)-O(100)	2.466(7)
Nd(5)-O(36)	2.462(8)	Nd(11)-O(95)	2.474(8)
Nd(5)-O(37)	2.470(8)	Nd(11)-O(96)	2.482(9)
Nd(5)-O(34)	2.481(8)	Nd(11)-O(99)	2.512(9)
Nd(5)-O(35)	2.502(9)	Nd(11)-O(98)	2.522(10)
Nd(5)-O(32)	2.519(8)	Nd(12)-O(114)	2.313(7)
Nd(6)-O(118)	2.342(8)	Nd(12)-O(112)	2.342(8)
Nd(6)-O(41)	2.344(8)	Nd(12)-O(107)	2.363(8)
Nd(6)-O(40)	2.351(8)	Nd(12)-O(100)	2.372(9)
Nd(6)-O(30)	2.360(9)	Nd(12)-O(106)	2.376(8)
Nd(6)-O(34)	2.405(8)	Nd(12)-O(20)	2.414(7)
Nd(6)-O(5)	2.422(7)	Nd(12)-O(105)	2.422(7)
Nd(6)-O(31)	2.424(8)	Nd(12)-O(19)	2.516(8)
Nd(6)-O(4)	2.488(9)	Nd(13)-O(39)	2.319(9)

Nd(13)-O(37)	2.335(8)	Nd(19)-O(8)	2.424(10)
Nd(13)-O(22)	2.359(9)	Nd(19)-O(55)	2.428(9)
Nd(13)-O(28)	2.373(8)	Nd(19)-O(52)	2.433(8)
Nd(13)-O(24)	2.385(8)	Nd(19)-O(62)	2.471(9)
Nd(13)-O(2)	2.417(7)	Nd(19)-O(54)	2.476(11)
Nd(13)-O(23)	2.445(8)	Nd(19)-O(63)	2.525(9)
Nd(13)-O(1)	2.489(8)	Nd(20)-O(38)	2.370(9)
Nd(14)-O(21)	2.388(9)	Nd(20)-O(40)	2.395(8)
Nd(14)-O(20)	2.399(8)	Nd(20)-O(45)	2.411(9)
Nd(14)-O(106)	2.404(7)	Nd(20)-O(42)	2.455(9)
Nd(14)-O(110)	2.428(10)	Nd(20)-O(48)	2.461(11)
Nd(14)-O(23)#1	2.439(8)	Nd(20)-O(51)	2.477(8)
Nd(14)-O(116)	2.461(11)	Nd(20)-O(41)	2.477(8)
Nd(14)-O(115)	2.479(9)	Nd(20)-O(50)	2.492(10)
Nd(14)-O(117)	2.480(15)	Nd(20)-O(49)	2.520(9)
Nd(14)-O(22)#1	2.551(8)	Nd(21)-O(104)	2.327(8)
Nd(15)-O(6)	2.368(9)	Nd(21)-O(106)	2.361(8)
Nd(15)-O(49)	2.377(11)	Nd(21)-O(112)	2.468(9)
Nd(15)-O(45)	2.410(8)	Nd(21)-O(113)	2.472(10)
Nd(15)-O(5)	2.414(9)	Nd(21)-O(111)	2.493(11)
Nd(15)-O(43)	2.422(10)	Nd(21)-O(109)	2.496(10)
Nd(15)-O(40)	2.440(7)	Nd(21)-O(110)	2.539(10)
Nd(15)-O(44)	2.450(10)	O(12)-Nd(1)-O(79)	87.9(3)
Nd(15)-O(46)	2.465(9)	O(12)-Nd(1)-O(76)	82.0(3)
Nd(15)-O(47)	2.519(10)	O(79)-Nd(1)-O(76)	120.3(3)
Nd(16)-O(65)	2.316(9)	O(12)-Nd(1)-O(68)	135.7(3)
Nd(16)-O(58)	2.353(9)	O(79)-Nd(1)-O(68)	70.0(3)
Nd(16)-O(51)	2.357(9)	O(76)-Nd(1)-O(68)	142.3(3)
Nd(16)-O(47)	2.368(9)	O(12)-Nd(1)-O(71)	128.4(3)
Nd(16)-O(52)	2.368(9)	O(79)-Nd(1)-O(71)	143.2(3)
Nd(16)-O(8)	2.417(9)	O(76)-Nd(1)-O(71)	76.7(3)
Nd(16)-O(45)	2.435(8)	O(68)-Nd(1)-O(71)	77.6(3)
Nd(16)-O(7)	2.491(10)	O(12)-Nd(1)-O(11)	70.6(3)
Nd(17)-O(91)	2.409(7)	O(79)-Nd(1)-O(11)	85.5(3)
Nd(17)-O(15)	2.409(9)	O(76)-Nd(1)-O(11)	141.9(3)
Nd(17)-O(90)	2.415(8)	O(68)-Nd(1)-O(11)	69.8(3)
Nd(17)-O(83)	2.417(9)	O(71)-Nd(1)-O(11)	99.7(3)
Nd(17)-O(81)	2.419(9)	O(12)-Nd(1)-O(74)	138.0(3)
Nd(17)-O(82)	2.438(9)	O(79)-Nd(1)-O(74)	70.2(3)
Nd(17)-O(14)	2.441(9)	O(76)-Nd(1)-O(74)	79.3(3)
Nd(17)-O(93)	2.473(9)	O(68)-Nd(1)-O(74)	70.5(3)
Nd(17)-O(92)	2.519(9)	O(71)-Nd(1)-O(74)	83.0(3)
Nd(18)-O(18)	2.393(10)	O(11)-Nd(1)-O(74)	138.5(3)
Nd(18)-O(105)	2.398(8)	O(12)-Nd(1)-O(72)	77.0(3)
Nd(18)-O(101)	2.404(10)	O(79)-Nd(1)-O(72)	157.8(3)
Nd(18)-O(99)	2.411(9)	O(76)-Nd(1)-O(72)	74.1(3)
Nd(18)-O(17)	2.424(8)	O(68)-Nd(1)-O(72)	110.0(3)
Nd(18)-O(97)	2.429(8)	O(71)-Nd(1)-O(72)	52.1(3)
Nd(18)-O(108)	2.469(9)	O(11)-Nd(1)-O(72)	74.3(3)
Nd(18)-O(102)	2.493(10)	O(74)-Nd(1)-O(72)	131.6(3)
Nd(18)-O(107)	2.570(8)	O(12)-Nd(1)-O(75)	70.9(3)
Nd(19)-O(53)	2.408(8)	O(79)-Nd(1)-O(75)	68.8(3)
Nd(19)-O(9)	2.415(10)	O(76)-Nd(1)-O(75)	52.2(3)
Nd(19)-O(60)	2.417(10)	O(68)-Nd(1)-O(75)	128.8(3)

O(71)-Nd(1)-O(75)	123.9(3)	O(69)-Nd(3)-O(81)	128.4(3)
O(11)-Nd(1)-O(75)	134.0(3)	O(91)-Nd(3)-O(81)	67.0(3)
O(74)-Nd(1)-O(75)	67.9(3)	O(85)-Nd(3)-O(81)	145.1(3)
O(72)-Nd(1)-O(75)	119.6(3)	O(88)-Nd(3)-O(81)	97.0(3)
O(90)-Nd(2)-O(75)	77.4(3)	O(84)-Nd(3)-O(81)	134.1(3)
O(90)-Nd(2)-O(78)	149.6(3)	O(89)-Nd(3)-O(81)	72.1(3)
O(75)-Nd(2)-O(78)	103.7(3)	O(90)-Nd(3)-O(80)	80.5(3)
O(90)-Nd(2)-O(86)	117.9(3)	O(69)-Nd(3)-O(80)	77.4(3)
O(75)-Nd(2)-O(86)	144.0(3)	O(91)-Nd(3)-O(80)	119.1(3)
O(78)-Nd(2)-O(86)	79.4(3)	O(85)-Nd(3)-O(80)	152.2(3)
O(90)-Nd(2)-O(84)	71.4(3)	O(88)-Nd(3)-O(80)	80.2(3)
O(75)-Nd(2)-O(84)	138.2(3)	O(84)-Nd(3)-O(80)	138.3(3)
O(78)-Nd(2)-O(84)	90.5(3)	O(89)-Nd(3)-O(80)	100.0(3)
O(86)-Nd(2)-O(84)	76.7(3)	O(81)-Nd(3)-O(80)	53.2(3)
O(90)-Nd(2)-O(14)	70.5(3)	O(28)-Nd(4)-O(3)	136.2(3)
O(75)-Nd(2)-O(14)	83.4(3)	O(28)-Nd(4)-O(31)	70.4(3)
O(78)-Nd(2)-O(14)	139.8(3)	O(3)-Nd(4)-O(31)	89.0(3)
O(86)-Nd(2)-O(14)	73.2(3)	O(28)-Nd(4)-O(32)	71.6(3)
O(84)-Nd(2)-O(14)	110.5(3)	O(3)-Nd(4)-O(32)	138.0(3)
O(90)-Nd(2)-O(79)	80.9(3)	O(31)-Nd(4)-O(32)	70.5(3)
O(75)-Nd(2)-O(79)	70.9(3)	O(28)-Nd(4)-O(27)	102.1(3)
O(78)-Nd(2)-O(79)	71.2(3)	O(3)-Nd(4)-O(27)	82.6(3)
O(86)-Nd(2)-O(79)	140.1(3)	O(31)-Nd(4)-O(27)	157.8(3)
O(84)-Nd(2)-O(79)	77.2(3)	O(32)-Nd(4)-O(27)	128.1(3)
O(14)-Nd(2)-O(79)	145.1(3)	O(28)-Nd(4)-O(26)	76.1(3)
O(90)-Nd(2)-O(13)	128.2(3)	O(3)-Nd(4)-O(26)	132.8(3)
O(75)-Nd(2)-O(13)	72.4(3)	O(31)-Nd(4)-O(26)	138.3(3)
O(78)-Nd(2)-O(13)	79.3(3)	O(32)-Nd(4)-O(26)	76.0(3)
O(86)-Nd(2)-O(13)	73.0(3)	O(27)-Nd(4)-O(26)	53.3(3)
O(84)-Nd(2)-O(13)	149.3(3)	O(28)-Nd(4)-O(2)	69.8(3)
O(14)-Nd(2)-O(13)	65.1(3)	O(3)-Nd(4)-O(2)	69.4(3)
O(79)-Nd(2)-O(13)	124.8(3)	O(31)-Nd(4)-O(2)	82.2(3)
O(90)-Nd(3)-O(69)	87.6(3)	O(32)-Nd(4)-O(2)	138.3(2)
O(90)-Nd(3)-O(91)	70.9(3)	O(27)-Nd(4)-O(2)	75.6(3)
O(69)-Nd(3)-O(91)	148.8(3)	O(26)-Nd(4)-O(2)	108.8(3)
O(90)-Nd(3)-O(85)	121.3(3)	O(28)-Nd(4)-O(29)	146.5(3)
O(69)-Nd(3)-O(85)	86.0(3)	O(3)-Nd(4)-O(29)	77.3(3)
O(91)-Nd(3)-O(85)	86.4(3)	O(31)-Nd(4)-O(29)	120.1(3)
O(90)-Nd(3)-O(88)	160.7(3)	O(32)-Nd(4)-O(29)	82.1(3)
O(69)-Nd(3)-O(88)	86.9(3)	O(27)-Nd(4)-O(29)	78.0(3)
O(91)-Nd(3)-O(88)	120.5(3)	O(26)-Nd(4)-O(29)	77.7(3)
O(85)-Nd(3)-O(88)	76.7(3)	O(2)-Nd(4)-O(29)	139.6(3)
O(90)-Nd(3)-O(84)	69.1(3)	O(28)-Nd(4)-O(30)	130.2(3)
O(69)-Nd(3)-O(84)	73.6(3)	O(3)-Nd(4)-O(30)	69.8(3)
O(91)-Nd(3)-O(84)	77.6(3)	O(31)-Nd(4)-O(30)	69.0(3)
O(85)-Nd(3)-O(84)	53.2(3)	O(32)-Nd(4)-O(30)	68.7(3)
O(88)-Nd(3)-O(84)	126.6(3)	O(27)-Nd(4)-O(30)	125.9(3)
O(90)-Nd(3)-O(89)	134.0(3)	O(26)-Nd(4)-O(30)	120.3(3)
O(69)-Nd(3)-O(89)	137.8(3)	O(2)-Nd(4)-O(30)	129.7(3)
O(91)-Nd(3)-O(89)	69.1(3)	O(29)-Nd(4)-O(30)	51.5(3)
O(85)-Nd(3)-O(89)	77.6(3)	O(28)-Nd(5)-O(25)	86.6(3)
O(88)-Nd(3)-O(89)	51.7(3)	O(28)-Nd(5)-O(31)	71.1(3)
O(84)-Nd(3)-O(89)	121.6(3)	O(25)-Nd(5)-O(31)	147.2(3)
O(90)-Nd(3)-O(81)	72.2(3)	O(28)-Nd(5)-O(33)	81.4(3)

O(25)-Nd(5)-O(33)	77.6(3)
O(31)-Nd(5)-O(33)	120.6(3)
O(28)-Nd(5)-O(36)	122.4(3)
O(25)-Nd(5)-O(36)	86.8(3)
O(31)-Nd(5)-O(36)	85.4(3)
O(33)-Nd(5)-O(36)	150.9(3)
O(28)-Nd(5)-O(37)	70.0(3)
O(25)-Nd(5)-O(37)	73.8(3)
O(31)-Nd(5)-O(37)	76.0(3)
O(33)-Nd(5)-O(37)	140.2(3)
O(36)-Nd(5)-O(37)	53.3(3)
O(28)-Nd(5)-O(34)	133.2(3)
O(25)-Nd(5)-O(34)	139.5(3)
O(31)-Nd(5)-O(34)	69.0(3)
O(33)-Nd(5)-O(34)	98.6(3)
O(36)-Nd(5)-O(34)	77.6(3)
O(37)-Nd(5)-O(34)	121.1(3)
O(28)-Nd(5)-O(35)	161.1(3)
O(25)-Nd(5)-O(35)	87.6(3)
O(31)-Nd(5)-O(35)	120.8(3)
O(33)-Nd(5)-O(35)	79.7(3)
O(36)-Nd(5)-O(35)	75.2(3)
O(37)-Nd(5)-O(35)	125.3(3)
O(34)-Nd(5)-O(35)	52.4(3)
O(28)-Nd(5)-O(32)	70.9(3)
O(25)-Nd(5)-O(32)	126.5(3)
O(31)-Nd(5)-O(32)	69.1(3)
O(33)-Nd(5)-O(32)	52.1(3)
O(36)-Nd(5)-O(32)	146.2(3)
O(37)-Nd(5)-O(32)	134.0(3)
O(34)-Nd(5)-O(32)	72.9(3)
O(35)-Nd(5)-O(32)	98.5(3)
O(118)-Nd(6)-O(41)	76.2(3)
O(118)-Nd(6)-O(40)	119.4(3)
O(41)-Nd(6)-O(40)	72.2(3)
O(118)-Nd(6)-O(30)	144.6(3)
O(41)-Nd(6)-O(30)	138.3(3)
O(40)-Nd(6)-O(30)	76.6(3)
O(118)-Nd(6)-O(34)	77.5(3)
O(41)-Nd(6)-O(34)	91.5(3)
O(40)-Nd(6)-O(34)	151.0(3)
O(30)-Nd(6)-O(34)	103.5(3)
O(118)-Nd(6)-O(5)	74.0(3)
O(41)-Nd(6)-O(5)	109.2(3)
O(40)-Nd(6)-O(5)	69.9(3)
O(30)-Nd(6)-O(5)	84.4(3)
O(34)-Nd(6)-O(5)	139.1(3)
O(118)-Nd(6)-O(31)	137.4(2)
O(41)-Nd(6)-O(31)	77.1(3)
O(40)-Nd(6)-O(31)	82.3(3)
O(30)-Nd(6)-O(31)	72.0(3)
O(34)-Nd(6)-O(31)	70.6(3)
O(5)-Nd(6)-O(31)	147.1(3)
O(118)-Nd(6)-O(4)	72.8(3)
O(41)-Nd(6)-O(4)	148.9(3)
O(40)-Nd(6)-O(4)	127.0(3)
O(30)-Nd(6)-O(4)	72.8(3)
O(34)-Nd(6)-O(4)	78.9(3)
O(5)-Nd(6)-O(4)	65.0(3)
O(31)-Nd(6)-O(4)	125.5(3)
O(103)-Nd(7)-O(92)	146.6(3)
O(103)-Nd(7)-O(95)	78.7(3)
O(92)-Nd(7)-O(95)	133.6(3)
O(103)-Nd(7)-O(97)	119.8(3)
O(92)-Nd(7)-O(97)	73.7(3)
O(95)-Nd(7)-O(97)	70.9(3)
O(103)-Nd(7)-O(89)	76.4(3)
O(92)-Nd(7)-O(89)	105.8(3)
O(95)-Nd(7)-O(89)	92.6(3)
O(97)-Nd(7)-O(89)	152.2(3)
O(103)-Nd(7)-O(91)	136.1(3)
O(92)-Nd(7)-O(91)	72.1(3)
O(95)-Nd(7)-O(91)	74.6(3)
O(97)-Nd(7)-O(91)	83.2(3)
O(89)-Nd(7)-O(91)	70.7(3)
O(103)-Nd(7)-O(17)	73.2(3)
O(92)-Nd(7)-O(17)	85.3(3)
O(95)-Nd(7)-O(17)	109.1(3)
O(97)-Nd(7)-O(17)	69.9(3)
O(89)-Nd(7)-O(17)	137.8(3)
O(91)-Nd(7)-O(17)	148.9(3)
O(103)-Nd(7)-O(16)	74.2(3)
O(92)-Nd(7)-O(16)	73.3(3)
O(95)-Nd(7)-O(16)	152.9(3)
O(97)-Nd(7)-O(16)	124.2(3)
O(89)-Nd(7)-O(16)	80.4(3)
O(91)-Nd(7)-O(16)	125.9(3)
O(17)-Nd(7)-O(16)	63.7(3)
O(119)-Nd(8)-O(52)	87.2(3)
O(119)-Nd(8)-O(53)	148.6(3)
O(52)-Nd(8)-O(53)	71.7(3)
O(119)-Nd(8)-O(56)	136.6(3)
O(52)-Nd(8)-O(56)	135.1(3)
O(53)-Nd(8)-O(56)	70.9(3)
O(119)-Nd(8)-O(59)	86.2(3)
O(52)-Nd(8)-O(59)	120.6(3)
O(53)-Nd(8)-O(59)	85.2(3)
O(56)-Nd(8)-O(59)	79.6(3)
O(119)-Nd(8)-O(61)	78.7(3)
O(52)-Nd(8)-O(61)	83.1(3)
O(53)-Nd(8)-O(61)	119.8(3)
O(56)-Nd(8)-O(61)	94.8(3)
O(59)-Nd(8)-O(61)	151.4(3)
O(119)-Nd(8)-O(58)	75.1(3)
O(52)-Nd(8)-O(58)	69.2(3)
O(53)-Nd(8)-O(58)	75.8(3)
O(56)-Nd(8)-O(58)	122.8(3)
O(59)-Nd(8)-O(58)	52.1(3)

O(61)-Nd(8)-O(58)	142.4(3)
O(119)-Nd(8)-O(57)	85.0(3)
O(52)-Nd(8)-O(57)	160.9(3)
O(53)-Nd(8)-O(57)	121.8(3)
O(56)-Nd(8)-O(57)	51.9(3)
O(59)-Nd(8)-O(57)	76.2(3)
O(61)-Nd(8)-O(57)	78.3(3)
O(58)-Nd(8)-O(57)	125.0(3)
O(119)-Nd(8)-O(60)	126.5(3)
O(52)-Nd(8)-O(60)	70.0(3)
O(53)-Nd(8)-O(60)	68.3(3)
O(56)-Nd(8)-O(60)	73.8(3)
O(59)-Nd(8)-O(60)	147.2(3)
O(61)-Nd(8)-O(60)	51.7(3)
O(58)-Nd(8)-O(60)	132.1(3)
O(57)-Nd(8)-O(60)	101.1(3)
O(70)-Nd(9)-O(68)	117.3(3)
O(70)-Nd(9)-O(66)	75.7(3)
O(68)-Nd(9)-O(66)	71.3(3)
O(70)-Nd(9)-O(63)	148.6(3)
O(68)-Nd(9)-O(63)	76.3(3)
O(66)-Nd(9)-O(63)	135.0(3)
O(70)-Nd(9)-O(56)	78.4(3)
O(68)-Nd(9)-O(56)	151.3(3)
O(66)-Nd(9)-O(56)	91.5(3)
O(63)-Nd(9)-O(56)	103.2(3)
O(70)-Nd(9)-O(11)	73.7(3)
O(68)-Nd(9)-O(11)	71.1(3)
O(66)-Nd(9)-O(11)	111.3(3)
O(63)-Nd(9)-O(11)	85.8(3)
O(56)-Nd(9)-O(11)	137.5(3)
O(70)-Nd(9)-O(53)	137.1(3)
O(68)-Nd(9)-O(53)	81.3(3)
O(66)-Nd(9)-O(53)	74.9(3)
O(63)-Nd(9)-O(53)	70.0(3)
O(56)-Nd(9)-O(53)	71.9(3)
O(11)-Nd(9)-O(53)	147.0(3)
O(70)-Nd(9)-O(10)	75.7(3)
O(68)-Nd(9)-O(10)	127.8(3)
O(66)-Nd(9)-O(10)	150.9(3)
O(63)-Nd(9)-O(10)	74.1(3)
O(56)-Nd(9)-O(10)	77.8(3)
O(11)-Nd(9)-O(10)	64.8(3)
O(53)-Nd(9)-O(10)	125.2(3)
O(64)-Nd(10)-O(68)	89.2(3)
O(64)-Nd(10)-O(79)	150.1(3)
O(68)-Nd(10)-O(79)	70.7(3)
O(64)-Nd(10)-O(73)	76.6(3)
O(68)-Nd(10)-O(73)	82.4(3)
O(79)-Nd(10)-O(73)	120.4(3)
O(64)-Nd(10)-O(67)	86.5(3)
O(68)-Nd(10)-O(67)	121.3(3)
O(79)-Nd(10)-O(67)	85.6(3)
O(73)-Nd(10)-O(67)	151.0(3)
O(64)-Nd(10)-O(66)	75.7(3)
O(68)-Nd(10)-O(66)	69.0(3)
O(79)-Nd(10)-O(66)	76.5(3)
O(73)-Nd(10)-O(66)	139.9(3)
O(67)-Nd(10)-O(66)	53.2(3)
O(64)-Nd(10)-O(77)	84.4(3)
O(68)-Nd(10)-O(77)	161.6(3)
O(79)-Nd(10)-O(77)	121.1(3)
O(73)-Nd(10)-O(77)	79.4(3)
O(67)-Nd(10)-O(77)	75.6(3)
O(66)-Nd(10)-O(77)	125.4(3)
O(64)-Nd(10)-O(78)	136.3(3)
O(68)-Nd(10)-O(78)	133.5(3)
O(79)-Nd(10)-O(78)	69.6(3)
O(73)-Nd(10)-O(78)	97.7(3)
O(67)-Nd(10)-O(78)	78.5(3)
O(66)-Nd(10)-O(78)	122.4(3)
O(77)-Nd(10)-O(78)	52.3(3)
O(64)-Nd(10)-O(74)	126.0(3)
O(68)-Nd(10)-O(74)	69.5(3)
O(79)-Nd(10)-O(74)	68.2(3)
O(73)-Nd(10)-O(74)	52.5(3)
O(67)-Nd(10)-O(74)	147.1(3)
O(66)-Nd(10)-O(74)	132.2(3)
O(77)-Nd(10)-O(74)	100.6(3)
O(78)-Nd(10)-O(74)	74.1(3)
O(87)-Nd(11)-O(97)	89.5(3)
O(87)-Nd(11)-O(105)	148.8(3)
O(97)-Nd(11)-O(105)	71.3(3)
O(87)-Nd(11)-O(94)	84.1(3)
O(97)-Nd(11)-O(94)	121.2(3)
O(105)-Nd(11)-O(94)	85.2(3)
O(87)-Nd(11)-O(100)	135.9(3)
O(97)-Nd(11)-O(100)	134.3(3)
O(105)-Nd(11)-O(100)	68.9(3)
O(94)-Nd(11)-O(100)	77.0(3)
O(87)-Nd(11)-O(95)	75.5(3)
O(97)-Nd(11)-O(95)	69.1(3)
O(105)-Nd(11)-O(95)	74.7(3)
O(94)-Nd(11)-O(95)	52.7(3)
O(100)-Nd(11)-O(95)	119.3(3)
O(87)-Nd(11)-O(96)	85.3(3)
O(97)-Nd(11)-O(96)	159.6(3)
O(105)-Nd(11)-O(96)	120.9(3)
O(94)-Nd(11)-O(96)	77.9(3)
O(100)-Nd(11)-O(96)	52.1(3)
O(95)-Nd(11)-O(96)	128.0(3)
O(87)-Nd(11)-O(99)	129.1(3)
O(97)-Nd(11)-O(99)	70.8(3)
O(105)-Nd(11)-O(99)	68.5(3)
O(94)-Nd(11)-O(99)	146.4(3)
O(100)-Nd(11)-O(99)	74.3(3)
O(95)-Nd(11)-O(99)	132.1(3)
O(96)-Nd(11)-O(99)	97.4(3)

O(87)-Nd(11)-O(98)	78.9(3)	O(28)-Nd(13)-O(23)	81.1(3)
O(97)-Nd(11)-O(98)	81.2(3)	O(24)-Nd(13)-O(23)	72.8(3)
O(105)-Nd(11)-O(98)	120.3(3)	O(2)-Nd(13)-O(23)	146.4(3)
O(94)-Nd(11)-O(98)	151.8(3)	O(39)-Nd(13)-O(1)	73.2(3)
O(100)-Nd(11)-O(98)	100.1(3)	O(37)-Nd(13)-O(1)	148.5(3)
O(95)-Nd(11)-O(98)	140.5(3)	O(22)-Nd(13)-O(1)	75.0(3)
O(96)-Nd(11)-O(98)	78.4(3)	O(28)-Nd(13)-O(1)	129.0(3)
O(99)-Nd(11)-O(98)	52.5(3)	O(24)-Nd(13)-O(1)	76.3(3)
O(114)-Nd(12)-O(112)	74.5(3)	O(2)-Nd(13)-O(1)	65.6(3)
O(114)-Nd(12)-O(107)	149.2(3)	O(23)-Nd(13)-O(1)	125.3(3)
O(112)-Nd(12)-O(107)	135.1(3)	O(21)-Nd(14)-O(20)	71.9(3)
O(114)-Nd(12)-O(100)	81.0(3)	O(21)-Nd(14)-O(106)	136.2(3)
O(112)-Nd(12)-O(100)	94.9(3)	O(20)-Nd(14)-O(106)	70.0(3)
O(107)-Nd(12)-O(100)	100.9(3)	O(21)-Nd(14)-O(110)	136.3(3)
O(114)-Nd(12)-O(106)	115.6(3)	O(20)-Nd(14)-O(110)	138.0(3)
O(112)-Nd(12)-O(106)	72.0(3)	O(106)-Nd(14)-O(110)	69.8(3)
O(107)-Nd(12)-O(106)	75.6(3)	O(21)-Nd(14)-O(23)#1	86.1(3)
O(100)-Nd(12)-O(106)	153.8(3)	O(20)-Nd(14)-O(23)#1	85.6(3)
O(114)-Nd(12)-O(20)	72.8(3)	O(106)-Nd(14)-O(23)#1	70.3(3)
O(112)-Nd(12)-O(20)	110.7(3)	O(110)-Nd(14)-O(23)#1	70.1(3)
O(107)-Nd(12)-O(20)	85.8(3)	O(21)-Nd(14)-O(116)	133.5(4)
O(100)-Nd(12)-O(20)	136.0(3)	O(20)-Nd(14)-O(116)	100.1(3)
O(106)-Nd(12)-O(20)	70.2(3)	O(106)-Nd(14)-O(116)	74.5(3)
O(114)-Nd(12)-O(105)	136.8(3)	O(110)-Nd(14)-O(116)	80.3(4)
O(112)-Nd(12)-O(105)	76.0(3)	O(21)-Nd(14)-O(115)	81.1(3)
O(107)-Nd(12)-O(105)	70.3(3)	O(20)-Nd(14)-O(115)	142.0(3)
O(100)-Nd(12)-O(105)	70.8(3)	O(106)-Nd(14)-O(115)	142.6(3)
O(106)-Nd(12)-O(105)	83.8(3)	O(110)-Nd(14)-O(115)	79.8(3)
O(20)-Nd(12)-O(105)	148.4(3)	O(116)-Nd(14)-O(115)	79.5(3)
O(114)-Nd(12)-O(19)	78.1(3)	O(21)-Nd(14)-O(117)	74.4(5)
O(112)-Nd(12)-O(19)	152.3(3)	O(20)-Nd(14)-O(117)	73.8(4)
O(107)-Nd(12)-O(19)	72.5(3)	O(106)-Nd(14)-O(117)	113.7(4)
O(100)-Nd(12)-O(19)	76.9(3)	O(110)-Nd(14)-O(117)	134.8(5)
O(106)-Nd(12)-O(19)	124.7(3)	O(116)-Nd(14)-O(117)	59.7(5)
O(20)-Nd(12)-O(19)	63.6(3)	O(115)-Nd(14)-O(117)	73.5(4)
O(105)-Nd(12)-O(19)	123.9(3)	O(21)-Nd(14)-O(22)#1	69.6(3)
O(39)-Nd(13)-O(37)	75.9(3)	O(20)-Nd(14)-O(22)#1	134.1(3)
O(39)-Nd(13)-O(22)	146.4(3)	O(106)-Nd(14)-O(22)#1	127.9(3)
O(37)-Nd(13)-O(22)	136.5(3)	O(110)-Nd(14)-O(22)#1	67.6(3)
O(39)-Nd(13)-O(28)	118.0(3)	O(6)-Nd(15)-O(49)	136.0(4)
O(37)-Nd(13)-O(28)	71.9(3)	O(6)-Nd(15)-O(45)	88.7(3)
O(22)-Nd(13)-O(28)	75.4(3)	O(49)-Nd(15)-O(45)	69.9(3)
O(39)-Nd(13)-O(24)	77.7(3)	O(6)-Nd(15)-O(5)	72.6(3)
O(37)-Nd(13)-O(24)	91.6(3)	O(49)-Nd(15)-O(5)	137.7(3)
O(22)-Nd(13)-O(24)	104.8(3)	O(45)-Nd(15)-O(5)	83.6(3)
O(28)-Nd(13)-O(24)	151.9(3)	O(6)-Nd(15)-O(43)	134.3(4)
O(39)-Nd(13)-O(2)	73.3(3)	O(49)-Nd(15)-O(43)	76.1(4)
O(37)-Nd(13)-O(2)	110.7(3)	O(45)-Nd(15)-O(43)	137.0(3)
O(22)-Nd(13)-O(2)	84.0(3)	O(5)-Nd(15)-O(43)	106.1(3)
O(28)-Nd(13)-O(2)	70.8(3)	O(6)-Nd(15)-O(40)	137.8(3)
O(24)-Nd(13)-O(2)	137.2(3)	O(49)-Nd(15)-O(40)	72.0(3)
O(39)-Nd(13)-O(23)	138.3(3)	O(45)-Nd(15)-O(40)	71.4(3)
O(37)-Nd(13)-O(23)	76.2(3)	O(5)-Nd(15)-O(40)	68.6(3)
O(22)-Nd(13)-O(23)	71.0(3)	O(43)-Nd(15)-O(40)	73.7(3)

O(6)-Nd(15)-O(44)	83.6(4)
O(49)-Nd(15)-O(44)	127.7(4)
O(45)-Nd(15)-O(44)	159.5(4)
O(5)-Nd(15)-O(44)	76.0(3)
O(43)-Nd(15)-O(44)	53.3(4)
O(40)-Nd(15)-O(44)	102.2(3)
O(6)-Nd(15)-O(46)	77.1(3)
O(49)-Nd(15)-O(46)	81.3(4)
O(45)-Nd(15)-O(46)	120.1(3)
O(5)-Nd(15)-O(46)	140.9(3)
O(43)-Nd(15)-O(46)	78.4(3)
O(40)-Nd(15)-O(46)	145.1(3)
O(44)-Nd(15)-O(46)	76.6(4)
O(6)-Nd(15)-O(47)	68.5(3)
O(49)-Nd(15)-O(47)	67.9(3)
O(45)-Nd(15)-O(47)	68.3(3)
O(5)-Nd(15)-O(47)	131.7(3)
O(43)-Nd(15)-O(47)	121.4(3)
O(40)-Nd(15)-O(47)	130.4(3)
O(44)-Nd(15)-O(47)	125.1(3)
O(46)-Nd(15)-O(47)	52.2(3)
O(65)-Nd(16)-O(58)	76.4(3)
O(65)-Nd(16)-O(51)	78.0(3)
O(58)-Nd(16)-O(51)	92.5(3)
O(65)-Nd(16)-O(47)	147.2(3)
O(58)-Nd(16)-O(47)	135.8(3)
O(51)-Nd(16)-O(47)	102.1(3)
O(65)-Nd(16)-O(52)	119.3(3)
O(58)-Nd(16)-O(52)	71.8(3)
O(51)-Nd(16)-O(52)	151.3(3)
O(47)-Nd(16)-O(52)	75.9(3)
O(65)-Nd(16)-O(8)	74.1(3)
O(58)-Nd(16)-O(8)	109.8(3)
O(51)-Nd(16)-O(8)	138.4(3)
O(47)-Nd(16)-O(8)	86.0(3)
O(52)-Nd(16)-O(8)	70.3(3)
O(65)-Nd(16)-O(45)	136.7(3)
O(58)-Nd(16)-O(45)	75.9(3)
O(51)-Nd(16)-O(45)	70.7(3)
O(47)-Nd(16)-O(45)	70.4(3)
O(52)-Nd(16)-O(45)	81.9(3)
O(8)-Nd(16)-O(45)	147.4(3)
O(65)-Nd(16)-O(7)	74.5(4)
O(58)-Nd(16)-O(7)	150.7(3)
O(51)-Nd(16)-O(7)	78.2(3)
O(47)-Nd(16)-O(7)	73.5(4)
O(52)-Nd(16)-O(7)	126.7(3)
O(8)-Nd(16)-O(7)	65.0(3)
O(45)-Nd(16)-O(7)	125.1(3)
O(91)-Nd(17)-O(15)	90.8(3)
O(91)-Nd(17)-O(90)	70.6(3)
O(15)-Nd(17)-O(90)	137.7(3)
O(91)-Nd(17)-O(83)	136.2(3)
O(15)-Nd(17)-O(83)	133.0(3)
O(90)-Nd(17)-O(83)	75.0(3)
O(91)-Nd(17)-O(81)	68.8(3)
O(15)-Nd(17)-O(81)	136.6(3)
O(90)-Nd(17)-O(81)	72.5(3)
O(83)-Nd(17)-O(81)	75.6(3)
O(91)-Nd(17)-O(82)	157.8(3)
O(15)-Nd(17)-O(82)	81.8(3)
O(90)-Nd(17)-O(82)	101.1(3)
O(83)-Nd(17)-O(82)	55.1(3)
O(81)-Nd(17)-O(82)	129.6(3)
O(91)-Nd(17)-O(14)	83.0(3)
O(15)-Nd(17)-O(14)	71.6(3)
O(90)-Nd(17)-O(14)	68.6(3)
O(83)-Nd(17)-O(14)	108.9(3)
O(81)-Nd(17)-O(14)	137.7(3)
O(82)-Nd(17)-O(14)	74.9(3)
O(91)-Nd(17)-O(93)	120.6(3)
O(15)-Nd(17)-O(93)	78.5(3)
O(90)-Nd(17)-O(93)	143.8(3)
O(83)-Nd(17)-O(93)	75.6(3)
O(81)-Nd(17)-O(93)	80.1(3)
O(82)-Nd(17)-O(93)	78.5(3)
O(14)-Nd(17)-O(93)	142.2(3)
O(91)-Nd(17)-O(92)	69.5(3)
O(15)-Nd(17)-O(92)	69.1(3)
O(90)-Nd(17)-O(92)	131.3(3)
O(83)-Nd(17)-O(92)	119.3(3)
O(81)-Nd(17)-O(92)	68.0(3)
O(82)-Nd(17)-O(92)	125.8(3)
O(14)-Nd(17)-O(92)	130.8(3)
O(93)-Nd(17)-O(92)	52.0(3)
O(18)-Nd(18)-O(105)	87.8(3)
O(18)-Nd(18)-O(101)	132.5(4)
O(105)-Nd(18)-O(101)	139.5(3)
O(18)-Nd(18)-O(99)	137.4(3)
O(105)-Nd(18)-O(99)	70.8(3)
O(101)-Nd(18)-O(99)	78.3(3)
O(18)-Nd(18)-O(17)	71.7(3)
O(105)-Nd(18)-O(17)	84.8(3)
O(101)-Nd(18)-O(17)	102.5(3)
O(99)-Nd(18)-O(17)	138.4(3)
O(18)-Nd(18)-O(97)	136.4(3)
O(105)-Nd(18)-O(97)	70.8(3)
O(101)-Nd(18)-O(97)	74.9(3)
O(99)-Nd(18)-O(97)	71.4(3)
O(17)-Nd(18)-O(97)	68.9(3)
O(18)-Nd(18)-O(108)	79.9(3)
O(105)-Nd(18)-O(108)	118.4(3)
O(101)-Nd(18)-O(108)	79.2(3)
O(99)-Nd(18)-O(108)	78.9(3)
O(17)-Nd(18)-O(108)	142.6(3)
O(97)-Nd(18)-O(108)	143.7(3)
O(18)-Nd(18)-O(102)	79.6(4)
O(105)-Nd(18)-O(102)	160.0(3)

O(101)-Nd(18)-O(102)	53.9(4)	O(40)-Nd(20)-O(42)	121.2(3)
O(99)-Nd(18)-O(102)	128.6(4)	O(45)-Nd(20)-O(42)	86.2(3)
O(17)-Nd(18)-O(102)	76.5(3)	O(38)-Nd(20)-O(48)	77.4(3)
O(97)-Nd(18)-O(102)	108.1(3)	O(40)-Nd(20)-O(48)	81.9(3)
O(108)-Nd(18)-O(102)	74.9(3)	O(45)-Nd(20)-O(48)	119.6(3)
O(18)-Nd(18)-O(107)	69.9(3)	O(42)-Nd(20)-O(48)	151.1(4)
O(105)-Nd(18)-O(107)	67.2(3)	O(38)-Nd(20)-O(51)	139.0(3)
O(101)-Nd(18)-O(107)	123.8(3)	O(40)-Nd(20)-O(51)	134.1(3)
O(99)-Nd(18)-O(107)	67.9(3)	O(45)-Nd(20)-O(51)	69.1(3)
O(17)-Nd(18)-O(107)	132.6(3)	O(42)-Nd(20)-O(51)	79.8(3)
O(97)-Nd(18)-O(107)	128.7(3)	O(48)-Nd(20)-O(51)	96.6(3)
O(108)-Nd(18)-O(107)	51.8(3)	O(38)-Nd(20)-O(41)	74.5(3)
O(102)-Nd(18)-O(107)	121.4(3)	O(40)-Nd(20)-O(41)	69.1(3)
O(53)-Nd(19)-O(9)	86.9(3)	O(45)-Nd(20)-O(41)	76.9(3)
O(53)-Nd(19)-O(60)	70.8(3)	O(42)-Nd(20)-O(41)	52.7(3)
O(9)-Nd(19)-O(60)	137.7(3)	O(48)-Nd(20)-O(41)	140.6(3)
O(53)-Nd(19)-O(8)	84.9(3)	O(51)-Nd(20)-O(41)	122.7(3)
O(9)-Nd(19)-O(8)	70.6(3)	O(38)-Nd(20)-O(50)	86.6(3)
O(60)-Nd(19)-O(8)	138.6(3)	O(40)-Nd(20)-O(50)	160.0(3)
O(53)-Nd(19)-O(55)	138.5(3)	O(45)-Nd(20)-O(50)	121.2(3)
O(9)-Nd(19)-O(55)	134.4(3)	O(42)-Nd(20)-O(50)	76.7(4)
O(60)-Nd(19)-O(55)	76.8(4)	O(48)-Nd(20)-O(50)	78.4(4)
O(8)-Nd(19)-O(55)	103.8(3)	O(51)-Nd(20)-O(50)	52.7(3)
O(53)-Nd(19)-O(52)	71.4(3)	O(41)-Nd(20)-O(50)	126.1(3)
O(9)-Nd(19)-O(52)	135.5(3)	O(38)-Nd(20)-O(49)	126.0(3)
O(60)-Nd(19)-O(52)	71.4(3)	O(40)-Nd(20)-O(49)	70.3(3)
O(8)-Nd(19)-O(52)	69.1(3)	O(45)-Nd(20)-O(49)	67.5(3)
O(55)-Nd(19)-O(52)	74.1(3)	O(42)-Nd(20)-O(49)	147.2(3)
O(53)-Nd(19)-O(62)	119.7(3)	O(48)-Nd(20)-O(49)	52.4(3)
O(9)-Nd(19)-O(62)	80.0(3)	O(51)-Nd(20)-O(49)	72.9(3)
O(60)-Nd(19)-O(62)	80.7(3)	O(41)-Nd(20)-O(49)	132.3(3)
O(8)-Nd(19)-O(62)	140.7(3)	O(50)-Nd(20)-O(49)	99.8(4)
O(55)-Nd(19)-O(62)	78.5(3)	O(104)-Nd(21)-O(106)	89.1(3)
O(52)-Nd(19)-O(62)	144.5(3)	O(104)-Nd(21)-O(112)	74.3(3)
O(53)-Nd(19)-O(54)	159.5(4)	O(106)-Nd(21)-O(112)	70.1(3)
O(9)-Nd(19)-O(54)	81.3(4)	O(104)-Nd(21)-O(113)	85.9(3)
O(60)-Nd(19)-O(54)	128.5(4)	O(106)-Nd(21)-O(113)	121.7(3)
O(8)-Nd(19)-O(54)	75.3(4)	O(112)-Nd(21)-O(113)	52.6(3)
O(55)-Nd(19)-O(54)	54.4(4)	O(104)-Nd(21)-O(111)	82.3(3)
O(52)-Nd(19)-O(54)	105.8(4)	O(106)-Nd(21)-O(111)	159.6(3)
O(62)-Nd(19)-O(54)	74.9(4)	O(112)-Nd(21)-O(111)	124.3(4)
O(53)-Nd(19)-O(63)	67.8(3)	O(113)-Nd(21)-O(111)	76.3(4)
O(9)-Nd(19)-O(63)	70.5(3)	O(104)-Nd(21)-O(109)	78.1(3)
O(60)-Nd(19)-O(63)	67.9(3)	O(106)-Nd(21)-O(109)	80.3(3)
O(8)-Nd(19)-O(63)	133.0(3)	O(112)-Nd(21)-O(109)	139.4(3)
O(55)-Nd(19)-O(63)	122.1(3)	O(113)-Nd(21)-O(109)	152.8(4)
O(52)-Nd(19)-O(63)	129.5(3)	O(111)-Nd(21)-O(109)	79.9(4)
O(62)-Nd(19)-O(63)	52.2(3)	O(104)-Nd(21)-O(110)	127.7(3)
O(54)-Nd(19)-O(63)	122.7(3)	O(106)-Nd(21)-O(110)	68.6(3)
O(38)-Nd(20)-O(40)	85.8(3)	O(112)-Nd(21)-O(110)	131.9(3)
O(38)-Nd(20)-O(45)	148.6(3)	O(113)-Nd(21)-O(110)	146.3(3)
O(40)-Nd(20)-O(45)	72.1(3)	O(111)-Nd(21)-O(110)	102.4(4)
O(38)-Nd(20)-O(42)	86.7(3)	O(109)-Nd(21)-O(110)	52.5(3)

Table S3. Selected Bond Lengths (Å) for **2**.

La(1)-O(12)	2.394(9)	La(7)-O(103)	2.313(7)
La(1)-O(11)	2.434(8)	La(7)-O(92)	2.367(8)
La(1)-O(76)	2.437(8)	La(7)-O(95)	2.369(7)
La(1)-O(68)	2.447(7)	La(7)-O(97)	2.383(8)
La(1)-O(74)	2.447(8)	La(7)-O(89)	2.414(9)
La(1)-O(79)	2.449(7)	La(7)-O(91)	2.444(7)
La(1)-O(71)	2.450(8)	La(7)-O(17)	2.453(7)
La(1)-O(72)	2.492(8)	La(7)-O(16)	2.561(8)
La(1)-O(75)	2.544(8)	La(8)-O(119)	2.364(7)
La(2)-O(86)	2.354(8)	La(8)-O(52)	2.404(7)
La(2)-O(90)	2.371(7)	La(8)-O(53)	2.429(7)
La(2)-O(75)	2.372(7)	La(8)-O(59)	2.475(8)
La(2)-O(78)	2.390(8)	La(8)-O(61)	2.482(9)
La(2)-O(84)	2.393(7)	La(8)-O(56)	2.488(8)
La(2)-O(14)	2.448(8)	La(8)-O(58)	2.499(8)
La(2)-O(79)	2.464(8)	La(8)-O(57)	2.513(8)
La(2)-O(13)	2.520(8)	La(8)-O(60)	2.566(9)
La(3)-O(69)	2.386(8)	La(9)-O(70)	2.359(8)
La(3)-O(90)	2.387(7)	La(9)-O(66)	2.363(7)
La(3)-O(91)	2.470(7)	La(9)-O(68)	2.367(7)
La(3)-O(85)	2.473(8)	La(9)-O(63)	2.385(8)
La(3)-O(84)	2.492(7)	La(9)-O(56)	2.386(8)
La(3)-O(81)	2.498(8)	La(9)-O(11)	2.419(8)
La(3)-O(89)	2.498(8)	La(9)-O(53)	2.447(8)
La(3)-O(88)	2.503(9)	La(9)-O(10)	2.532(8)
La(3)-O(80)	2.524(8)	La(10)-O(64)	2.372(8)
La(4)-O(3)	2.417(8)	La(10)-O(68)	2.389(7)
La(4)-O(32)	2.422(7)	La(10)-O(79)	2.418(7)
La(4)-O(31)	2.424(7)	La(10)-O(73)	2.473(9)
La(4)-O(28)	2.430(7)	La(10)-O(66)	2.486(7)
La(4)-O(27)	2.456(9)	La(10)-O(78)	2.502(8)
La(4)-O(26)	2.464(9)	La(10)-O(77)	2.508(9)
La(4)-O(2)	2.488(8)	La(10)-O(67)	2.515(9)
La(4)-O(29)	2.508(8)	La(10)-O(74)	2.535(8)
La(4)-O(30)	2.546(7)	La(11)-O(87)	2.342(8)
La(5)-O(28)	2.378(7)	La(11)-O(97)	2.387(7)
La(5)-O(25)	2.392(7)	La(11)-O(105)	2.453(7)
La(5)-O(31)	2.477(7)	La(11)-O(100)	2.480(7)
La(5)-O(36)	2.486(8)	La(11)-O(94)	2.485(8)
La(5)-O(33)	2.489(8)	La(11)-O(95)	2.504(7)
La(5)-O(37)	2.492(7)	La(11)-O(96)	2.505(8)
La(5)-O(34)	2.496(7)	La(11)-O(98)	2.544(9)
La(5)-O(35)	2.522(8)	La(11)-O(99)	2.546(8)
La(5)-O(32)	2.533(8)	La(12)-O(114)	2.346(7)
La(6)-O(118)	2.343(7)	La(12)-O(106)	2.364(7)
La(6)-O(41)	2.365(8)	La(12)-O(112)	2.364(8)
La(6)-O(40)	2.368(7)	La(12)-O(107)	2.400(8)
La(6)-O(30)	2.395(8)	La(12)-O(100)	2.404(7)
La(6)-O(34)	2.427(7)	La(12)-O(105)	2.435(7)
La(6)-O(5)	2.450(7)	La(12)-O(20)	2.447(7)
La(6)-O(31)	2.457(7)	La(12)-O(19)	2.525(8)
La(6)-O(4)	2.521(8)	La(13)-O(39)	2.355(8)

La(13)-O(37)	2.359(7)	La(19)-O(8)	2.440(9)
La(13)-O(22)	2.363(9)	La(19)-O(52)	2.451(8)
La(13)-O(24)	2.378(8)	La(19)-O(54)	2.491(11)
La(13)-O(28)	2.386(7)	La(19)-O(62)	2.499(9)
La(13)-O(2)	2.424(7)	La(19)-O(63)	2.557(8)
La(13)-O(23)	2.440(7)	La(20)-O(38)	2.359(8)
La(13)-O(1)	2.522(8)	La(20)-O(40)	2.386(8)
La(14)-O(20)	2.410(8)	La(20)-O(45)	2.437(8)
La(14)-O(21)	2.420(8)	La(20)-O(42)	2.459(9)
La(14)-O(110)	2.442(9)	La(20)-O(41)	2.493(8)
La(14)-O(106)	2.448(7)	La(20)-O(51)	2.503(8)
La(14)-O(23)#1	2.464(8)	La(20)-O(50)	2.508(9)
La(14)-O(116)	2.468(10)	La(20)-O(48)	2.519(9)
La(14)-O(115)	2.494(8)	La(20)-O(49)	2.560(9)
La(14)-O(117)	2.525(13)	La(21)-O(104)	2.346(8)
La(14)-O(22)#1	2.568(8)	La(21)-O(106)	2.392(8)
La(15)-O(6)	2.413(9)	La(21)-O(23)#1	2.440(8)
La(15)-O(49)	2.419(9)	La(21)-O(113)	2.476(9)
La(15)-O(43)	2.422(9)	La(21)-O(24)#1	2.492(8)
La(15)-O(45)	2.446(7)	La(21)-O(112)	2.508(7)
La(15)-O(5)	2.448(8)	La(21)-O(111)	2.511(10)
La(15)-O(40)	2.449(7)	La(21)-O(109)	2.512(9)
La(15)-O(44)	2.458(10)	La(21)-O(110)	2.575(9)
La(15)-O(46)	2.512(8)	O(12)-La(1)-O(11)	70.8(3)
La(15)-O(47)	2.558(8)	O(12)-La(1)-O(76)	82.2(3)
La(16)-O(65)	2.331(9)	O(11)-La(1)-O(76)	141.9(3)
La(16)-O(58)	2.364(8)	O(12)-La(1)-O(68)	135.7(3)
La(16)-O(47)	2.374(9)	O(11)-La(1)-O(68)	69.7(3)
La(16)-O(51)	2.386(9)	O(76)-La(1)-O(68)	142.1(3)
La(16)-O(52)	2.405(8)	O(12)-La(1)-O(74)	138.0(3)
La(16)-O(8)	2.441(8)	O(11)-La(1)-O(74)	137.8(3)
La(16)-O(45)	2.464(7)	O(76)-La(1)-O(74)	80.0(3)
La(16)-O(7)	2.522(9)	O(68)-La(1)-O(74)	69.9(3)
La(17)-O(91)	2.417(7)	O(12)-La(1)-O(79)	87.5(3)
La(17)-O(15)	2.417(9)	O(11)-La(1)-O(79)	85.4(2)
La(17)-O(81)	2.423(9)	O(76)-La(1)-O(79)	120.6(3)
La(17)-O(83)	2.432(8)	O(68)-La(1)-O(79)	70.1(2)
La(17)-O(90)	2.435(7)	O(74)-La(1)-O(79)	69.9(2)
La(17)-O(14)	2.447(8)	O(12)-La(1)-O(71)	129.1(3)
La(17)-O(82)	2.455(8)	O(11)-La(1)-O(71)	100.4(3)
La(17)-O(93)	2.501(8)	O(76)-La(1)-O(71)	76.0(3)
La(17)-O(92)	2.545(8)	O(68)-La(1)-O(71)	77.7(3)
La(18)-O(18)	2.412(8)	O(74)-La(1)-O(71)	82.4(3)
La(18)-O(17)	2.413(8)	O(79)-La(1)-O(71)	143.0(3)
La(18)-O(99)	2.414(8)	O(12)-La(1)-O(72)	77.2(3)
La(18)-O(105)	2.427(7)	O(11)-La(1)-O(72)	74.7(3)
La(18)-O(97)	2.427(7)	O(76)-La(1)-O(72)	73.4(3)
La(18)-O(101)	2.428(9)	O(68)-La(1)-O(72)	110.4(3)
La(18)-O(108)	2.497(9)	O(74)-La(1)-O(72)	131.8(3)
La(18)-O(102)	2.511(9)	O(79)-La(1)-O(72)	157.9(3)
La(18)-O(107)	2.593(7)	O(71)-La(1)-O(72)	52.8(3)
La(19)-O(60)	2.392(9)	O(12)-La(1)-O(75)	70.6(3)
La(19)-O(9)	2.406(10)	O(11)-La(1)-O(75)	133.9(2)
La(19)-O(53)	2.427(8)	O(76)-La(1)-O(75)	52.5(2)
La(19)-O(55)	2.437(10)	O(68)-La(1)-O(75)	128.8(2)

O(74)-La(1)-O(75)	68.3(3)	O(91)-La(3)-O(88)	120.5(3)
O(79)-La(1)-O(75)	68.8(2)	O(85)-La(3)-O(88)	77.5(3)
O(71)-La(1)-O(75)	123.4(3)	O(84)-La(3)-O(88)	126.5(3)
O(72)-La(1)-O(75)	119.2(3)	O(81)-La(3)-O(88)	97.3(3)
O(86)-La(2)-O(90)	118.6(3)	O(89)-La(3)-O(88)	51.9(3)
O(86)-La(2)-O(75)	144.3(3)	O(69)-La(3)-O(80)	76.6(3)
O(90)-La(2)-O(75)	76.8(3)	O(90)-La(3)-O(80)	79.3(3)
O(86)-La(2)-O(78)	79.2(3)	O(91)-La(3)-O(80)	118.5(3)
O(90)-La(2)-O(78)	149.3(3)	O(85)-La(3)-O(80)	153.4(3)
O(75)-La(2)-O(78)	103.7(3)	O(84)-La(3)-O(80)	138.5(3)
O(86)-La(2)-O(84)	76.1(3)	O(81)-La(3)-O(80)	53.2(3)
O(90)-La(2)-O(84)	71.9(2)	O(89)-La(3)-O(80)	100.5(3)
O(75)-La(2)-O(84)	138.6(3)	O(88)-La(3)-O(80)	80.8(3)
O(78)-La(2)-O(84)	90.6(3)	O(3)-La(4)-O(32)	137.8(3)
O(86)-La(2)-O(14)	73.3(3)	O(3)-La(4)-O(31)	88.4(3)
O(90)-La(2)-O(14)	70.5(3)	O(32)-La(4)-O(31)	70.9(2)
O(75)-La(2)-O(14)	83.8(3)	O(3)-La(4)-O(28)	136.4(3)
O(78)-La(2)-O(14)	140.1(3)	O(32)-La(4)-O(28)	71.5(2)
O(84)-La(2)-O(14)	109.7(3)	O(31)-La(4)-O(28)	70.8(2)
O(86)-La(2)-O(79)	139.3(3)	O(3)-La(4)-O(27)	82.9(3)
O(90)-La(2)-O(79)	80.8(2)	O(32)-La(4)-O(27)	128.3(3)
O(75)-La(2)-O(79)	71.3(2)	O(31)-La(4)-O(27)	157.3(3)
O(78)-La(2)-O(79)	70.7(2)	O(28)-La(4)-O(27)	101.6(3)
O(84)-La(2)-O(79)	77.4(2)	O(3)-La(4)-O(26)	133.3(3)
O(14)-La(2)-O(79)	145.7(2)	O(32)-La(4)-O(26)	75.4(3)
O(86)-La(2)-O(13)	72.7(3)	O(31)-La(4)-O(26)	138.2(3)
O(90)-La(2)-O(13)	128.2(3)	O(28)-La(4)-O(26)	75.7(3)
O(75)-La(2)-O(13)	73.0(3)	O(27)-La(4)-O(26)	53.8(3)
O(78)-La(2)-O(13)	79.4(3)	O(3)-La(4)-O(2)	70.0(3)
O(84)-La(2)-O(13)	148.5(2)	O(32)-La(4)-O(2)	137.9(2)
O(14)-La(2)-O(13)	65.3(3)	O(31)-La(4)-O(2)	82.0(2)
O(79)-La(2)-O(13)	125.4(2)	O(28)-La(4)-O(2)	69.5(2)
O(69)-La(3)-O(90)	87.4(3)	O(27)-La(4)-O(2)	75.2(3)
O(69)-La(3)-O(91)	149.6(3)	O(26)-La(4)-O(2)	108.9(3)
O(90)-La(3)-O(91)	71.3(2)	O(3)-La(4)-O(29)	77.6(3)
O(69)-La(3)-O(85)	86.9(3)	O(32)-La(4)-O(29)	82.4(3)
O(90)-La(3)-O(85)	121.2(3)	O(31)-La(4)-O(29)	121.0(2)
O(91)-La(3)-O(85)	86.1(3)	O(28)-La(4)-O(29)	145.9(3)
O(69)-La(3)-O(84)	75.1(3)	O(27)-La(4)-O(29)	77.6(3)
O(90)-La(3)-O(84)	69.9(2)	O(26)-La(4)-O(29)	76.8(3)
O(91)-La(3)-O(84)	77.3(2)	O(2)-La(4)-O(29)	139.7(2)
O(85)-La(3)-O(84)	52.1(3)	O(3)-La(4)-O(30)	69.7(3)
O(69)-La(3)-O(81)	127.8(3)	O(32)-La(4)-O(30)	68.7(2)
O(90)-La(3)-O(81)	71.7(2)	O(31)-La(4)-O(30)	69.5(2)
O(91)-La(3)-O(81)	66.5(3)	O(28)-La(4)-O(30)	130.7(2)
O(85)-La(3)-O(81)	144.9(3)	O(27)-La(4)-O(30)	125.7(3)
O(84)-La(3)-O(81)	133.7(3)	O(26)-La(4)-O(30)	119.3(3)
O(69)-La(3)-O(89)	137.7(3)	O(2)-La(4)-O(30)	130.6(3)
O(90)-La(3)-O(89)	134.1(3)	O(29)-La(4)-O(30)	51.8(2)
O(91)-La(3)-O(89)	68.9(3)	O(28)-La(5)-O(25)	86.6(2)
O(85)-La(3)-O(89)	77.9(3)	O(28)-La(5)-O(31)	70.8(2)
O(84)-La(3)-O(89)	120.8(3)	O(25)-La(5)-O(31)	147.4(2)
O(81)-La(3)-O(89)	72.2(3)	O(28)-La(5)-O(36)	122.2(3)
O(69)-La(3)-O(88)	86.5(3)	O(25)-La(5)-O(36)	87.0(3)
O(90)-La(3)-O(88)	160.0(3)	O(31)-La(5)-O(36)	85.9(2)

O(28)-La(5)-O(33)	81.4(3)	O(34)-La(6)-O(4)	79.0(3)
O(25)-La(5)-O(33)	77.2(3)	O(5)-La(6)-O(4)	64.9(3)
O(31)-La(5)-O(33)	120.2(2)	O(31)-La(6)-O(4)	125.0(3)
O(36)-La(5)-O(33)	150.9(3)	O(103)-La(7)-O(92)	146.2(3)
O(28)-La(5)-O(37)	70.0(2)	O(103)-La(7)-O(95)	78.7(3)
O(25)-La(5)-O(37)	74.1(2)	O(92)-La(7)-O(95)	134.2(3)
O(31)-La(5)-O(37)	76.2(2)	O(103)-La(7)-O(97)	119.8(3)
O(36)-La(5)-O(37)	53.1(2)	O(92)-La(7)-O(97)	74.6(3)
O(33)-La(5)-O(37)	140.3(3)	O(95)-La(7)-O(97)	71.4(3)
O(28)-La(5)-O(34)	133.9(2)	O(103)-La(7)-O(89)	76.1(3)
O(25)-La(5)-O(34)	138.9(2)	O(92)-La(7)-O(89)	105.1(3)
O(31)-La(5)-O(34)	69.6(2)	O(95)-La(7)-O(89)	92.0(3)
O(36)-La(5)-O(34)	77.2(3)	O(97)-La(7)-O(89)	152.5(3)
O(33)-La(5)-O(34)	98.8(3)	O(103)-La(7)-O(91)	136.2(3)
O(37)-La(5)-O(34)	120.8(2)	O(92)-La(7)-O(91)	71.8(3)
O(28)-La(5)-O(35)	160.5(3)	O(95)-La(7)-O(91)	74.8(2)
O(25)-La(5)-O(35)	87.3(2)	O(97)-La(7)-O(91)	83.6(2)
O(31)-La(5)-O(35)	121.4(2)	O(89)-La(7)-O(91)	70.6(3)
O(36)-La(5)-O(35)	75.8(3)	O(103)-La(7)-O(17)	73.8(3)
O(33)-La(5)-O(35)	79.2(3)	O(92)-La(7)-O(17)	85.5(3)
O(37)-La(5)-O(35)	125.7(3)	O(95)-La(7)-O(17)	109.1(2)
O(34)-La(5)-O(35)	52.2(2)	O(97)-La(7)-O(17)	68.8(3)
O(28)-La(5)-O(32)	70.4(2)	O(89)-La(7)-O(17)	138.6(3)
O(25)-La(5)-O(32)	126.6(3)	O(91)-La(7)-O(17)	148.2(3)
O(31)-La(5)-O(32)	68.2(2)	O(103)-La(7)-O(16)	74.2(3)
O(36)-La(5)-O(32)	146.1(3)	O(92)-La(7)-O(16)	72.7(3)
O(33)-La(5)-O(32)	52.7(2)	O(95)-La(7)-O(16)	152.9(2)
O(37)-La(5)-O(32)	133.3(2)	O(97)-La(7)-O(16)	123.8(3)
O(34)-La(5)-O(32)	73.6(2)	O(89)-La(7)-O(16)	80.6(3)
O(35)-La(5)-O(32)	98.9(3)	O(91)-La(7)-O(16)	125.6(2)
O(118)-La(6)-O(41)	76.1(3)	O(17)-La(7)-O(16)	64.2(2)
O(118)-La(6)-O(40)	118.2(3)	O(119)-La(8)-O(52)	87.3(3)
O(41)-La(6)-O(40)	71.5(3)	O(119)-La(8)-O(53)	149.5(3)
O(118)-La(6)-O(30)	144.6(3)	O(52)-La(8)-O(53)	72.2(3)
O(41)-La(6)-O(30)	138.4(3)	O(119)-La(8)-O(59)	86.4(3)
O(40)-La(6)-O(30)	77.5(3)	O(52)-La(8)-O(59)	121.8(3)
O(118)-La(6)-O(34)	77.8(3)	O(53)-La(8)-O(59)	85.7(3)
O(41)-La(6)-O(34)	91.2(3)	O(119)-La(8)-O(61)	78.2(3)
O(40)-La(6)-O(34)	150.9(3)	O(52)-La(8)-O(61)	82.3(3)
O(30)-La(6)-O(34)	103.7(3)	O(53)-La(8)-O(61)	119.5(3)
O(118)-La(6)-O(5)	73.3(3)	O(59)-La(8)-O(61)	150.9(3)
O(41)-La(6)-O(5)	109.4(3)	O(119)-La(8)-O(56)	136.4(3)
O(40)-La(6)-O(5)	70.3(3)	O(52)-La(8)-O(56)	134.8(3)
O(30)-La(6)-O(5)	84.5(3)	O(53)-La(8)-O(56)	70.5(3)
O(34)-La(6)-O(5)	138.7(3)	O(59)-La(8)-O(56)	79.8(3)
O(118)-La(6)-O(31)	138.2(2)	O(61)-La(8)-O(56)	94.5(3)
O(41)-La(6)-O(31)	77.4(2)	O(119)-La(8)-O(58)	75.4(3)
O(40)-La(6)-O(31)	82.2(2)	O(52)-La(8)-O(58)	69.4(3)
O(30)-La(6)-O(31)	71.5(2)	O(53)-La(8)-O(58)	76.3(3)
O(34)-La(6)-O(31)	71.1(2)	O(59)-La(8)-O(58)	53.0(2)
O(5)-La(6)-O(31)	146.8(2)	O(61)-La(8)-O(58)	141.8(3)
O(118)-La(6)-O(4)	73.4(3)	O(56)-La(8)-O(58)	123.6(3)
O(41)-La(6)-O(4)	149.2(3)	O(119)-La(8)-O(57)	83.9(3)
O(40)-La(6)-O(4)	127.4(3)	O(52)-La(8)-O(57)	160.3(3)
O(30)-La(6)-O(4)	72.3(3)	O(53)-La(8)-O(57)	122.1(3)

O(59)-La(8)-O(57)	75.3(3)	O(64)-La(10)-O(77)	84.2(3)
O(61)-La(8)-O(57)	78.7(3)	O(68)-La(10)-O(77)	160.9(3)
O(56)-La(8)-O(57)	52.7(3)	O(79)-La(10)-O(77)	121.2(3)
O(58)-La(8)-O(57)	124.6(3)	O(73)-La(10)-O(77)	78.9(3)
O(119)-La(8)-O(60)	126.7(3)	O(66)-La(10)-O(77)	125.8(3)
O(52)-La(8)-O(60)	69.1(3)	O(78)-La(10)-O(77)	52.4(3)
O(53)-La(8)-O(60)	67.2(3)	O(64)-La(10)-O(67)	86.1(3)
O(59)-La(8)-O(60)	146.8(3)	O(68)-La(10)-O(67)	121.2(3)
O(61)-La(8)-O(60)	52.5(3)	O(79)-La(10)-O(67)	84.7(3)
O(56)-La(8)-O(60)	73.4(3)	O(73)-La(10)-O(67)	151.2(3)
O(58)-La(8)-O(60)	131.1(3)	O(66)-La(10)-O(67)	53.4(3)
O(57)-La(8)-O(60)	102.5(3)	O(78)-La(10)-O(67)	78.3(3)
O(70)-La(9)-O(66)	76.6(3)	O(77)-La(10)-O(67)	76.1(3)
O(70)-La(9)-O(68)	118.3(3)	O(64)-La(10)-O(74)	126.3(3)
O(66)-La(9)-O(68)	71.2(2)	O(68)-La(10)-O(74)	69.3(2)
O(70)-La(9)-O(63)	147.7(3)	O(79)-La(10)-O(74)	69.0(2)
O(66)-La(9)-O(63)	135.0(3)	O(73)-La(10)-O(74)	52.1(3)
O(68)-La(9)-O(63)	75.9(3)	O(66)-La(10)-O(74)	131.9(2)
O(70)-La(9)-O(56)	77.9(3)	O(78)-La(10)-O(74)	74.7(3)
O(66)-La(9)-O(56)	92.1(3)	O(77)-La(10)-O(74)	100.8(3)
O(68)-La(9)-O(56)	151.5(3)	O(67)-La(10)-O(74)	147.3(3)
O(63)-La(9)-O(56)	103.2(3)	O(87)-La(11)-O(97)	90.1(3)
O(70)-La(9)-O(11)	73.7(3)	O(87)-La(11)-O(105)	148.2(3)
O(66)-La(9)-O(11)	111.2(3)	O(97)-La(11)-O(105)	71.1(2)
O(68)-La(9)-O(11)	71.3(3)	O(87)-La(11)-O(100)	135.6(3)
O(63)-La(9)-O(11)	85.4(3)	O(97)-La(11)-O(100)	134.1(3)
O(56)-La(9)-O(11)	137.2(3)	O(105)-La(11)-O(100)	68.9(2)
O(70)-La(9)-O(53)	137.2(3)	O(87)-La(11)-O(94)	83.4(3)
O(66)-La(9)-O(53)	75.0(3)	O(97)-La(11)-O(94)	121.4(3)
O(68)-La(9)-O(53)	81.3(2)	O(105)-La(11)-O(94)	84.9(3)
O(63)-La(9)-O(53)	70.3(3)	O(100)-La(11)-O(94)	76.5(3)
O(56)-La(9)-O(53)	72.0(3)	O(87)-La(11)-O(95)	74.8(3)
O(11)-La(9)-O(53)	147.1(3)	O(97)-La(11)-O(95)	69.0(2)
O(70)-La(9)-O(10)	74.8(3)	O(105)-La(11)-O(95)	74.6(2)
O(66)-La(9)-O(10)	151.0(3)	O(100)-La(11)-O(95)	119.2(2)
O(68)-La(9)-O(10)	127.6(3)	O(94)-La(11)-O(95)	53.0(2)
O(63)-La(9)-O(10)	74.0(3)	O(87)-La(11)-O(96)	85.3(3)
O(56)-La(9)-O(10)	77.5(3)	O(97)-La(11)-O(96)	159.5(3)
O(11)-La(9)-O(10)	64.6(3)	O(105)-La(11)-O(96)	120.8(2)
O(53)-La(9)-O(10)	125.3(3)	O(100)-La(11)-O(96)	52.1(2)
O(64)-La(10)-O(68)	88.8(3)	O(94)-La(11)-O(96)	78.0(3)
O(64)-La(10)-O(79)	149.7(3)	O(95)-La(11)-O(96)	128.3(3)
O(68)-La(10)-O(79)	71.6(2)	O(87)-La(11)-O(98)	80.2(3)
O(64)-La(10)-O(73)	77.4(3)	O(97)-La(11)-O(98)	81.2(3)
O(68)-La(10)-O(73)	82.2(3)	O(105)-La(11)-O(98)	120.2(3)
O(79)-La(10)-O(73)	120.8(3)	O(100)-La(11)-O(98)	100.0(3)
O(64)-La(10)-O(66)	75.0(3)	O(94)-La(11)-O(98)	152.1(3)
O(68)-La(10)-O(66)	68.8(2)	O(95)-La(11)-O(98)	140.6(3)
O(79)-La(10)-O(66)	76.4(2)	O(96)-La(11)-O(98)	78.3(3)
O(73)-La(10)-O(66)	139.9(3)	O(87)-La(11)-O(99)	130.4(3)
O(64)-La(10)-O(78)	136.1(3)	O(97)-La(11)-O(99)	70.5(3)
O(68)-La(10)-O(78)	134.2(3)	O(105)-La(11)-O(99)	68.1(2)
O(79)-La(10)-O(78)	69.6(3)	O(100)-La(11)-O(99)	74.3(3)
O(73)-La(10)-O(78)	97.5(3)	O(94)-La(11)-O(99)	145.8(2)
O(66)-La(10)-O(78)	122.6(3)	O(95)-La(11)-O(99)	131.6(2)

O(96)-La(11)-O(99)	97.5(3)
O(98)-La(11)-O(99)	52.7(3)
O(114)-La(12)-O(106)	116.8(3)
O(114)-La(12)-O(112)	74.5(3)
O(106)-La(12)-O(112)	72.6(3)
O(114)-La(12)-O(107)	148.9(3)
O(106)-La(12)-O(107)	75.7(3)
O(112)-La(12)-O(107)	135.7(3)
O(114)-La(12)-O(100)	80.2(3)
O(106)-La(12)-O(100)	153.2(3)
O(112)-La(12)-O(100)	94.3(3)
O(107)-La(12)-O(100)	100.7(3)
O(114)-La(12)-O(105)	136.0(3)
O(106)-La(12)-O(105)	83.5(2)
O(112)-La(12)-O(105)	75.8(3)
O(107)-La(12)-O(105)	70.6(3)
O(100)-La(12)-O(105)	70.5(2)
O(114)-La(12)-O(20)	73.1(3)
O(106)-La(12)-O(20)	70.6(3)
O(112)-La(12)-O(20)	110.7(3)
O(107)-La(12)-O(20)	86.2(3)
O(100)-La(12)-O(20)	136.2(3)
O(105)-La(12)-O(20)	148.9(2)
O(114)-La(12)-O(19)	77.2(3)
O(106)-La(12)-O(19)	126.0(3)
O(112)-La(12)-O(19)	151.3(3)
O(107)-La(12)-O(19)	73.0(3)
O(100)-La(12)-O(19)	76.1(3)
O(105)-La(12)-O(19)	123.8(2)
O(20)-La(12)-O(19)	64.6(2)
O(39)-La(13)-O(37)	76.6(3)
O(39)-La(13)-O(22)	145.6(3)
O(37)-La(13)-O(22)	136.9(3)
O(39)-La(13)-O(24)	77.7(3)
O(37)-La(13)-O(24)	91.0(3)
O(22)-La(13)-O(24)	104.3(3)
O(39)-La(13)-O(28)	118.9(3)
O(37)-La(13)-O(28)	72.2(3)
O(22)-La(13)-O(28)	75.7(3)
O(24)-La(13)-O(28)	151.1(3)
O(39)-La(13)-O(2)	73.3(3)
O(37)-La(13)-O(2)	111.1(2)
O(22)-La(13)-O(2)	84.2(3)
O(24)-La(13)-O(2)	137.6(3)
O(28)-La(13)-O(2)	71.3(2)
O(39)-La(13)-O(23)	138.5(3)
O(37)-La(13)-O(23)	75.9(2)
O(22)-La(13)-O(23)	71.1(3)
O(24)-La(13)-O(23)	72.3(3)
O(28)-La(13)-O(23)	80.7(2)
O(2)-La(13)-O(23)	146.5(3)
O(39)-La(13)-O(1)	72.6(3)
O(37)-La(13)-O(1)	148.6(3)
O(22)-La(13)-O(1)	74.5(3)
O(24)-La(13)-O(1)	76.8(3)
O(28)-La(13)-O(1)	129.0(3)
O(2)-La(13)-O(1)	65.4(2)
O(23)-La(13)-O(1)	125.5(3)
O(20)-La(14)-O(21)	71.4(3)
O(20)-La(14)-O(110)	138.7(3)
O(21)-La(14)-O(110)	136.3(3)
O(20)-La(14)-O(106)	69.8(2)
O(21)-La(14)-O(106)	135.8(3)
O(110)-La(14)-O(106)	70.8(3)
O(20)-La(14)-O(23)#1	85.7(3)
O(21)-La(14)-O(23)#1	85.9(3)
O(110)-La(14)-O(23)#1	70.4(3)
O(106)-La(14)-O(23)#1	71.1(2)
O(20)-La(14)-O(116)	101.2(3)
O(21)-La(14)-O(116)	133.8(4)
O(110)-La(14)-O(116)	79.5(4)
O(106)-La(14)-O(116)	74.6(3)
O(23)#1-La(14)-O(116)	140.0(3)
O(20)-La(14)-O(115)	142.1(3)
O(21)-La(14)-O(115)	81.8(3)
O(110)-La(14)-O(115)	78.9(3)
O(106)-La(14)-O(115)	142.3(3)
O(23)#1-La(14)-O(115)	119.2(3)
O(116)-La(14)-O(115)	78.3(3)
O(20)-La(14)-O(117)	74.5(3)
O(21)-La(14)-O(117)	75.0(4)
O(110)-La(14)-O(117)	133.7(4)
O(106)-La(14)-O(117)	113.1(4)
O(23)#1-La(14)-O(117)	156.0(4)
O(116)-La(14)-O(117)	59.4(4)
O(115)-La(14)-O(117)	73.0(4)
O(20)-La(14)-O(22)#1	134.1(3)
O(21)-La(14)-O(22)#1	70.2(3)
O(110)-La(14)-O(22)#1	66.9(3)
O(106)-La(14)-O(22)#1	128.1(3)
O(23)#1-La(14)-O(22)#1	67.4(3)
O(116)-La(14)-O(22)#1	123.6(3)
O(115)-La(14)-O(22)#1	52.4(3)
O(117)-La(14)-O(22)#1	117.6(4)
O(6)-La(15)-O(49)	135.8(3)
O(6)-La(15)-O(43)	134.9(3)
O(49)-La(15)-O(43)	75.4(4)
O(6)-La(15)-O(45)	88.5(3)
O(49)-La(15)-O(45)	70.4(3)
O(43)-La(15)-O(45)	136.6(3)
O(6)-La(15)-O(5)	71.7(3)
O(49)-La(15)-O(5)	138.6(3)
O(43)-La(15)-O(5)	107.4(3)
O(45)-La(15)-O(5)	82.8(3)
O(6)-La(15)-O(40)	137.1(3)
O(49)-La(15)-O(40)	72.4(3)
O(43)-La(15)-O(40)	74.4(3)
O(45)-La(15)-O(40)	70.3(2)
O(5)-La(15)-O(40)	69.0(2)
O(6)-La(15)-O(44)	82.6(3)

O(49)-La(15)-O(44)	128.1(3)	O(15)-La(17)-O(90)	138.0(3)
O(43)-La(15)-O(44)	54.8(4)	O(81)-La(17)-O(90)	72.2(3)
O(45)-La(15)-O(44)	159.2(3)	O(83)-La(17)-O(90)	74.6(3)
O(5)-La(15)-O(44)	76.5(3)	O(91)-La(17)-O(14)	83.1(2)
O(40)-La(15)-O(44)	104.0(3)	O(15)-La(17)-O(14)	71.2(3)
O(6)-La(15)-O(46)	78.0(3)	O(81)-La(17)-O(14)	137.9(3)
O(49)-La(15)-O(46)	80.1(3)	O(83)-La(17)-O(14)	109.3(3)
O(43)-La(15)-O(46)	77.9(3)	O(90)-La(17)-O(14)	69.5(3)
O(45)-La(15)-O(46)	120.4(3)	O(91)-La(17)-O(82)	158.4(3)
O(5)-La(15)-O(46)	141.3(3)	O(15)-La(17)-O(82)	82.6(3)
O(40)-La(15)-O(46)	144.9(3)	O(81)-La(17)-O(82)	129.6(3)
O(44)-La(15)-O(46)	76.2(3)	O(83)-La(17)-O(82)	54.5(3)
O(6)-La(15)-O(47)	69.0(3)	O(90)-La(17)-O(82)	100.9(3)
O(49)-La(15)-O(47)	67.2(3)	O(14)-La(17)-O(82)	75.3(3)
O(43)-La(15)-O(47)	120.7(3)	O(91)-La(17)-O(93)	120.8(3)
O(45)-La(15)-O(47)	68.6(3)	O(15)-La(17)-O(93)	78.4(3)
O(5)-La(15)-O(47)	131.2(3)	O(81)-La(17)-O(93)	80.8(3)
O(40)-La(15)-O(47)	129.6(3)	O(83)-La(17)-O(93)	75.4(3)
O(44)-La(15)-O(47)	124.4(3)	O(90)-La(17)-O(93)	143.5(3)
O(46)-La(15)-O(47)	52.2(3)	O(14)-La(17)-O(93)	141.3(3)
O(65)-La(16)-O(58)	77.0(3)	O(82)-La(17)-O(93)	77.7(3)
O(65)-La(16)-O(47)	146.4(3)	O(91)-La(17)-O(92)	69.3(2)
O(58)-La(16)-O(47)	135.9(3)	O(15)-La(17)-O(92)	69.3(3)
O(65)-La(16)-O(51)	77.8(3)	O(81)-La(17)-O(92)	67.3(3)
O(58)-La(16)-O(51)	93.1(3)	O(83)-La(17)-O(92)	118.7(3)
O(47)-La(16)-O(51)	102.2(3)	O(90)-La(17)-O(92)	131.3(3)
O(65)-La(16)-O(52)	119.7(3)	O(14)-La(17)-O(92)	131.0(3)
O(58)-La(16)-O(52)	71.7(3)	O(82)-La(17)-O(92)	125.6(3)
O(47)-La(16)-O(52)	75.8(3)	O(93)-La(17)-O(92)	52.2(3)
O(51)-La(16)-O(52)	151.6(3)	O(18)-La(18)-O(17)	72.2(3)
O(65)-La(16)-O(8)	74.1(3)	O(18)-La(18)-O(99)	136.9(3)
O(58)-La(16)-O(8)	109.9(3)	O(17)-La(18)-O(99)	139.0(3)
O(47)-La(16)-O(8)	85.5(3)	O(18)-La(18)-O(105)	88.3(3)
O(51)-La(16)-O(8)	138.1(3)	O(17)-La(18)-O(105)	85.5(2)
O(52)-La(16)-O(8)	70.3(3)	O(99)-La(18)-O(105)	70.7(3)
O(65)-La(16)-O(45)	136.6(3)	O(18)-La(18)-O(97)	136.7(3)
O(58)-La(16)-O(45)	75.1(3)	O(17)-La(18)-O(97)	68.7(2)
O(47)-La(16)-O(45)	71.4(2)	O(99)-La(18)-O(97)	72.1(2)
O(51)-La(16)-O(45)	71.2(3)	O(105)-La(18)-O(97)	70.9(2)
O(52)-La(16)-O(45)	81.6(3)	O(18)-La(18)-O(101)	132.1(3)
O(8)-La(16)-O(45)	147.3(3)	O(17)-La(18)-O(101)	102.4(3)
O(65)-La(16)-O(7)	74.5(3)	O(99)-La(18)-O(101)	78.3(3)
O(58)-La(16)-O(7)	151.2(3)	O(105)-La(18)-O(101)	139.5(3)
O(47)-La(16)-O(7)	72.8(3)	O(97)-La(18)-O(101)	75.2(3)
O(51)-La(16)-O(7)	77.8(3)	O(18)-La(18)-O(108)	79.2(3)
O(52)-La(16)-O(7)	126.6(3)	O(17)-La(18)-O(108)	141.7(3)
O(8)-La(16)-O(7)	65.1(3)	O(99)-La(18)-O(108)	79.1(3)
O(45)-La(16)-O(7)	125.3(3)	O(105)-La(18)-O(108)	118.9(2)
O(91)-La(17)-O(15)	90.0(3)	O(97)-La(18)-O(108)	144.1(3)
O(91)-La(17)-O(81)	68.5(3)	O(101)-La(18)-O(108)	78.6(3)
O(15)-La(17)-O(81)	136.0(3)	O(18)-La(18)-O(102)	79.3(3)
O(91)-La(17)-O(83)	136.7(3)	O(17)-La(18)-O(102)	76.1(3)
O(15)-La(17)-O(83)	133.3(3)	O(99)-La(18)-O(102)	128.5(3)
O(81)-La(17)-O(83)	76.1(3)	O(105)-La(18)-O(102)	160.2(3)
O(91)-La(17)-O(90)	71.5(2)	O(97)-La(18)-O(102)	108.0(3)

O(101)-La(18)-O(102)	53.9(3)	O(45)-La(20)-O(41)	76.4(2)
O(108)-La(18)-O(102)	74.1(3)	O(42)-La(20)-O(41)	53.1(3)
O(18)-La(18)-O(107)	70.0(3)	O(38)-La(20)-O(51)	138.8(3)
O(17)-La(18)-O(107)	133.5(2)	O(40)-La(20)-O(51)	133.8(3)
O(99)-La(18)-O(107)	67.2(2)	O(45)-La(20)-O(51)	69.7(3)
O(105)-La(18)-O(107)	67.6(2)	O(42)-La(20)-O(51)	79.6(3)
O(97)-La(18)-O(107)	129.0(2)	O(41)-La(20)-O(51)	123.0(3)
O(101)-La(18)-O(107)	122.9(3)	O(38)-La(20)-O(50)	86.5(3)
O(108)-La(18)-O(107)	51.9(2)	O(40)-La(20)-O(50)	160.3(3)
O(102)-La(18)-O(107)	121.1(3)	O(45)-La(20)-O(50)	121.7(3)
O(60)-La(19)-O(9)	137.0(3)	O(42)-La(20)-O(50)	76.5(3)
O(60)-La(19)-O(53)	70.0(3)	O(41)-La(20)-O(50)	126.1(3)
O(9)-La(19)-O(53)	87.1(3)	O(51)-La(20)-O(50)	52.7(3)
O(60)-La(19)-O(55)	77.3(3)	O(38)-La(20)-O(48)	77.9(3)
O(9)-La(19)-O(55)	134.4(3)	O(40)-La(20)-O(48)	82.4(3)
O(53)-La(19)-O(55)	138.5(3)	O(45)-La(20)-O(48)	120.5(3)
O(60)-La(19)-O(8)	138.8(3)	O(42)-La(20)-O(48)	150.7(3)
O(9)-La(19)-O(8)	70.8(3)	O(41)-La(20)-O(48)	140.4(3)
O(53)-La(19)-O(8)	85.6(3)	O(51)-La(20)-O(48)	96.5(3)
O(55)-La(19)-O(8)	103.8(3)	O(50)-La(20)-O(48)	78.1(3)
O(60)-La(19)-O(52)	71.3(3)	O(38)-La(20)-O(49)	127.2(3)
O(9)-La(19)-O(52)	135.9(3)	O(40)-La(20)-O(49)	71.0(3)
O(53)-La(19)-O(52)	71.4(2)	O(45)-La(20)-O(49)	68.2(3)
O(55)-La(19)-O(52)	74.4(3)	O(42)-La(20)-O(49)	146.5(3)
O(8)-La(19)-O(52)	69.6(3)	O(41)-La(20)-O(49)	132.9(3)
O(60)-La(19)-O(54)	128.9(4)	O(51)-La(20)-O(49)	72.1(3)
O(9)-La(19)-O(54)	81.0(4)	O(50)-La(20)-O(49)	99.1(3)
O(53)-La(19)-O(54)	160.1(4)	O(48)-La(20)-O(49)	52.8(3)
O(55)-La(19)-O(54)	54.6(4)	O(104)-La(21)-O(106)	88.2(3)
O(8)-La(19)-O(54)	75.5(3)	O(104)-La(21)-O(23)#1	149.5(3)
O(52)-La(19)-O(54)	106.7(3)	O(106)-La(21)-O(23)#1	72.4(2)
O(60)-La(19)-O(62)	80.5(3)	O(104)-La(21)-O(113)	87.0(3)
O(9)-La(19)-O(62)	80.0(3)	O(106)-La(21)-O(113)	121.0(3)
O(53)-La(19)-O(62)	119.2(3)	O(23)#1-La(21)-O(113)	83.6(3)
O(55)-La(19)-O(62)	78.3(3)	O(104)-La(21)-O(24)#1	135.7(3)
O(8)-La(19)-O(62)	140.7(3)	O(104)-La(21)-O(112)	74.7(3)
O(52)-La(19)-O(62)	144.2(3)	O(106)-La(21)-O(112)	69.6(2)
O(54)-La(19)-O(62)	74.5(4)	O(113)-La(21)-O(112)	52.5(3)
O(60)-La(19)-O(63)	67.6(3)	O(104)-La(21)-O(111)	82.5(3)
O(9)-La(19)-O(63)	70.1(3)	O(106)-La(21)-O(111)	161.0(3)
O(53)-La(19)-O(63)	67.9(2)	O(113)-La(21)-O(111)	75.1(4)
O(55)-La(19)-O(63)	121.8(3)	O(112)-La(21)-O(111)	122.9(3)
O(8)-La(19)-O(63)	133.2(3)	O(104)-La(21)-O(109)	76.9(3)
O(52)-La(19)-O(63)	129.5(2)	O(106)-La(21)-O(109)	81.5(3)
O(54)-La(19)-O(63)	121.7(3)	O(113)-La(21)-O(109)	152.2(3)
O(62)-La(19)-O(63)	51.8(3)	O(112)-La(21)-O(109)	139.7(3)
O(38)-La(20)-O(40)	86.4(3)	O(111)-La(21)-O(109)	80.3(4)
O(38)-La(20)-O(45)	147.6(3)	O(104)-La(21)-O(110)	126.8(3)
O(40)-La(20)-O(45)	71.5(3)	O(106)-La(21)-O(110)	69.4(3)
O(38)-La(20)-O(42)	86.0(3)	O(113)-La(21)-O(110)	146.1(3)
O(40)-La(20)-O(42)	121.3(3)	O(24)#1-La(21)-O(110)	74.0(3)
O(45)-La(20)-O(42)	85.7(3)	O(112)-La(21)-O(110)	132.2(3)
O(38)-La(20)-O(41)	73.6(3)	O(111)-La(21)-O(110)	103.3(3)
O(40)-La(20)-O(41)	69.0(3)	O(109)-La(21)-O(110)	53.1(3)