Supporting Information

Self-assembly of luminescent 42-metal lanthanide nanowheels with sensing properties towards metal ions and nitro explosives

Dongliang Shi, Xiaoping Yang, Hongfen Chen, Yanan Ma, Desmond Schipper and Richard A. Jones

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

$[Yb_{42}(L)_{14}(OH)_{28}(OAc)_{84}]$ (1) $Yb(OAc)_3$ (0.40 mmol, 0.1401 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, washed with EtOH (3×5 ml) and dried in the air for one week. Yield (based on $Yb(OAc)_3$): 0.0549 g (40 %). m. p. > 199 ^oC (dec.). Elemental analysis: Found: C, 20.03; H, 2.64 %. Calc. for $C_{280}H_{378}Yb_{42}O_{238}$: C, 19.97; H, 2.66 %. IR (CH_3CN, cm^{-1}): 1620 (s), 1475 (s),1385 (w), 1355 (w), 1265 (s), 1200 (s), 1136 (m), 1106 (w), 1070 (m), 1043 (w), 967 (vs), 873 (m), 843 (m), 823 (m), 781 (s), 735 (vs), 694 (w), 626 (w).

$[Sm_{42}(L)_{14}(OH)_{28}(OAc)_{84}]$ (2) $Sm(OAc)_3$ (0.40 mmol, 0.1309 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, washed with EtOH (3×5 ml) and dried in the air for one week. Yield (based on $Sm(OAc)_3$): 0.0474 g (37 %). m. p. > 197 ^oC (dec.). Elemental analysis: Found: C, 21.32; H, 2.86 %. Calc. for $C_{280}H_{378}Sm_{42}O_{238}$: C, 21.39; H, 2.85 %. IR (KBr, cm^{-1}):1640 (s), 1560 (s), 1443 (m),1414 (s), 1310 (m), 1240 (s), 1211 (s), 1103 (m), 1271 (m), 1028 (w),957 (s),876 (s), 762 (w), 751 (m), 724 (w), 680 (m), 652 (m),607 (w).

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

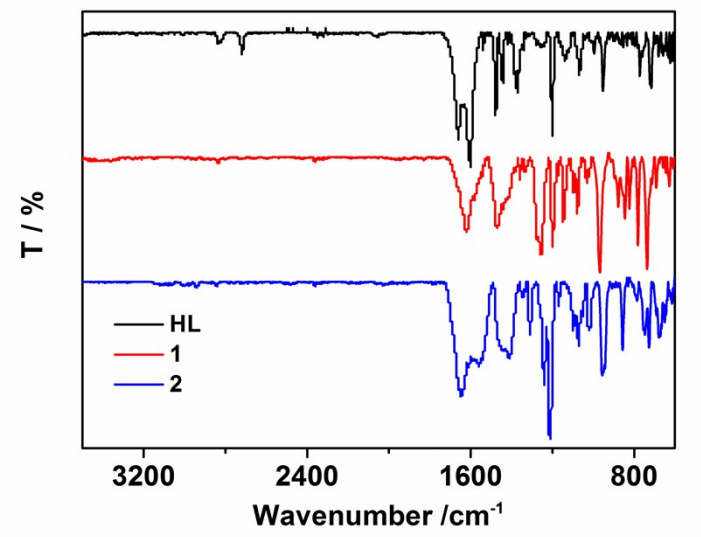


Figure S1. IR spectra of free ligand HL and clusters **1** and **2**.

4. The thermogravimetric analysis of 1

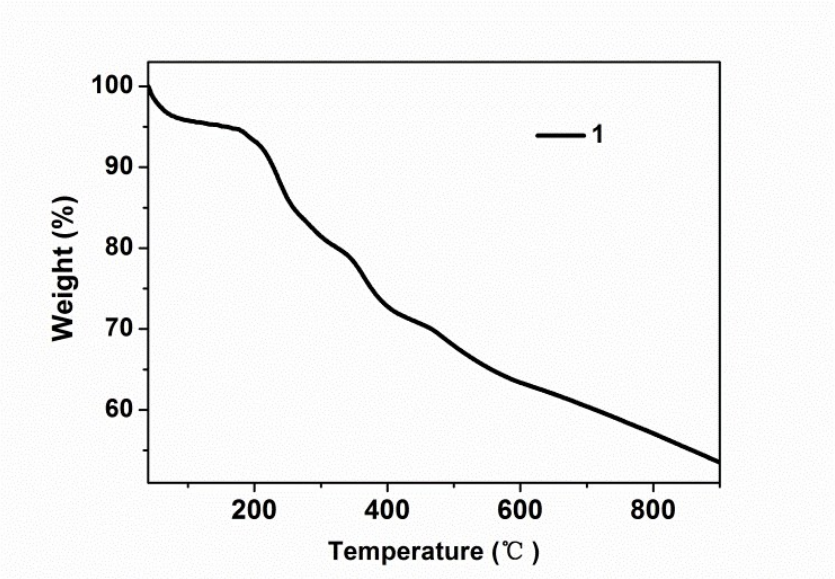


Figure S2. The thermogravimetric analysis of **1**.

5. Powder XRD patterns of 1 and 2

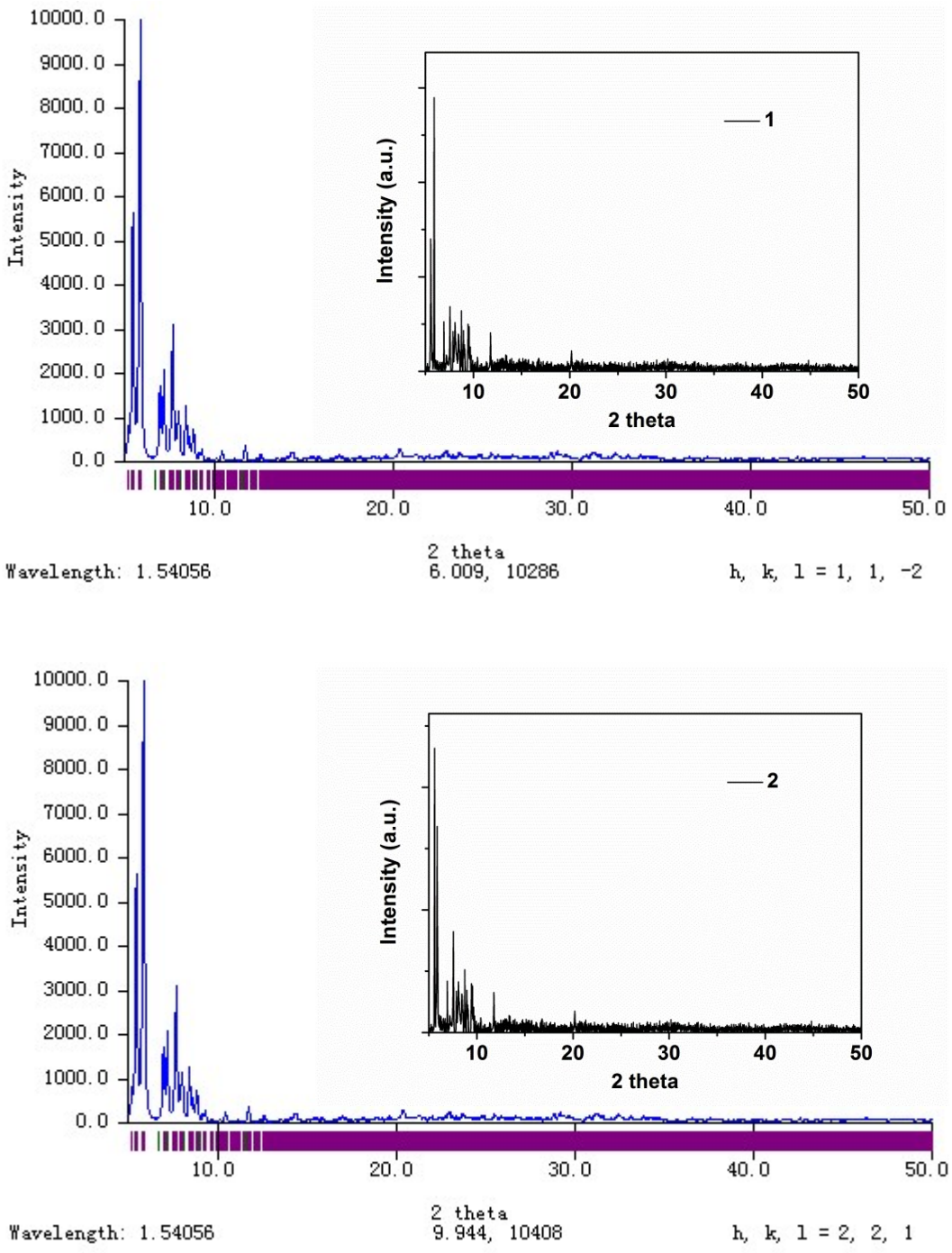


Figure S3. Powder XRD patterns of **1** and **2**.

6. Dynamic light scattering (DLS) measurements of 1

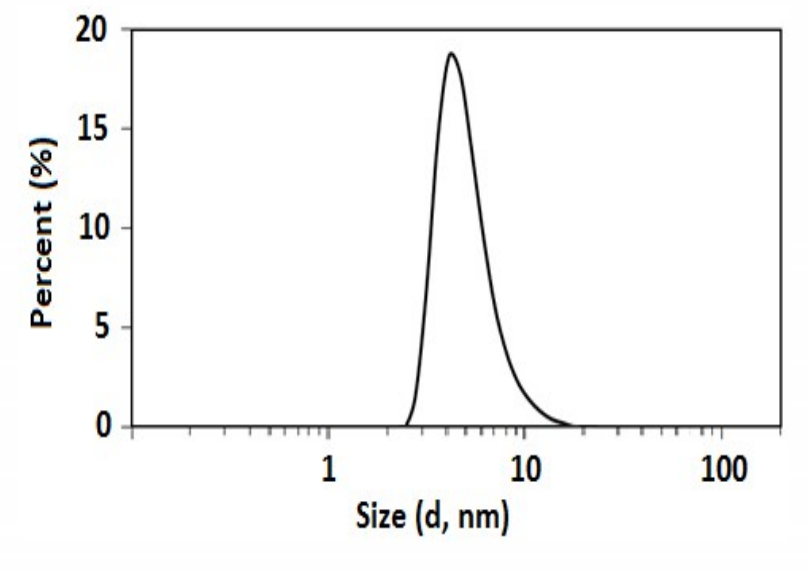


Figure S4. Dynamic light scattering (DLS) measurements of **1** in CH_3CN.

7. Photophysical properties of 1 and 2

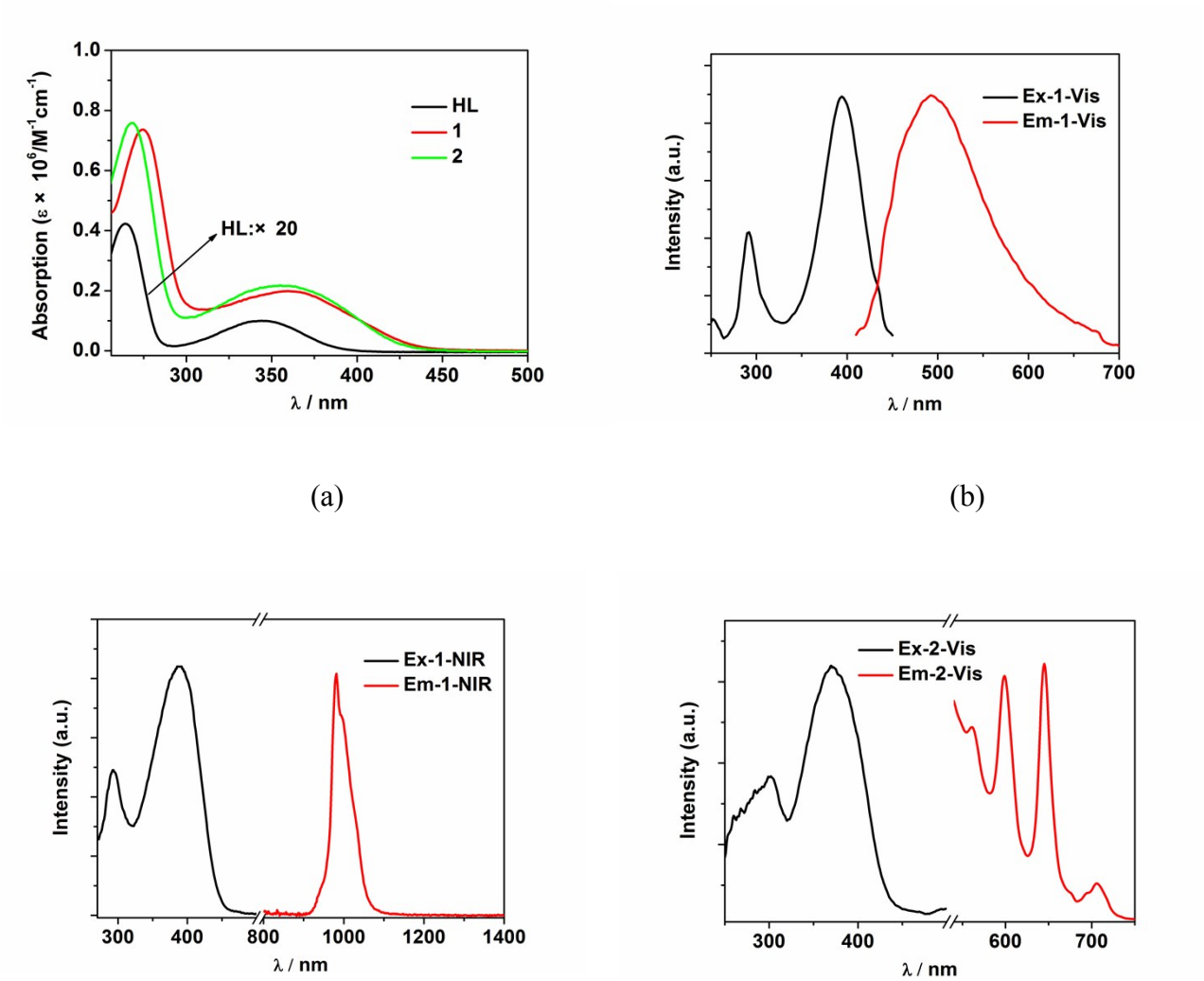


Figure S5. (a) UV-vis absorption spectra of the free ligand HL and clusters **1** and **2** in CH_3CN; (b) The excitation and visible emission spectra of **1** in CH_3CN; (c) The excitation and NIR emission spectra of **1** in CH_3CN; (d) The excitation and visible emission spectra of **2** in CH_3CN.

8. The lanthanide emission lifetimes of 1 and 2

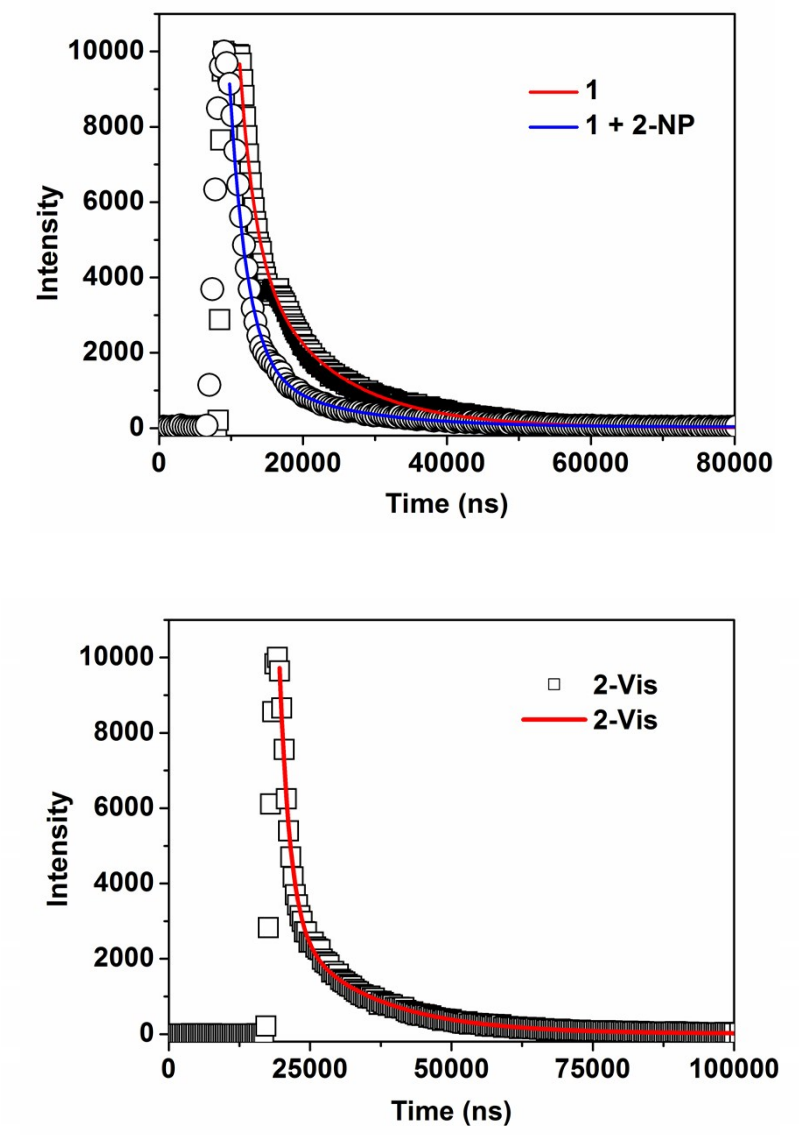


Figure S6. The lanthanide emission lifetimes of **1** (without the addition of 2-NP and with the addition of 700 μM 2-NP) and **2** in CH_3CN.

9. Chemical structures of nitro explosives

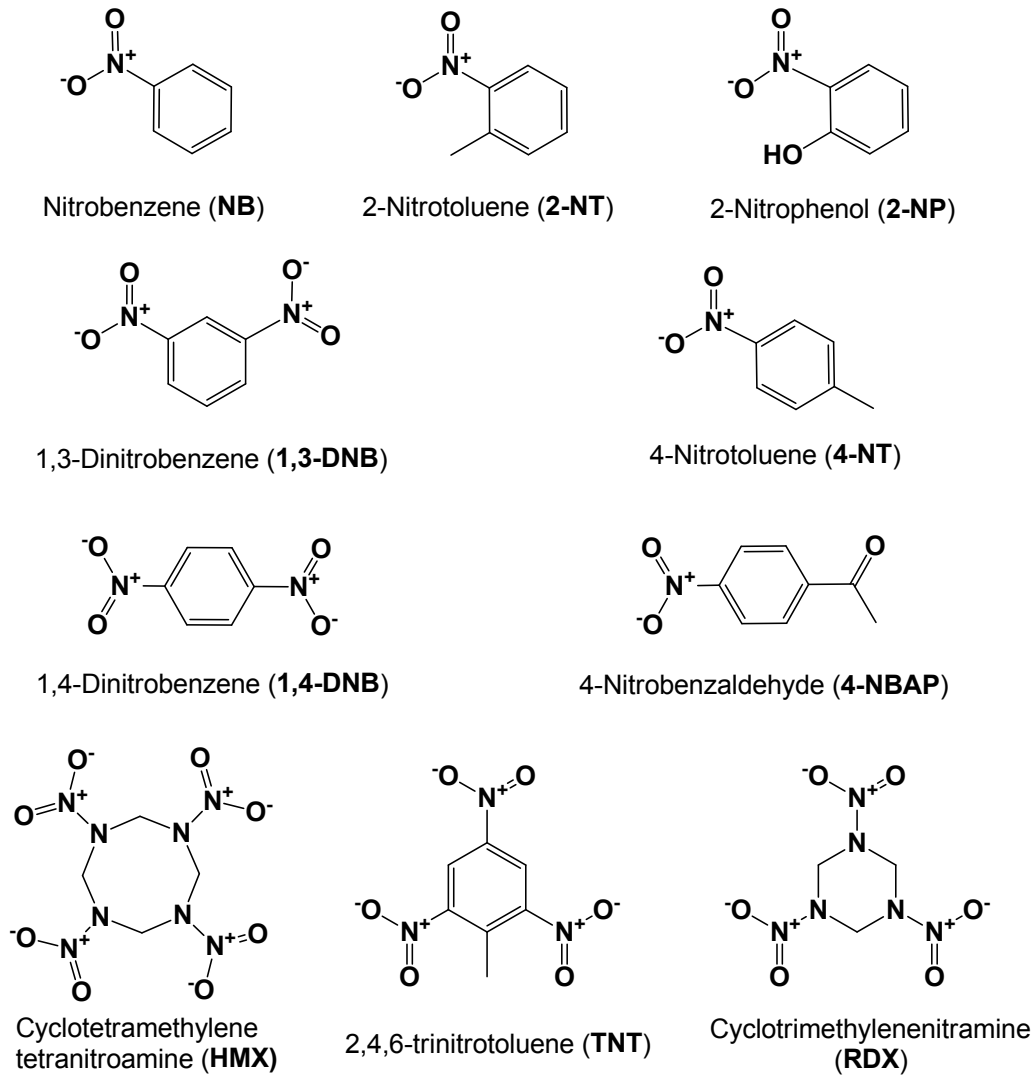
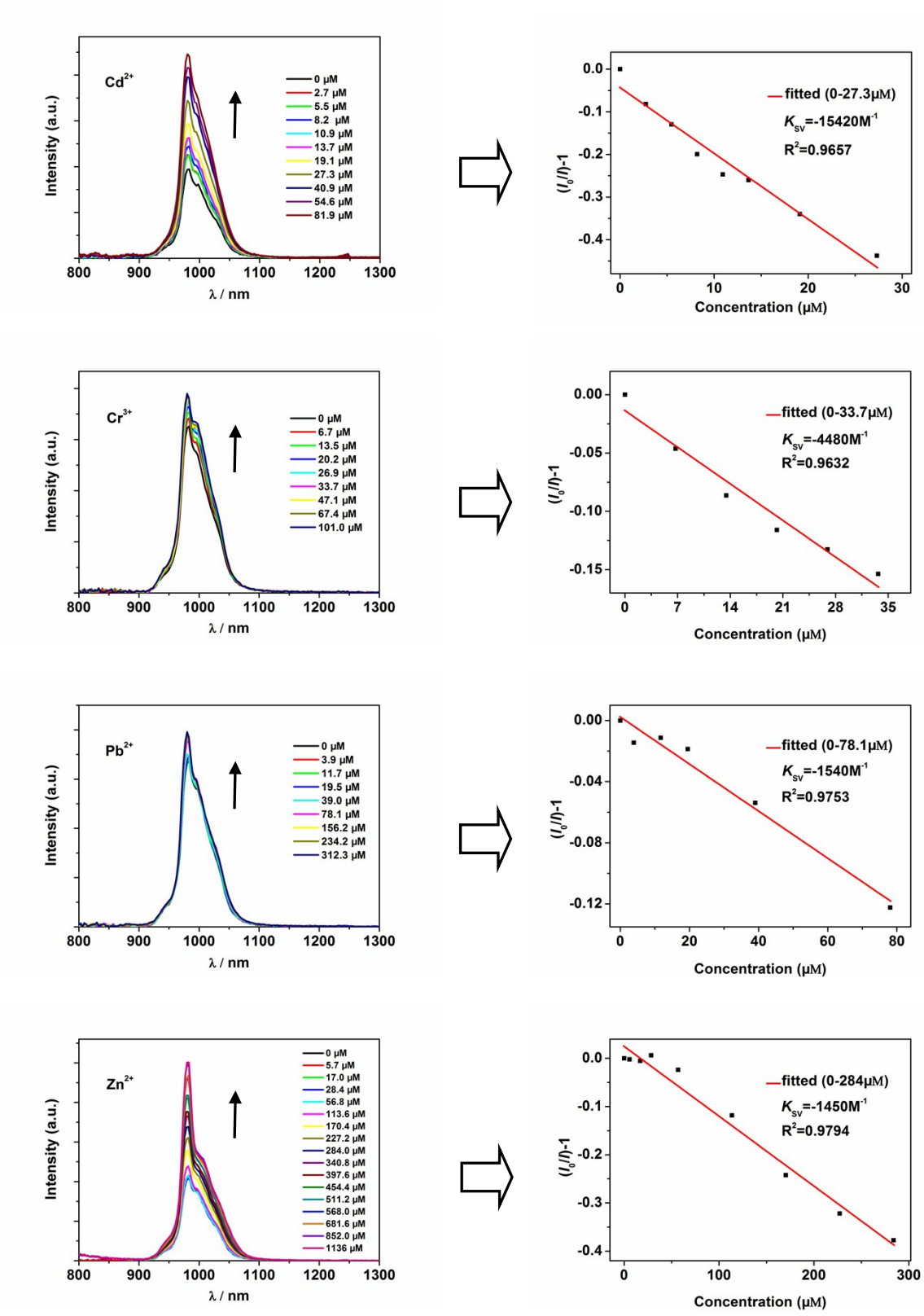
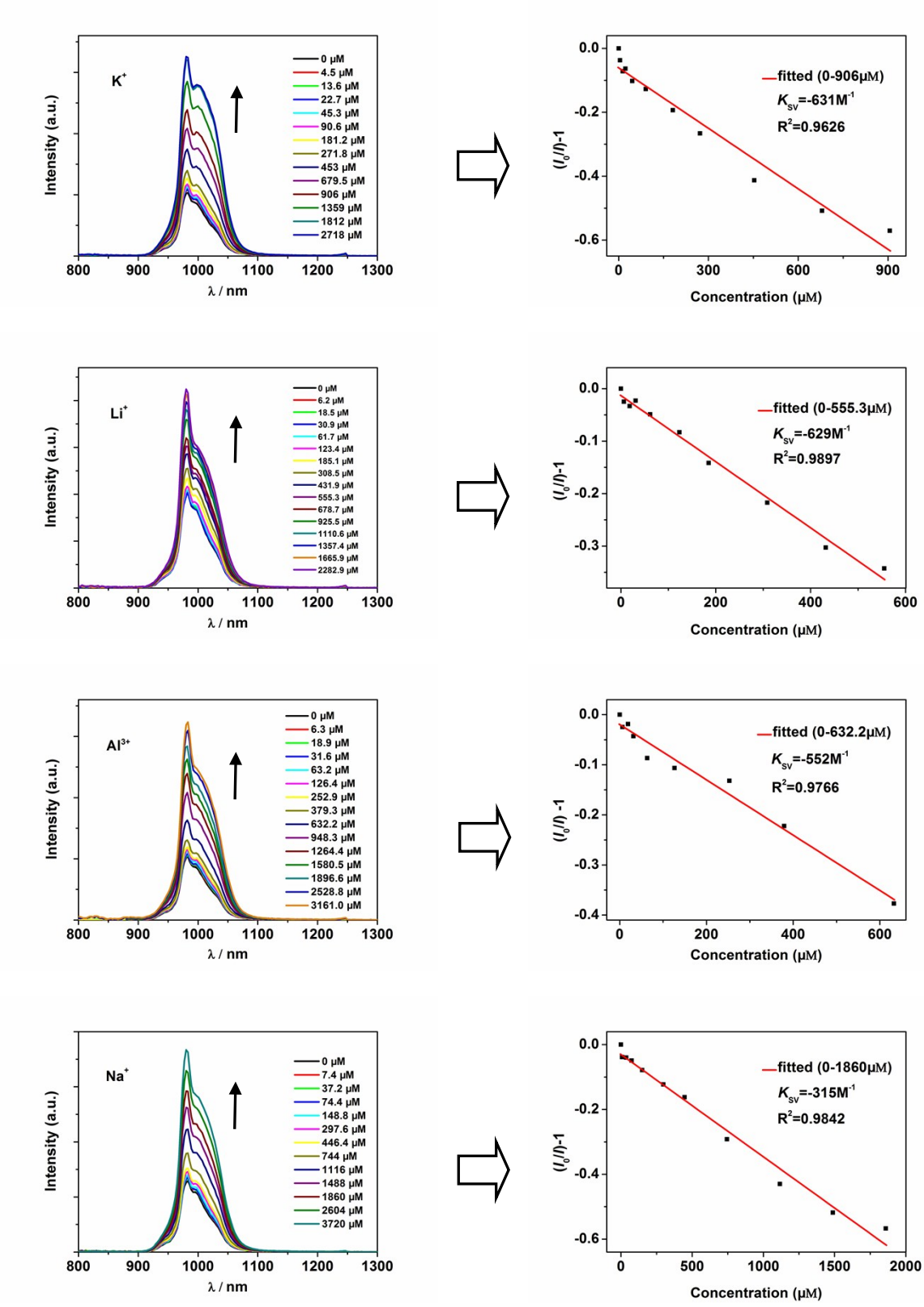
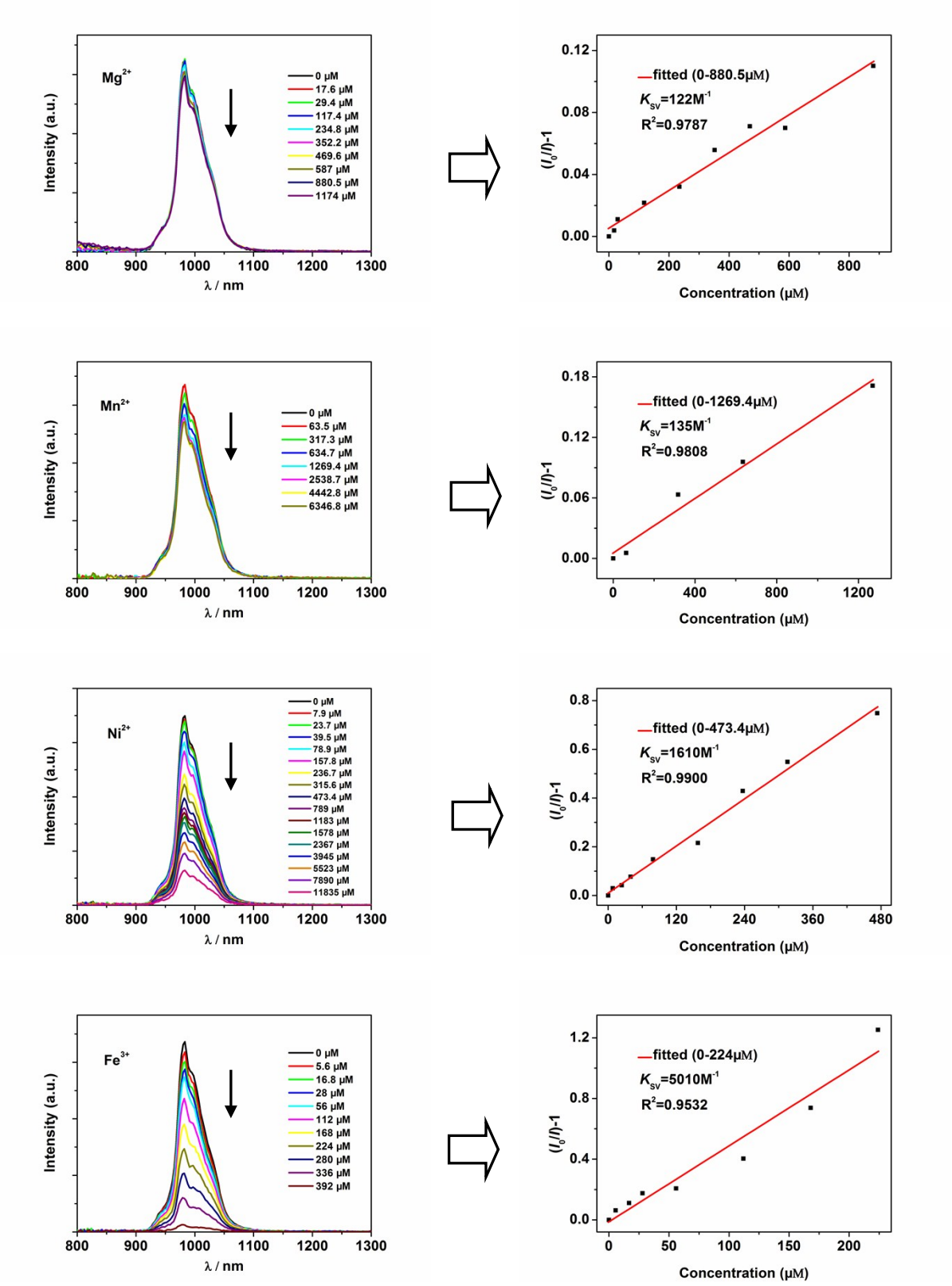


Figure S7. Chemical structures of nitro explosives.

10. NIR luminescent sensing of 1 to metal ions




K+
0 μM
4.5 μM
13.6 μM
22.7 μM
45.3 μM
90.6 μM
181.2 μM
271.8 μM
453 μM
679.5 μM
906 μM
1359 μM
1812 μM
2718 μM
Intensity (a.u.)
λ / nm
fitted (0-906μM)
K_{SV}=-631M^{-1}
R^2=0.9626
(I_0/I)-1
Concentration (μM)
Li+
0 μM
6.2 μM
18.5 μM
30.9 μM
61.7 μM
123.4 μM
185.1 μM
308.5 μM
431.9 μM
555.3 μM
678.7 μM
925.5 μM
1110.6 μM
1357.4 μM
1665.9 μM
2282.9 μM
fitted (0-555.3μM)
K_{SV}=-629M^{-1}
R^2=0.9897
Al3+
0 μM
6.3 μM
18.9 μM
31.6 μM
63.2 μM
126.4 μM
252.9 μM
379.3 μM
632.2 μM
948.3 μM
1264.4 μM
1580.5 μM
1896.6 μM
2528.8 μM
3161.0 μM
fitted (0-632.2μM)
K_{SV}=-552M^{-1}
R^2=0.9766
Na+
0 μM
7.4 μM
37.2 μM
74.4 μM
148.8 μM
297.6 μM
446.4 μM
744 μM
1116 μM
1488 μM
1860 μM
2604 μM
3720 μM
fitted (0-1860μM)
K_{SV}=-315M^{-1}
R^2=0.9842


Mg2+
0 μM
17.6 μM
29.4 μM
117.4 μM
234.8 μM
352.2 μM
469.6 μM
587 μM
880.5 μM
1174 μM
Intensity (a.u.)
λ / nm
fitted (0-880.5μM)
Ksv=122M-1
R2=0.9787
(I0/I)-1
Concentration (μM)
Mn2+
0 μM
63.5 μM
317.3 μM
634.7 μM
1269.4 μM
2538.7 μM
4442.8 μM
6346.8 μM
fitted (0-1269.4μM)
Ksv=135M-1
R2=0.9808
Ni2+
0 μM
7.9 μM
23.7 μM
39.5 μM
78.9 μM
157.8 μM
236.7 μM
315.6 μM
473.4 μM
789 μM
1183 μM
1578 μM
2367 μM
3945 μM
5523 μM
7890 μM
11835 μM
fitted (0-473.4μM)
Ksv=1610M-1
R2=0.9900
Fe3+
0 μM
5.6 μM
16.8 μM
28 μM
56 μM
112 μM
168 μM
224 μM
280 μM
336 μM
392 μM
fitted (0-224μM)
Ksv=5010M-1
R2=0.9532

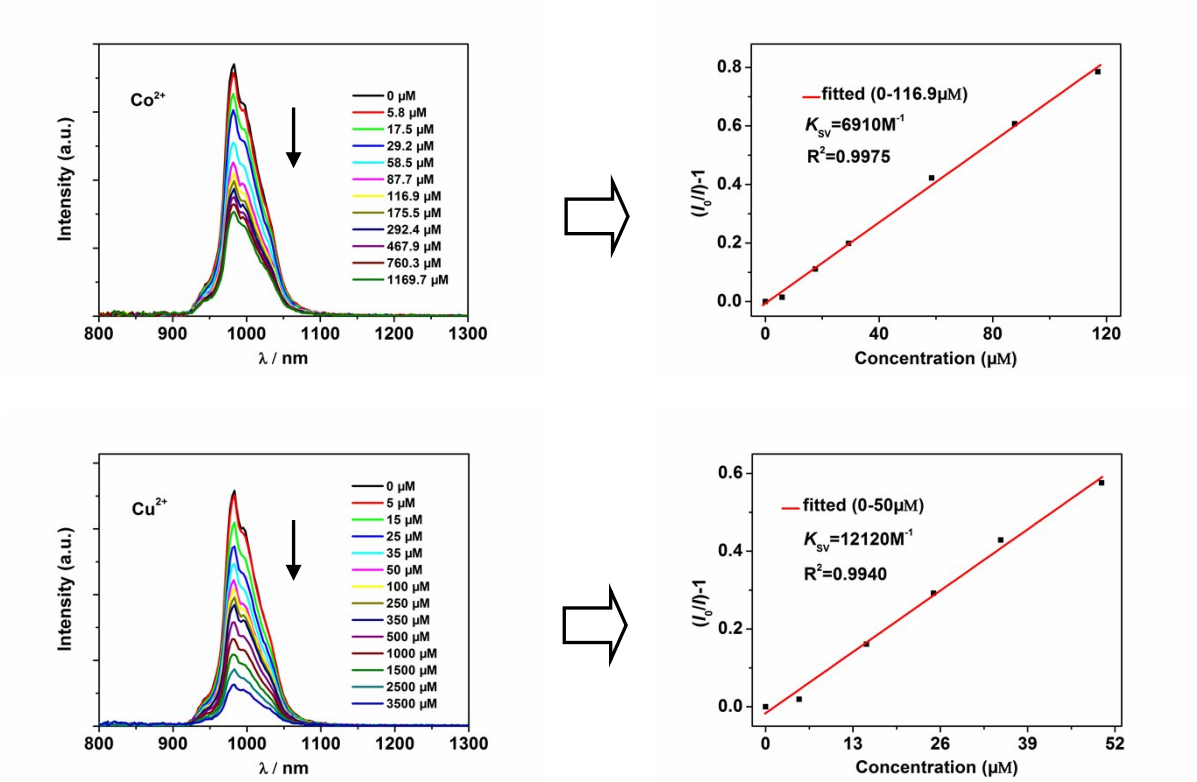
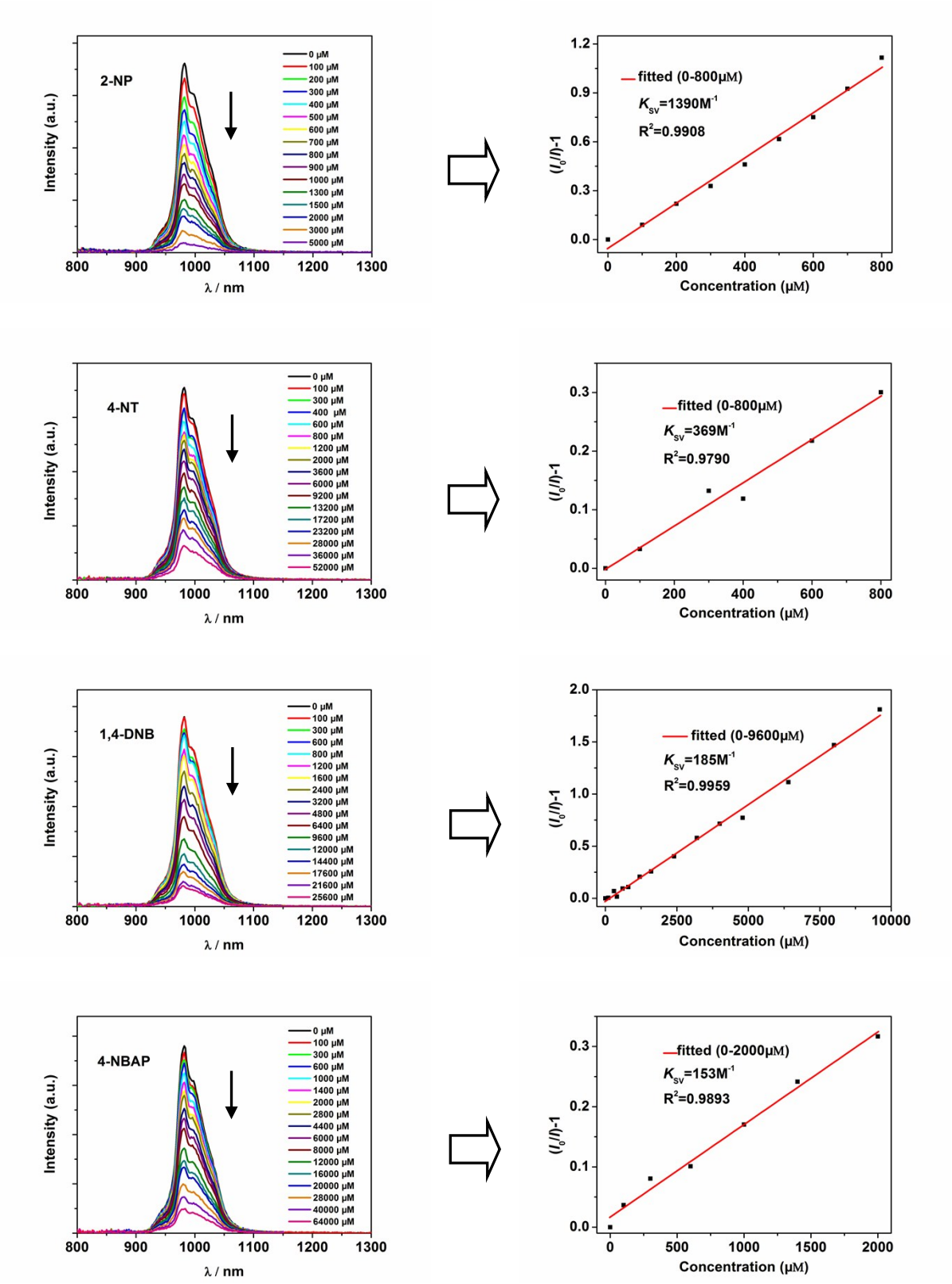
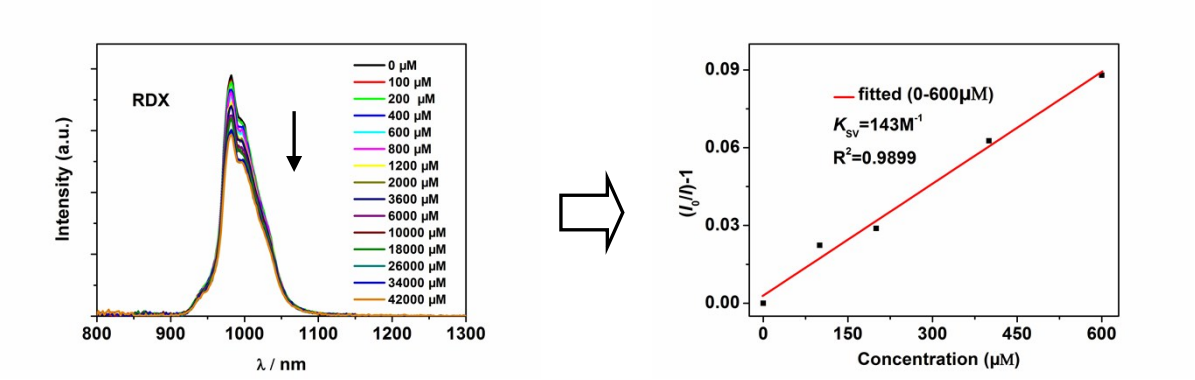
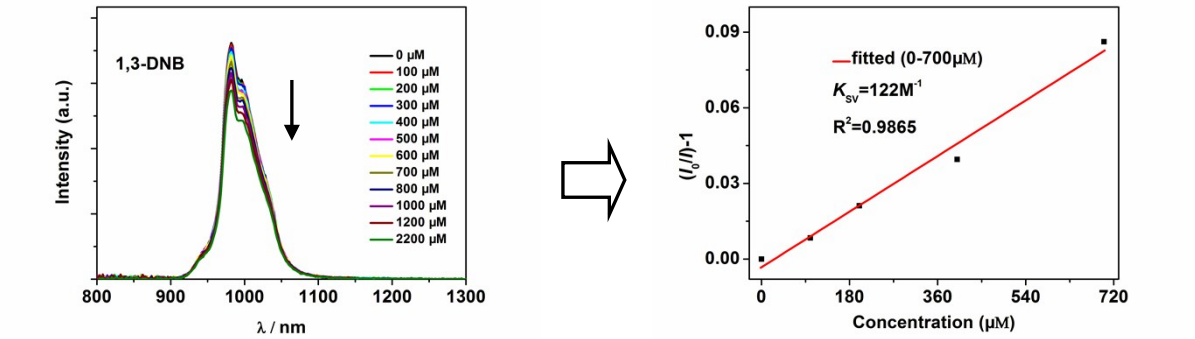


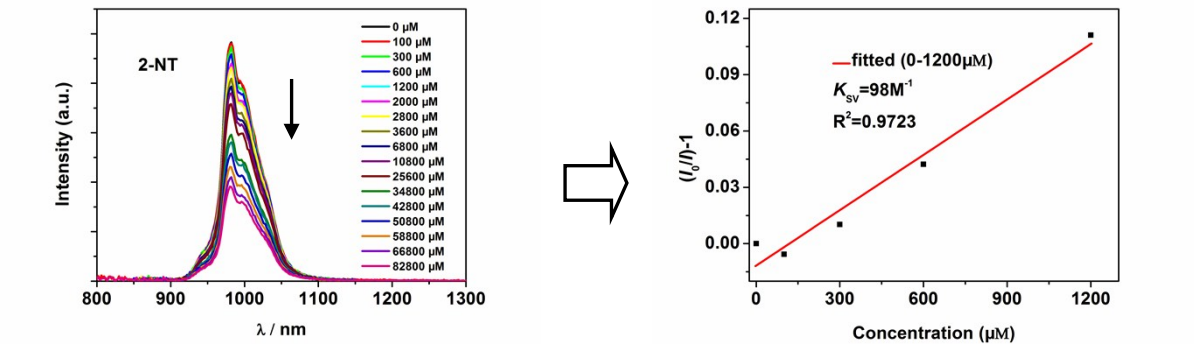
Figure S8. NIR luminescent sensing of **1** (15 μM) to metal ions in CH_3CN (λ_{ex} = 390 nm).

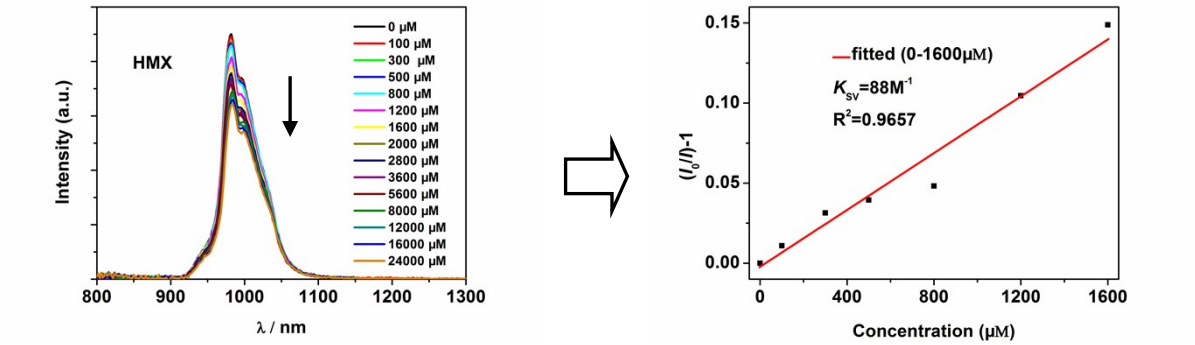
11. NIR luminescent sensing of 1 to nitro explosives




RDX
Intensity (a.u.)
λ / nm
0 μM
100 μM
200 μM
400 μM
600 μM
800 μM
1200 μM
2000 μM
3600 μM
6000 μM
10000 μM
18000 μM
26000 μM
34000 μM
42000 μM
fitted (0-600μM)
K_{SV}=143M^{-1}
R^2=0.9899
(I_0/I)-1
Concentration (μM)


1,3-DNB
Intensity (a.u.)
λ / nm
0 μM
100 μM
200 μM
300 μM
400 μM
500 μM
600 μM
700 μM
800 μM
1000 μM
1200 μM
2200 μM
fitted (0-700μM)
K_{SV}=122M^{-1}
R^2=0.9865
(I_0/I)-1
Concentration (μM)


2-NT
Intensity (a.u.)
λ / nm
0 μM
100 μM
300 μM
600 μM
1200 μM
2000 μM
2800 μM
3600 μM
6800 μM
10800 μM
25600 μM
34800 μM
42800 μM
50800 μM
58800 μM
66800 μM
82800 μM
fitted (0-1200μM)
K_{SV}=98M^{-1}
R^2=0.9723
(I_0/I)-1
Concentration (μM)


HMX
Intensity (a.u.)
λ / nm
0 μM
100 μM
300 μM
500 μM
800 μM
1200 μM
1600 μM
2000 μM
2800 μM
3600 μM
5600 μM
8000 μM
12000 μM
16000 μM
24000 μM
fitted (0-1600μM)
K_{SV}=88M^{-1}
R^2=0.9657
(I_0/I)-1
Concentration (μM)

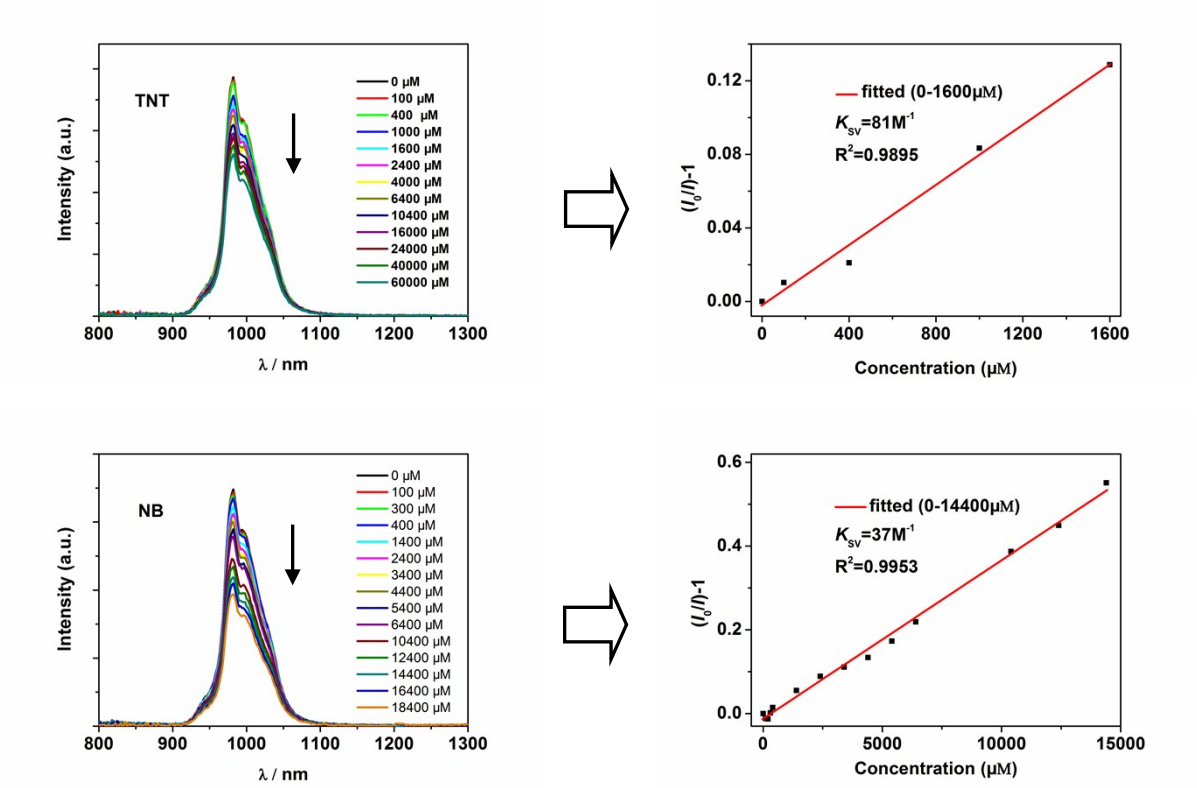


Figure S9. NIR luminescent sensing of **1** (15 μM) to nitro explosives in CH_3CN (λ_{ex} = 390 nm).

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

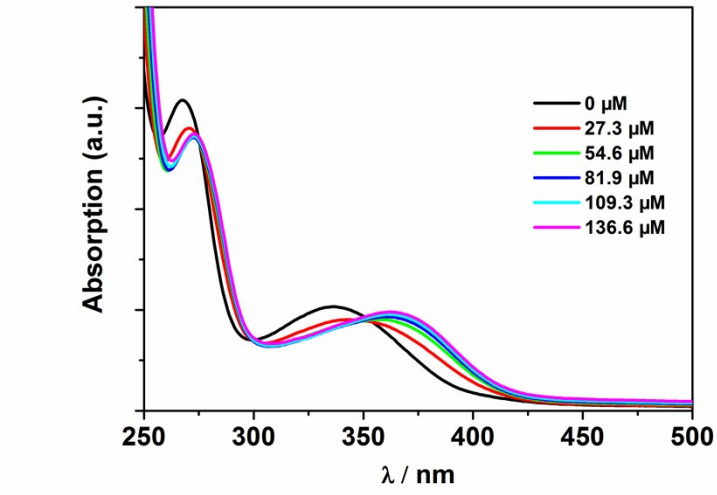


Figure S10. UV-Vis spectra of **1** with the addition of different concentrations of Cd^{2+} in CH_3CN.

13. UV-Vis spectra of 1 with the additional of 2-NP

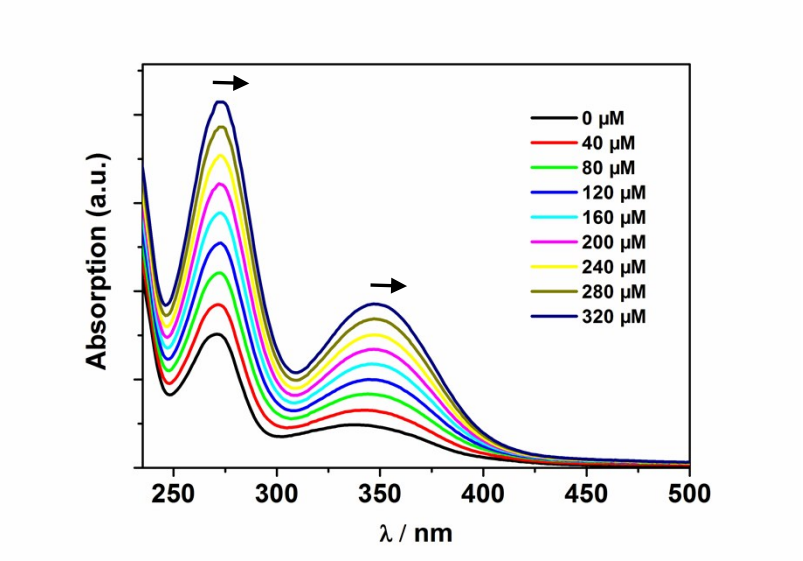


Figure S11. UV-Vis spectra of **1** with the additional of 2-NP in CH_3CN.

14. UV-Vis absorption spectra of explosives

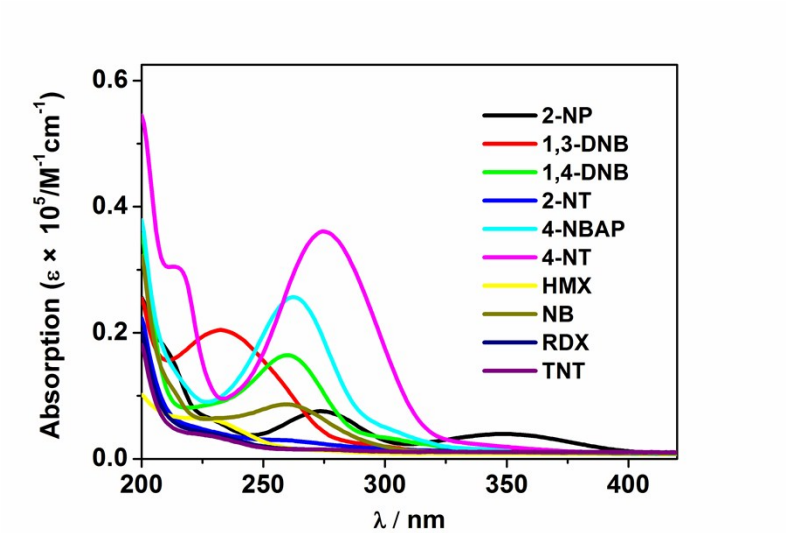


Figure S12. UV-Vis absorption spectra of explosives in CH_3CN.

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). Selected bond lengths are given in Tables S1 and S2. See http://www.rsc.org/suppdata/cc/ for crystallographic data in CIF format (CCDC reference numbers 1947262-1947263).

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. Selected Bond Lengths (Å) for **1**.

Yb(1)-O(11)	2.377(14)	Yb(7)-O(6)	2.387(13)
Yb(1)-O(2)	2.407(13)	Yb(7)-O(42)	2.397(13)
Yb(1)-O(23)	2.411(13)	Yb(7)-O(103)	2.416(10)
Yb(1)-O(17)	2.425(11)	Yb(7)-O(43)	2.418(14)
Yb(1)-O(99)	2.432(11)	Yb(7)-O(119)	2.420(10)
Yb(1)-O(100)	2.442(11)	Yb(7)-O(116)	2.422(13)
Yb(1)-O(18)	2.463(12)	Yb(7)-O(41)	2.460(13)
Yb(1)-O(15)	2.464(12)	Yb(7)-O(38)	2.503(13)
Yb(1)-O(16)	2.522(13)	Yb(7)-O(37)	2.551(12)
Yb(2)-O(25)	2.341(12)	Yb(8)-O(55)	2.361(12)
Yb(2)-O(99)	2.392(10)	Yb(8)-O(119)	2.385(11)
Yb(2)-O(100)	2.438(11)	Yb(8)-O(40)	2.429(15)
Yb(2)-O(21)	2.464(12)	Yb(8)-O(103)	2.439(11)
Yb(2)-O(20)	2.467(12)	Yb(8)-O(46)	2.467(12)
Yb(2)-O(19)	2.483(13)	Yb(8)-O(39)	2.493(11)
Yb(2)-O(23)	2.491(12)	Yb(8)-O(45)	2.494(13)
Yb(2)-O(24)	2.500(13)	Yb(8)-O(44)	2.494(13)
Yb(2)-O(115)	2.500(12)	Yb(8)-O(43)	2.515(11)
Yb(3)-O(99)	2.323(12)	Yb(9)-O(49)	2.316(13)
Yb(3)-O(98)#1	2.328(11)	Yb(9)-O(119)	2.329(12)
Yb(3)-O(21)	2.356(11)	Yb(9)-O(46)	2.350(12)
Yb(3)-O(27)	2.365(12)	Yb(9)-O(36)	2.363(11)
Yb(3)-O(95)	2.405(13)	Yb(9)-O(116)	2.390(11)
Yb(3)-O(11)	2.427(12)	Yb(9)-O(47)	2.410(13)
Yb(3)-O(101)	2.441(11)	Yb(9)-O(105)	2.454(10)
Yb(3)-O(1)	2.471(12)	Yb(9)-O(5)	2.495(13)
Yb(4)-O(102)	2.365(11)	Yb(10)-O(106)	2.368(10)
Yb(4)-O(4)	2.373(14)	Yb(10)-O(8)	2.391(14)
Yb(4)-O(101)	2.412(11)	Yb(10)-O(56)	2.423(14)
Yb(4)-O(32)	2.440(13)	Yb(10)-O(51)	2.431(13)
Yb(4)-O(22)	2.449(13)	Yb(10)-O(53)	2.442(13)
Yb(4)-O(96)	2.451(12)	Yb(10)-O(105)	2.468(10)
Yb(4)-O(31)	2.460(13)	Yb(10)-O(48)	2.505(12)
Yb(4)-O(33)	2.474(13)	Yb(10)-O(52)	2.508(14)
Yb(4)-O(95)	2.575(12)	Yb(10)-O(47)	2.521(12)
Yb(5)-O(102)	2.352(11)	Yb(11)-O(59)	2.375(11)
Yb(5)-O(101)	2.404(11)	Yb(11)-O(106)	2.379(12)
Yb(5)-O(35)	2.410(13)	Yb(11)-O(105)	2.459(11)
Yb(5)-O(30)	2.422(11)	Yb(11)-O(58)	2.461(12)
Yb(5)-O(29)	2.464(11)	Yb(11)-O(57)	2.480(13)
Yb(5)-O(28)	2.468(12)	Yb(11)-O(49)	2.486(12)
Yb(5)-O(27)	2.498(11)	Yb(11)-O(50)	2.489(13)
Yb(5)-O(34)	2.517(13)	Yb(11)-O(53)	2.513(13)
Yb(5)-O(33)	2.518(11)	Yb(11)-O(54)	2.514(12)
Yb(6)-O(26)	2.334(13)	Yb(12)-O(106)	2.349(12)
Yb(6)-O(102)	2.336(12)	Yb(12)-O(117)	2.349(13)
Yb(6)-O(39)	2.374(11)	Yb(12)-O(56)	2.375(12)
Yb(6)-O(37)	2.374(12)	Yb(12)-O(63)	2.383(13)
Yb(6)-O(30)	2.406(11)	Yb(12)-O(58)	2.384(12)
Yb(6)-O(103)	2.437(10)	Yb(12)-O(61)	2.388(13)
Yb(6)-O(22)	2.456(12)	Yb(12)-O(107)	2.488(11)
Yb(6)-O(3)	2.513(13)	Yb(12)-O(7)	2.524(13)

Yb(13)-O(107)	2.376(11)	Yb(17)-O(75)	2.458(12)
Yb(13)-O(10)	2.393(12)	Yb(17)-O(74)	2.462(13)
Yb(13)-O(114)	2.395(12)	Yb(17)-O(77)	2.487(13)
Yb(13)-O(69)	2.433(14)	Yb(17)-O(76)	2.495(12)
Yb(13)-O(108)	2.440(10)	Yb(17)-O(78)	2.561(13)
Yb(13)-O(68)	2.454(13)	Yb(18)-O(82)	2.302(13)
Yb(13)-O(64)	2.461(12)	Yb(18)-O(110)	2.337(13)
Yb(13)-O(70)	2.488(17)	Yb(18)-O(76)	2.382(12)
Yb(13)-O(63)	2.584(12)	Yb(18)-O(94)	2.388(14)
Yb(14)-O(108)	2.368(11)	Yb(18)-O(85)	2.392(11)
Yb(14)-O(81)	2.369(12)	Yb(18)-O(118)	2.424(11)
Yb(14)-O(107)	2.427(10)	Yb(18)-O(111)	2.434(10)
Yb(14)-O(66)	2.481(12)	Yb(18)-O(113)	2.508(12)
Yb(14)-O(61)	2.482(12)	Yb(19)-O(104)	2.367(13)
Yb(14)-O(65)	2.484(12)	Yb(19)-O(111)	2.406(10)
Yb(14)-O(67)	2.491(13)	Yb(19)-O(14)	2.415(14)
Yb(14)-O(62)	2.511(15)	Yb(19)-O(88)	2.421(11)
Yb(14)-O(68)	2.559(12)	Yb(19)-O(92)	2.431(14)
Yb(15)-O(108)	2.346(11)	Yb(19)-O(112)	2.441(12)
Yb(15)-O(60)	2.351(11)	Yb(19)-O(87)	2.462(12)
Yb(15)-O(66)	2.354(12)	Yb(19)-O(86)	2.485(12)
Yb(15)-O(71)	2.366(13)	Yb(19)-O(85)	2.516(11)
Yb(15)-O(109)	2.388(11)	Yb(20)-O(112)	2.352(12)
Yb(15)-O(114)	2.409(11)	Yb(20)-O(97)	2.368(12)
Yb(15)-O(73)	2.417(12)	Yb(20)-O(111)	2.432(11)
Yb(15)-O(9)	2.513(14)	Yb(20)-O(94)	2.455(12)
Yb(16)-O(118)	2.350(13)	Yb(20)-O(90)	2.466(11)
Yb(16)-O(12)	2.408(12)	Yb(20)-O(93)	2.471(12)
Yb(16)-O(109)	2.415(11)	Yb(20)-O(89)	2.475(11)
Yb(16)-O(110)	2.422(11)	Yb(20)-O(91)	2.483(13)
Yb(16)-O(78)	2.425(14)	Yb(20)-O(92)	2.554(12)
Yb(16)-O(80)	2.471(14)	Yb(21)-O(84)	2.312(12)
Yb(16)-O(72)	2.481(12)	Yb(21)-O(90)	2.335(12)
Yb(16)-O(79)	2.491(13)	Yb(21)-O(112)	2.352(12)
Yb(16)-O(71)	2.520(12)	Yb(21)-O(16)#1	2.384(12)
Yb(17)-O(83)	2.351(11)	Yb(21)-O(20)#1	2.394(12)
Yb(17)-O(110)	2.404(12)	Yb(21)-O(104)	2.405(13)
Yb(17)-O(73)	2.407(11)	Yb(21)-O(100)#1	2.427(12)
Yb(17)-O(109)	2.417(10)	Yb(21)-O(13)	2.508(13)

Table S2. Selected Bond Lengths (Å) for **2**.

Sm(1)-O(99)	2.393(9)	Sm(7)-O(6)	2.360(12)
Sm(1)-O(2)	2.401(10)	Sm(7)-O(116)	2.382(14)
Sm(1)-O(100)	2.403(9)	Sm(7)-O(42)	2.394(13)
Sm(1)-O(23)	2.419(11)	Sm(7)-O(103)	2.399(9)
Sm(1)-O(17)	2.423(9)	Sm(7)-O(38)	2.425(11)
Sm(1)-O(11)	2.436(11)	Sm(7)-O(119)	2.437(10)
Sm(1)-O(18)	2.452(11)	Sm(7)-O(41)	2.455(13)
Sm(1)-O(15)	2.473(9)	Sm(7)-O(37)	2.482(15)
Sm(1)-O(16)	2.495(11)	Sm(7)-O(43)	2.493(12)
Sm(2)-O(25)	2.292(10)	Sm(8)-O(119)	2.340(10)
Sm(2)-O(99)	2.367(9)	Sm(8)-O(55)	2.356(10)
Sm(2)-O(100)	2.416(9)	Sm(8)-O(46)	2.455(11)
Sm(2)-O(21)	2.447(11)	Sm(8)-O(103)	2.458(10)
Sm(2)-O(115)	2.453(11)	Sm(8)-O(45)	2.468(11)
Sm(2)-O(24)	2.459(12)	Sm(8)-O(39)	2.496(10)
Sm(2)-O(19)	2.465(12)	Sm(8)-O(40)	2.496(11)
Sm(2)-O(20)	2.502(10)	Sm(8)-O(44)	2.499(13)
Sm(2)-O(23)	2.527(10)	Sm(8)-O(43)	2.552(10)
Sm(3)-O(98)#1	2.298(11)	Sm(9)-O(46)	2.270(11)
Sm(3)-O(99)	2.316(10)	Sm(9)-O(119)	2.297(10)
Sm(3)-O(21)	2.317(10)	Sm(9)-O(49)	2.343(12)
Sm(3)-O(27)	2.320(11)	Sm(9)-O(36)	2.353(11)
Sm(3)-O(95)	2.347(10)	Sm(9)-O(47)	2.361(11)
Sm(3)-O(11)	2.411(10)	Sm(9)-O(116)	2.403(12)
Sm(3)-O(101)	2.442(10)	Sm(9)-O(105)	2.471(9)
Sm(3)-O(1)	2.511(11)	Sm(9)-O(5)	2.489(12)
Sm(4)-O(102)	2.353(10)	Sm(10)-O(8)	2.361(11)
Sm(4)-O(4)	2.356(11)	Sm(10)-O(105)	2.368(10)
Sm(4)-O(22)	2.392(11)	Sm(10)-O(51)	2.389(9)
Sm(4)-O(33)	2.398(11)	Sm(10)-O(106)	2.392(10)
Sm(4)-O(101)	2.401(11)	Sm(10)-O(53)	2.417(11)
Sm(4)-O(32)	2.418(13)	Sm(10)-O(56)	2.429(10)
Sm(4)-O(96)	2.451(12)	Sm(10)-O(52)	2.448(11)
Sm(4)-O(31)	2.483(11)	Sm(10)-O(48)	2.471(9)
Sm(4)-O(95)	2.521(10)	Sm(10)-O(47)	2.525(11)
Sm(5)-O(35)	2.337(9)	Sm(11)-O(59)	2.332(10)
Sm(5)-O(102)	2.354(10)	Sm(11)-O(106)	2.348(10)
Sm(5)-O(30)	2.412(9)	Sm(11)-O(58)	2.416(10)
Sm(5)-O(101)	2.416(10)	Sm(11)-O(105)	2.420(10)
Sm(5)-O(34)	2.458(13)	Sm(11)-O(54)	2.433(10)
Sm(5)-O(28)	2.467(12)	Sm(11)-O(50)	2.434(11)
Sm(5)-O(27)	2.490(10)	Sm(11)-O(57)	2.470(11)
Sm(5)-O(29)	2.495(11)	Sm(11)-O(49)	2.487(10)
Sm(5)-O(33)	2.545(11)	Sm(11)-O(53)	2.528(10)
Sm(6)-O(26)	2.287(10)	Sm(12)-O(117)	2.299(11)
Sm(6)-O(30)	2.353(9)	Sm(12)-O(106)	2.349(11)
Sm(6)-O(39)	2.368(12)	Sm(12)-O(58)	2.357(11)
Sm(6)-O(102)	2.368(10)	Sm(12)-O(63)	2.357(10)
Sm(6)-O(37)	2.389(13)	Sm(12)-O(61)	2.361(9)
Sm(6)-O(103)	2.425(9)	Sm(12)-O(56)	2.390(10)
Sm(6)-O(22)	2.427(10)	Sm(12)-O(107)	2.440(10)
Sm(6)-O(3)	2.511(11)	Sm(12)-O(7)	2.542(11)

Sm(13)-O(10)	2.343(11)	Sm(17)-O(77)	2.457(11)
Sm(13)-O(114)	2.377(11)	Sm(17)-O(76)	2.463(10)
Sm(13)-O(107)	2.385(10)	Sm(17)-O(75)	2.466(11)
Sm(13)-O(108)	2.403(10)	Sm(17)-O(73)	2.484(9)
Sm(13)-O(69)	2.433(11)	Sm(17)-O(78)	2.624(10)
Sm(13)-O(68)	2.435(13)	Sm(18)-O(82)	2.273(10)
Sm(13)-O(64)	2.438(10)	Sm(18)-O(76)	2.338(10)
Sm(13)-O(70)	2.508(13)	Sm(18)-O(94)	2.346(11)
Sm(13)-O(63)	2.552(9)	Sm(18)-O(110)	2.355(10)
Sm(14)-O(81)	2.340(10)	Sm(18)-O(85)	2.371(10)
Sm(14)-O(108)	2.365(9)	Sm(18)-O(118)	2.392(9)
Sm(14)-O(107)	2.428(9)	Sm(18)-O(111)	2.395(9)
Sm(14)-O(62)	2.444(13)	Sm(18)-O(113)	2.521(11)
Sm(14)-O(65)	2.456(11)	Sm(19)-O(14)	2.367(11)
Sm(14)-O(66)	2.458(10)	Sm(19)-O(112)	2.381(9)
Sm(14)-O(67)	2.477(11)	Sm(19)-O(104)	2.383(10)
Sm(14)-O(61)	2.483(9)	Sm(19)-O(88)	2.384(12)
Sm(14)-O(68)	2.497(11)	Sm(19)-O(111)	2.396(9)
Sm(15)-O(60)	2.296(10)	Sm(19)-O(92)	2.403(13)
Sm(15)-O(73)	2.316(10)	Sm(19)-O(86)	2.405(10)
Sm(15)-O(108)	2.316(9)	Sm(19)-O(87)	2.503(11)
Sm(15)-O(66)	2.331(11)	Sm(19)-O(85)	2.531(9)
Sm(15)-O(71)	2.343(11)	Sm(20)-O(97)	2.340(9)
Sm(15)-O(114)	2.424(10)	Sm(20)-O(112)	2.394(9)
Sm(15)-O(109)	2.427(9)	Sm(20)-O(111)	2.410(11)
Sm(15)-O(9)	2.465(11)	Sm(20)-O(90)	2.455(10)
Sm(16)-O(118)	2.374(10)	Sm(20)-O(89)	2.463(9)
Sm(16)-O(109)	2.386(9)	Sm(20)-O(94)	2.470(10)
Sm(16)-O(12)	2.402(12)	Sm(20)-O(91)	2.471(11)
Sm(16)-O(78)	2.416(12)	Sm(20)-O(93)	2.479(12)
Sm(16)-O(72)	2.426(10)	Sm(20)-O(92)	2.505(11)
Sm(16)-O(79)	2.428(12)	Sm(21)-O(112)	2.300(9)
Sm(16)-O(80)	2.456(11)	Sm(21)-O(84)	2.306(9)
Sm(16)-O(110)	2.456(9)	Sm(21)-O(20)#1	2.336(10)
Sm(16)-O(71)	2.556(9)	Sm(21)-O(90)	2.374(10)
Sm(17)-O(110)	2.306(9)	Sm(21)-O(16)#1	2.385(10)
Sm(17)-O(83)	2.320(10)	Sm(21)-O(104)	2.407(10)
Sm(17)-O(109)	2.438(9)	Sm(21)-O(100)#1	2.447(10)
Sm(17)-O(74)	2.447(12)	Sm(21)-O(13)	2.483(10)