# Supporting Information

## Self-assembly of Luminescent 12-metal Zn-Ln Planar Nanoclusters with Sensing Properties towards Nitro Explosives

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### Contents

## 1. $^1$H NMR spectra of $H_2L$

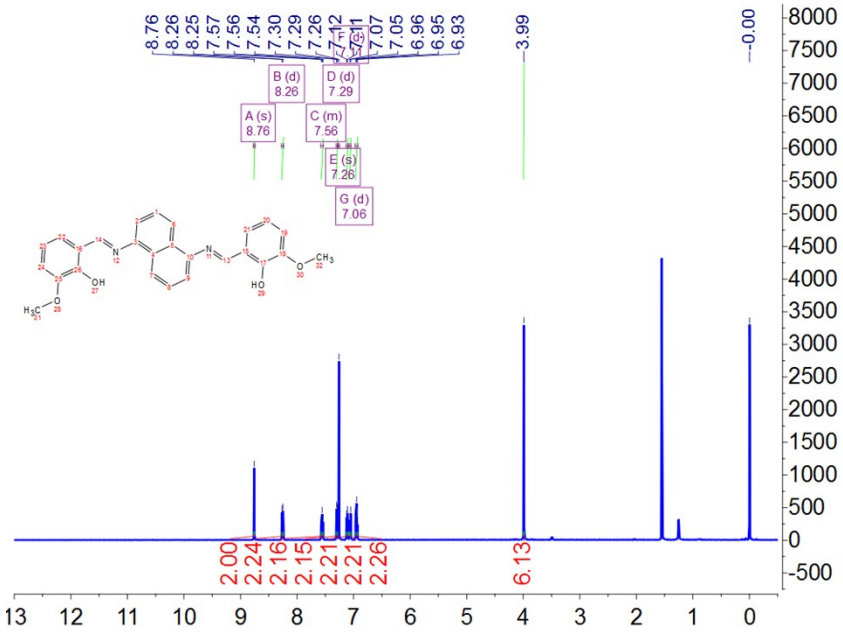



**Figure S1.** $^1$H NMR spectrum of $H_2L$ in $CDCl_3$.

## 2. IR spectra of $H_2L$ and clusters 1-3

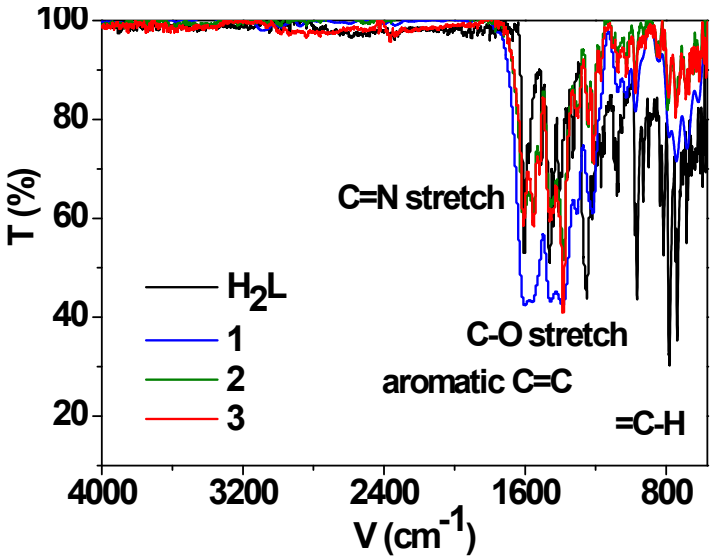



**Figure S2.** IR spectra of $H_2L$ and **1-3**.

## 3. Powder XRD patterns of 1-3

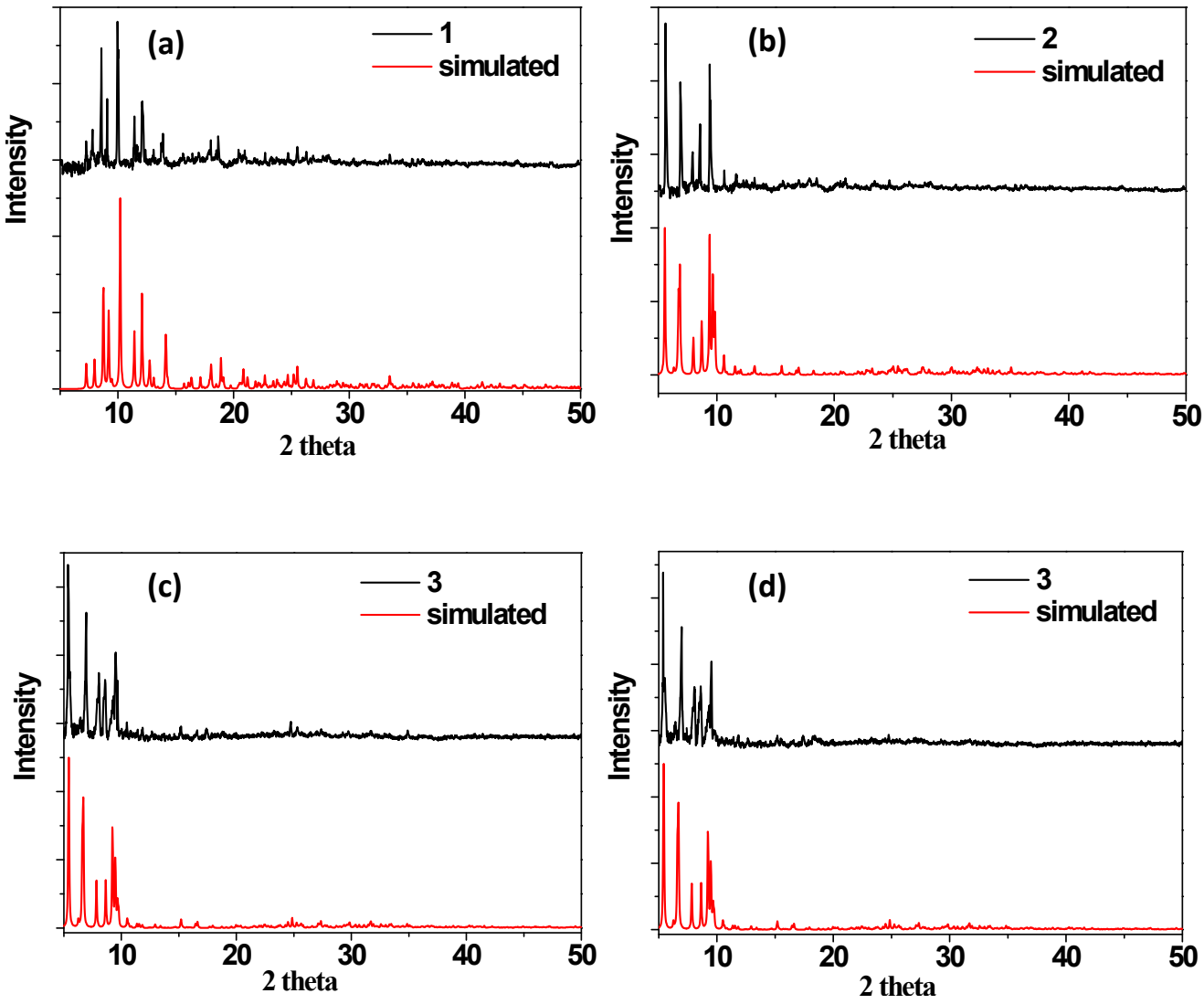
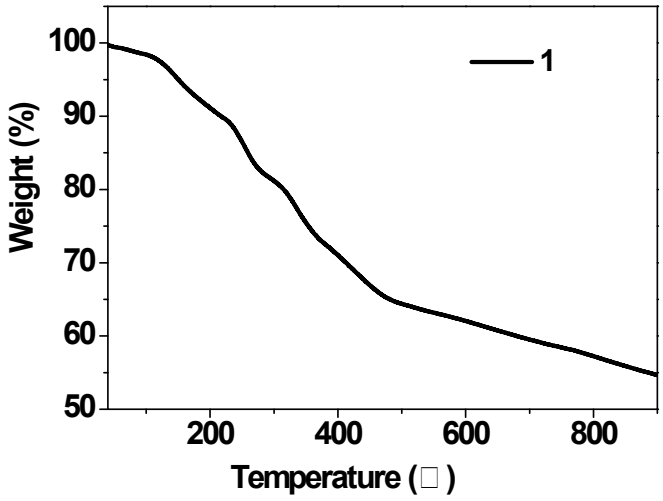
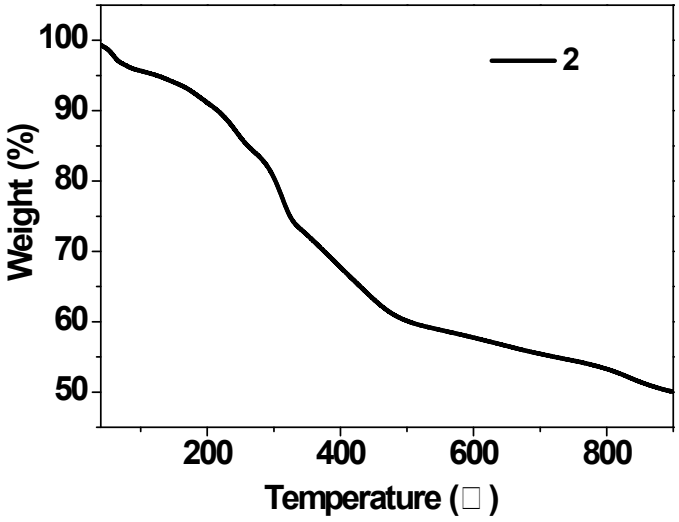



**Figure S3**. Powder XRD patterns of **1**-**3**: (a)-(c) are samples of **1**-**3** before treated with explosives, and (d) is the sample of **3** after treated with 1,4-DNB.

**4. The thermogravimetric analysis of 1-3**



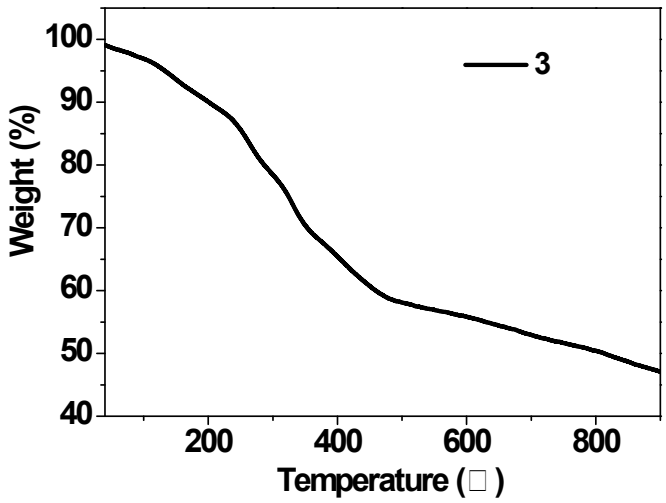



**Figure S4**. The thermogravimetric analysis of **1-3**.

## 5. The excitation and emission spectra of the free $H_2L$

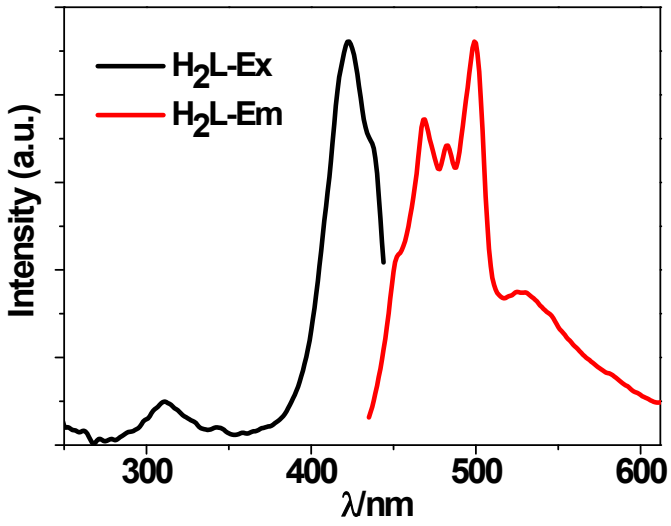
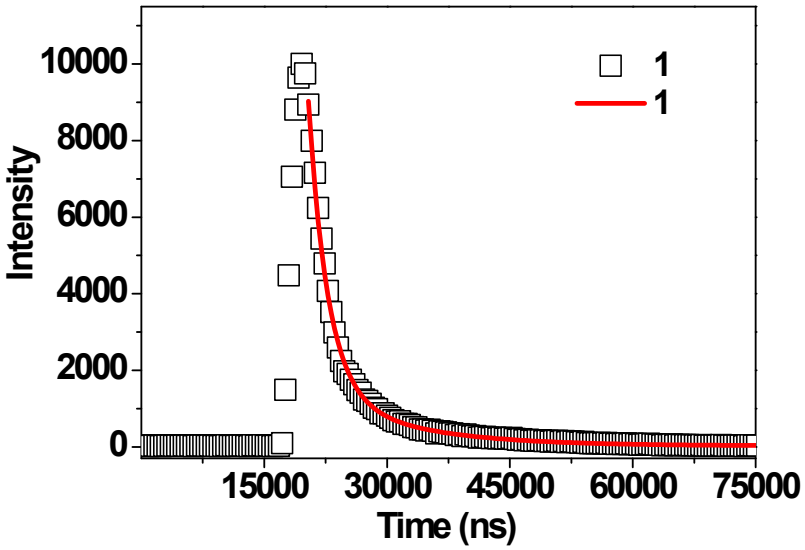
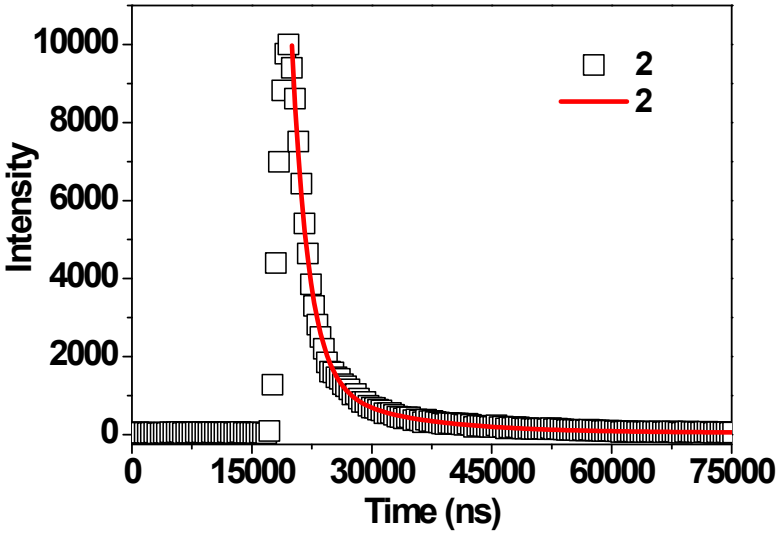



**Figure S5**. The excitation and emission spectra of the free $H_2L$ in DMF.

**6. The emission lifetimes of 1-3**



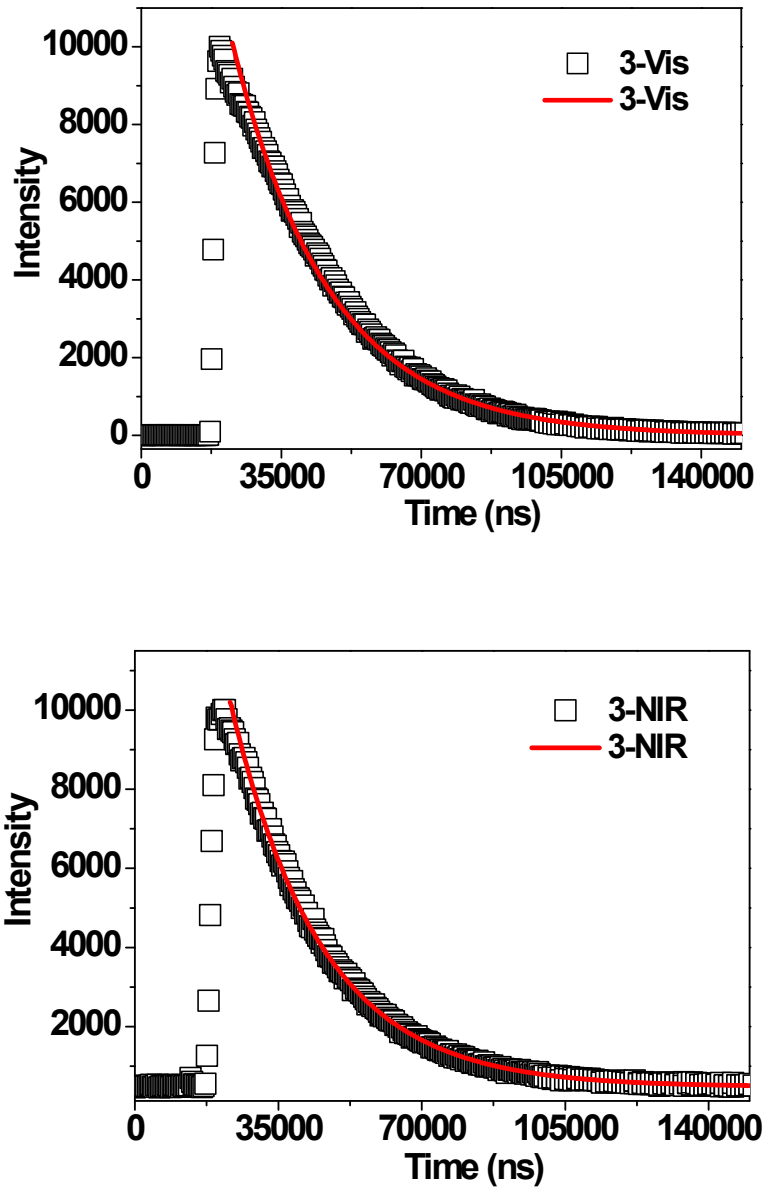
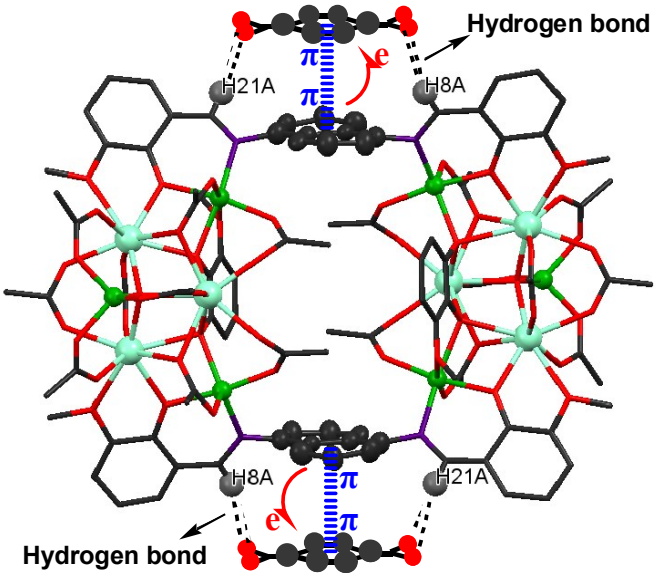
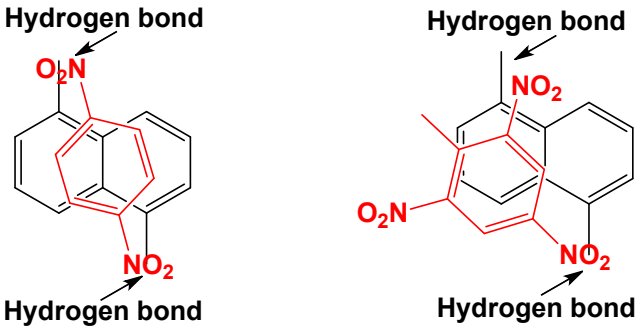



**Figure S6.** The visible and NIR emission lifetimes of **1**-**3** in DMF.

## 7. Interactions between the Schiff base ligands and guest molecules



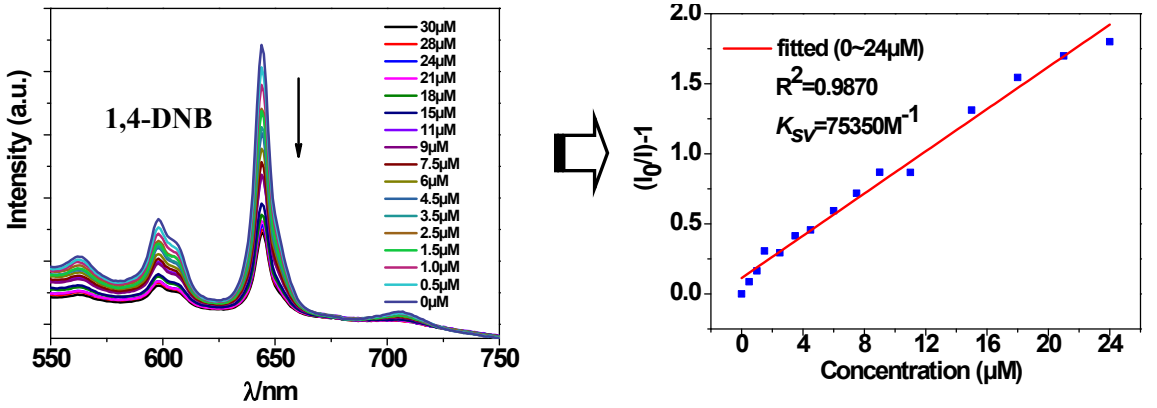

**(a)**

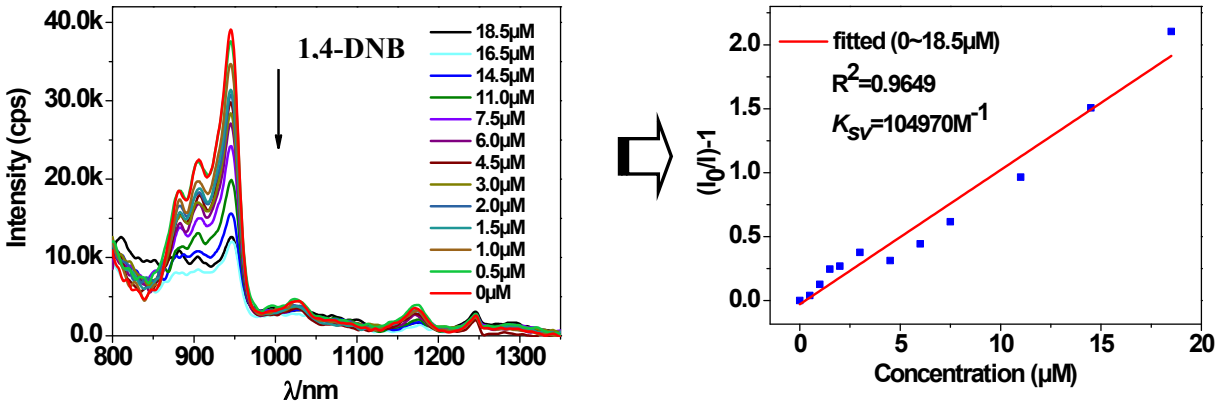


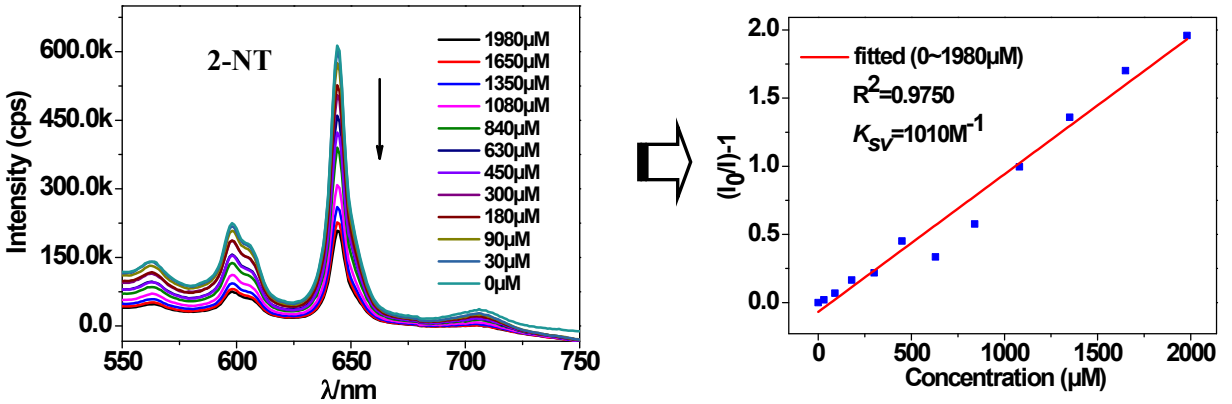

**(b)**

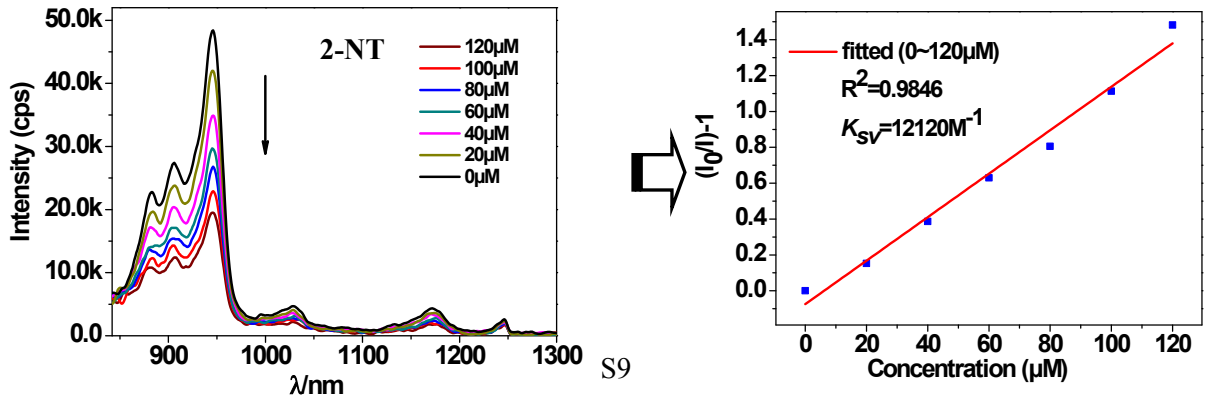
**Figure S7.** (a) π···π interactions and hydrogen bondings formed between the Schiff base ligands and guest molecules. (b) The overlapping manners of 1,4-DNB (left) and TNT (right) with the naphthyl ring of the Schiff base ligand.

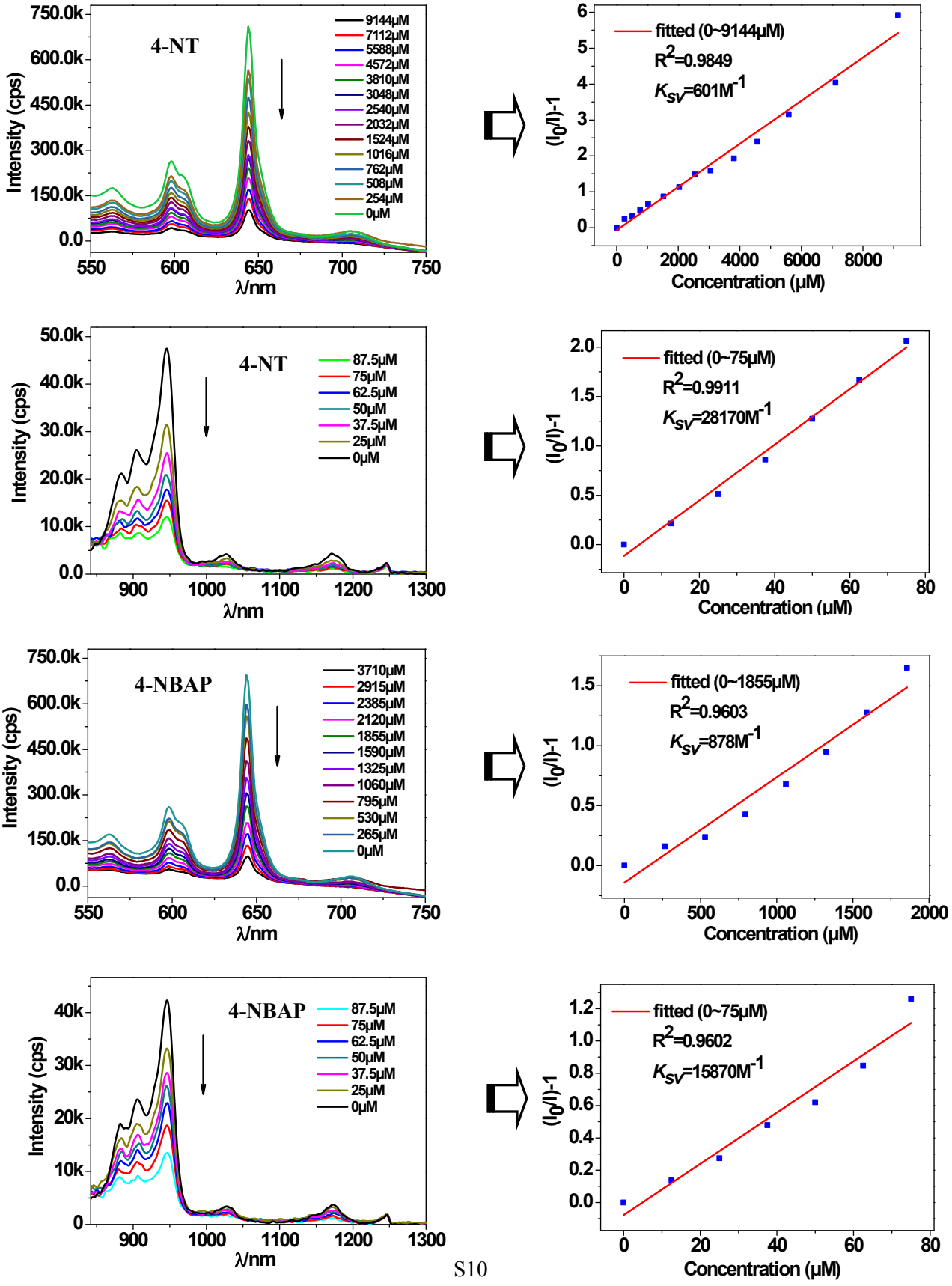
## 8. Luminescent sensing of 3 toward nitro explosives

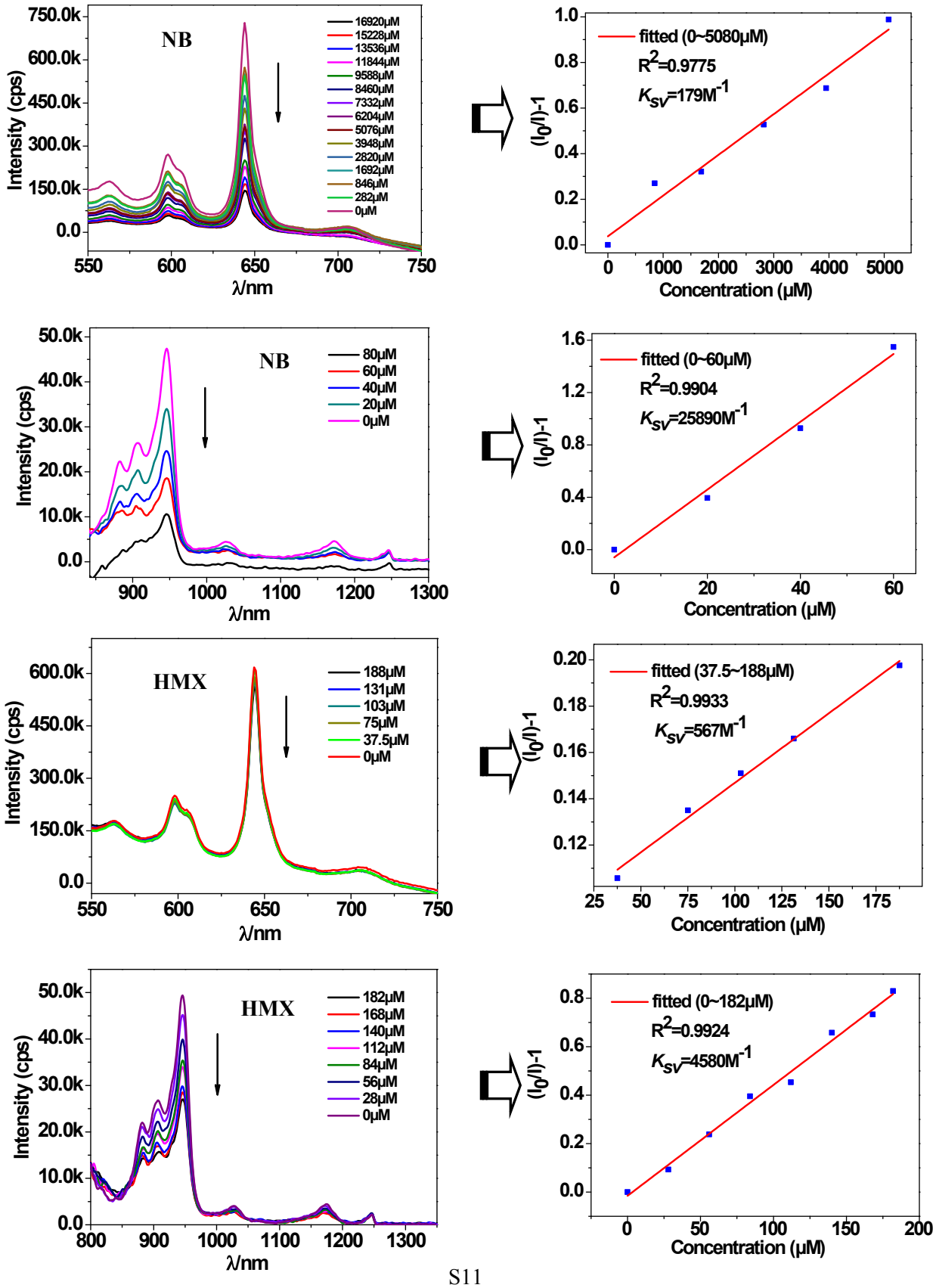



4-NT
Intensity (cps)
λ/nm
9144μM
7112μM
5588μM
4572μM
3810μM
3048μM
2540μM
2032μM
1524μM
1016μM
762μM
508μM
254μM
0μM
fitted (0~9144μM)
R2=0.9849
KSV=601M-1
(I0/I)-1
Concentration (μM)
4-NT
87.5μM
75μM
62.5μM
50μM
37.5μM
25μM
0μM
fitted (0~75μM)
R2=0.9911
KSV=28170M-1
4-NBAP
3710μM
2915μM
2385μM
2120μM
1855μM
1590μM
1325μM
1060μM
795μM
530μM
265μM
0μM
fitted (0~1855μM)
R2=0.9603
KSV=878M-1
4-NBAP
87.5μM
75μM
62.5μM
50μM
37.5μM
25μM
0μM
fitted (0~75μM)
R2=0.9602
KSV=15870M-1


NB
16920μM
15228μM
13536μM
11844μM
9588μM
8460μM
7332μM
6204μM
5076μM
3948μM
2820μM
1692μM
846μM
282μM
0μM
Intensity (cps)
λ/nm
fitted (0~5080μM)
R2=0.9775
KSV=179M-1
(I0/I)-1
Concentration (μM)
NB
80μM
60μM
40μM
20μM
0μM
Intensity (cps)
λ/nm
fitted (0~60μM)
R2=0.9904
KSV=25890M-1
(I0/I)-1
Concentration (μM)
HMX
188μM
131μM
103μM
75μM
37.5μM
0μM
Intensity (cps)
λ/nm
fitted (37.5~188μM)
R2=0.9933
KSV=567M-1
(I0/I)-1
Concentration (μM)
HMX
182μM
168μM
140μM
112μM
84μM
56μM
28μM
0μM
Intensity (cps)
λ/nm
fitted (0~182μM)
R2=0.9924
KSV=4580M-1
(I0/I)-1
Concentration (μM)

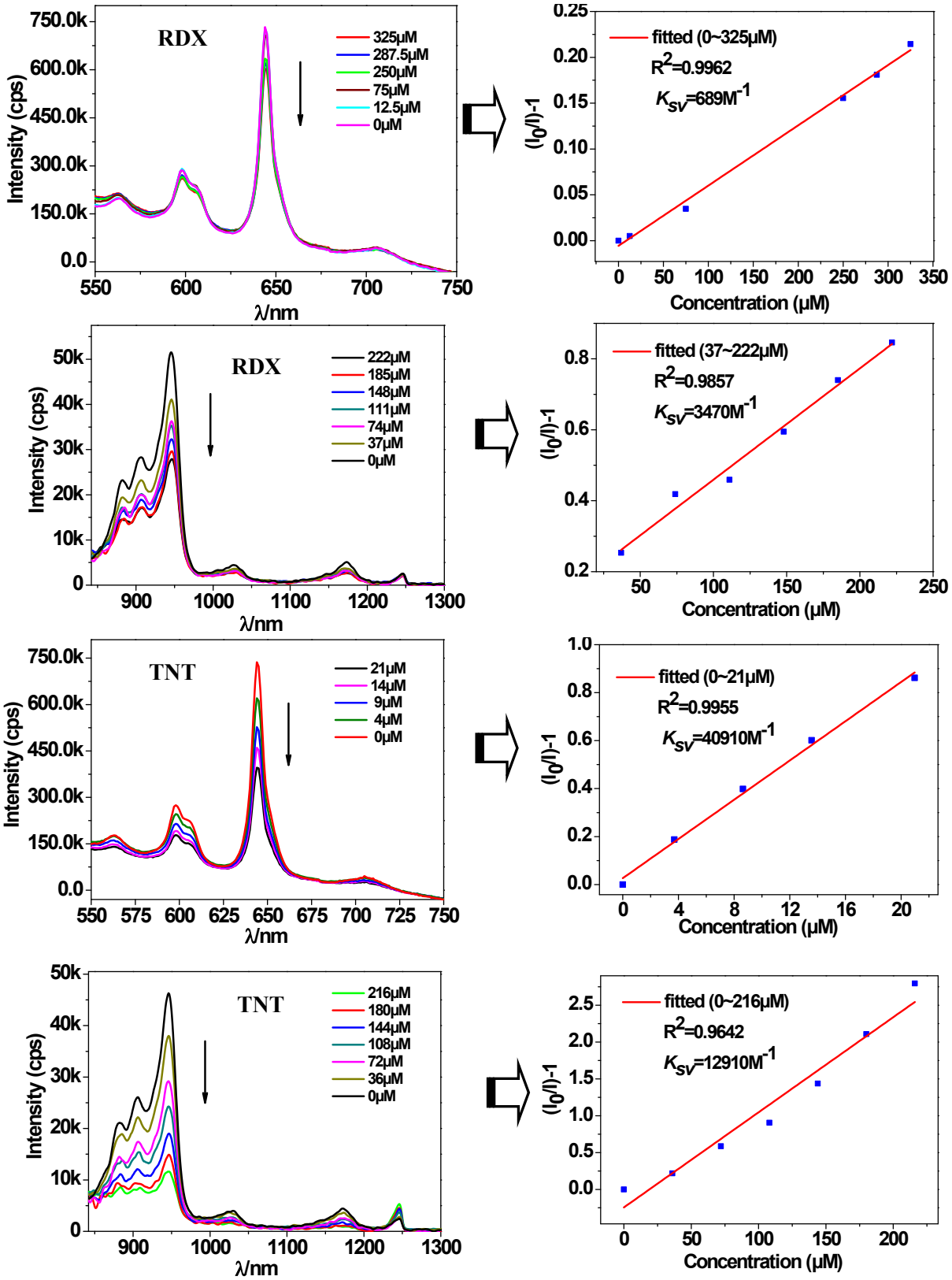



**Figure S8.** Visible and NIR luminescent sensing of **3** (15 μM) toward nitro explosives in DMF.

## 9. The NIR luminescence quenching efficiencies of 3 towards explosives

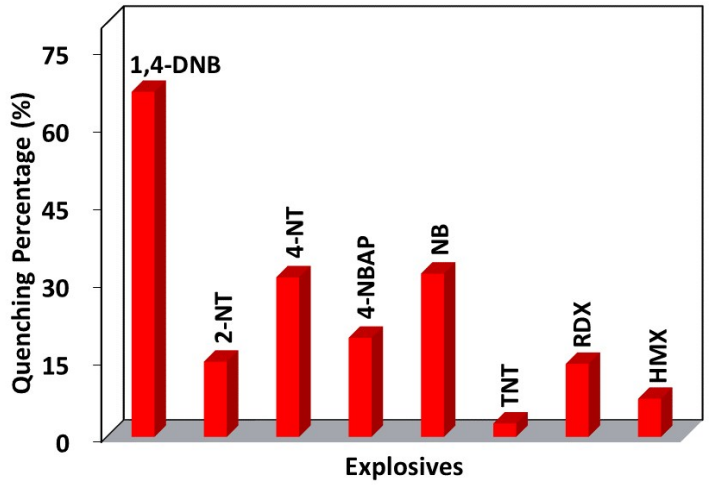
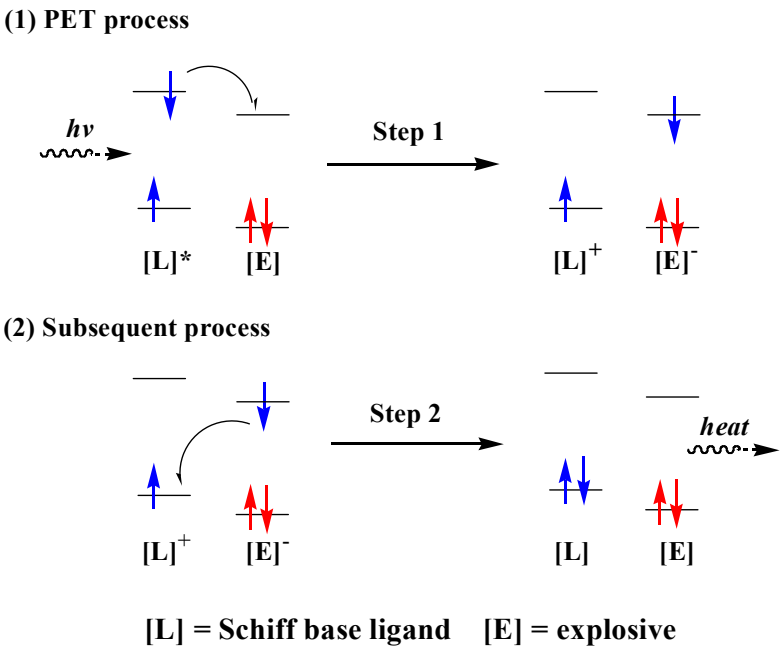



**Figure S9**. The NIR luminescence quenching efficiencies of **3** (15 μM) towards explosives (20 μM).

## 10. PET and subsequent processes.




**Scheme S1.** PET and subsequent processes.

## 11. UV-Vis spectra of 3 with the additional of 1,4-DNB

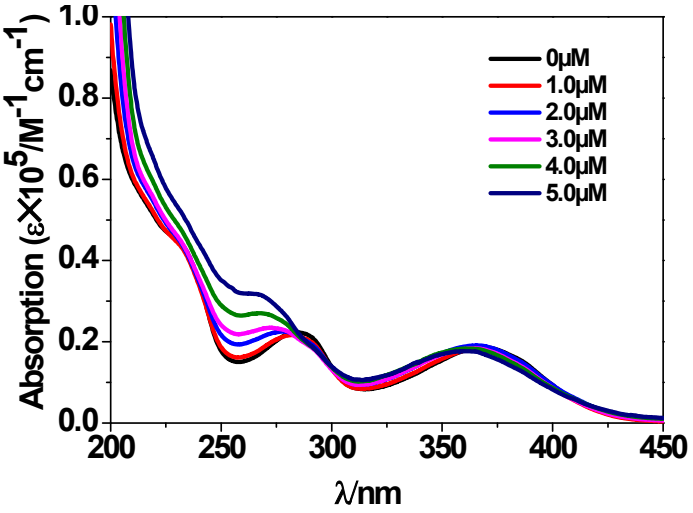



**Figure S10**. UV-Vis spectra of **3** with the additional of different concentrations of 1,4-DNB in DMF.

## 12. Excitation spectra of 3 with the additional of 1,4-DNB

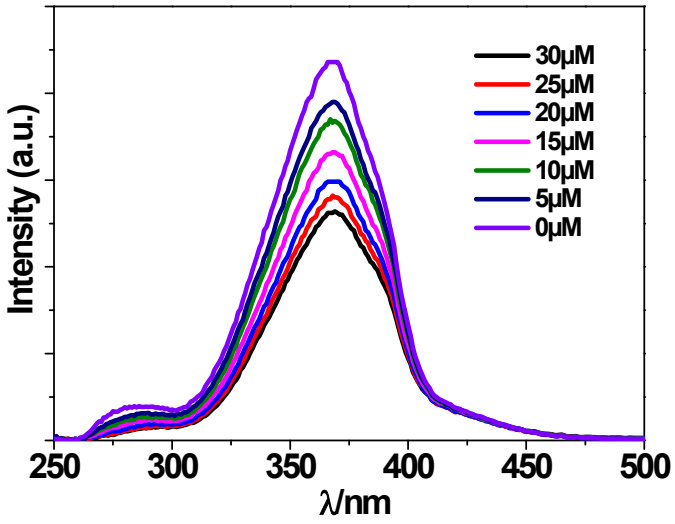



**Figure S11**. Excitation spectra of **3** ($\lambda_{em}$ = 645 nm) with the additional of different concentrations of 1,4-DNB in DMF.

## 13. X-Ray Crystallography

**Table S1**. Selected Bond Lengths (Å) and Angles (°) for **1**.

| | | | |
|---|---|---|---|
| Nd(1)-O(5) | 2.286(7) | O(5)-Nd(1)-O(10) | 75.7(3) |
| Nd(1)-O(6) | 2.285(8) | O(6)-Nd(1)-O(10) | 137.7(3) |
| Nd(1)-O(8) | 2.294(8) | O(8)-Nd(1)-O(10) | 71.2(3) |
| Nd(1)-O(3) | 2.304(8) | O(3)-Nd(1)-O(10) | 146.8(3) |
| Nd(1)-O(2)#1 | 2.310(8) | O(2)#1-Nd(1)-O(10) | 108.6(3) |
| Nd(1)-O(9) | 2.458(10) | O(9)-Nd(1)-O(10) | 52.3(3) |
| Nd(1)-O(10) | 2.480(8) | O(5)-Nd(1)-O(4) | 74.0(3) |
| Nd(1)-O(4) | 2.525(9) | O(6)-Nd(1)-O(4) | 79.0(3) |
| Nd(1)-O(1)#1 | 2.536(8) | O(8)-Nd(1)-O(4) | 109.5(3) |
| Nd(1)-N(3) | 2.860(13) | O(3)-Nd(1)-O(4) | 64.0(3) |
| Zn(1)-O(7) | 1.922(10) | O(2)#1-Nd(1)-O(4) | 131.4(3) |
| Zn(1)-O(2)#1 | 2.091(8) | O(9)-Nd(1)-O(4) | 69.2(3) |
| Zn(1)-N(2) | 2.130(3) | O(10)-Nd(1)-O(4) | 118.1(3) |
| Zn(1)-O(3) | 2.124(8) | O(5)-Nd(1)-O(1)#1 | 77.0(3) |
| Zn(1)-N(1)#1 | 2.196(7) | O(6)-Nd(1)-O(1)#1 | 78.3(3) |
| Zn(1)-O(1W) | 2.400(16) | O(8)-Nd(1)-O(1)#1 | 102.8(3) |
| O(5)-Nd(1)-O(6) | 72.8(3) | O(3)-Nd(1)-O(1)#1 | 130.6(3) |
| O(5)-Nd(1)-O(8) | 143.9(3) | O(2)#1-Nd(1)-O(1)#1 | 63.6(3) |
| O(6)-Nd(1)-O(8) | 143.2(3) | O(9)-Nd(1)-O(1)#1 | 118.7(3) |
| O(5)-Nd(1)-O(3) | 130.9(3) | O(10)-Nd(1)-O(1)#1 | 67.6(3) |
| O(6)-Nd(1)-O(3) | 75.1(3) | O(4)-Nd(1)-O(1)#1 | 147.3(3) |
| O(8)-Nd(1)-O(3) | 77.0(3) | O(5)-Nd(1)-N(3) | 75.4(3) |
| O(5)-Nd(1)-O(2)#1 | 133.3(3) | O(6)-Nd(1)-N(3) | 148.1(3) |
| O(6)-Nd(1)-O(2)#1 | 75.5(3) | O(8)-Nd(1)-N(3) | 68.5(3) |
| O(8)-Nd(1)-O(2)#1 | 72.5(3) | O(3)-Nd(1)-N(3) | 130.5(3) |
| O(3)-Nd(1)-O(2)#1 | 69.7(3) | O(2)#1-Nd(1)-N(3) | 127.1(3) |
| O(5)-Nd(1)-O(9) | 77.7(3) | O(9)-Nd(1)-N(3) | 27.5(4) |
| O(6)-Nd(1)-O(9) | 141.3(3) | O(10)-Nd(1)-N(3) | 24.7(3) |
| O(8)-Nd(1)-O(9) | 70.8(3) | O(4)-Nd(1)-N(3) | 95.1(3) |
| O(3)-Nd(1)-O(9) | 108.0(3) | O(1)#1-Nd(1)-N(3) | 91.9(3) |
| O(2)#1-Nd(1)-O(9) | 142.7(3) | | |

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

| | | | |
|---|---|---|---|
| Nd(1)-O(31) | 2.219(10) | O(16)-Nd(1)-O(22) | 134.8(4) |
| Nd(1)-O(14) | 2.276(12) | O(3)-Nd(1)-O(22) | 70.5(4) |
| Nd(1)-O(12) | 2.283(11) | O(31)-Nd(1)-O(19) | 68.0(4) |
| Nd(1)-O(16) | 2.299(14) | O(14)-Nd(1)-O(19) | 139.4(4) |
| Nd(1)-O(3) | 2.301(10) | O(12)-Nd(1)-O(19) | 131.5(4) |
| Nd(1)-O(22) | 2.406(9) | O(16)-Nd(1)-O(19) | 71.4(4) |
| Nd(1)-O(19) | 2.468(11) | O(3)-Nd(1)-O(19) | 82.3(4) |
| Nd(1)-O(4) | 2.603(12) | O(22)-Nd(1)-O(19) | 64.4(3) |
| Nd(2)-O(30) | 2.232(11) | O(31)-Nd(1)-O(4) | 153.3(3) |
| Nd(2)-O(17) | 2.260(12) | O(14)-Nd(1)-O(4) | 87.7(4) |
| Nd(2)-O(31) | 2.292(8) | O(12)-Nd(1)-O(4) | 74.4(4) |
| Nd(2)-O(6) | 2.322(11) | O(16)-Nd(1)-O(4) | 68.6(4) |
| Nd(2)-O(21) | 2.336(11) | O(3)-Nd(1)-O(4) | 62.9(3) |
| Nd(2)-O(19) | 2.374(12) | O(22)-Nd(1)-O(4) | 130.1(4) |
| Nd(2)-O(22) | 2.421(11) | O(19)-Nd(1)-O(4) | 122.6(4) |
| Nd(2)-O(8) | 2.471(11) | O(30)-Nd(2)-O(17) | 97.9(4) |
| Nd(3)-O(31) | 2.216(10) | O(30)-Nd(2)-O(31) | 94.1(4) |
| Nd(3)-O(13) | 2.245(12) | O(17)-Nd(2)-O(31) | 144.3(4) |
| Nd(3)-O(2) | 2.272(12) | O(30)-Nd(2)-O(6) | 79.4(4) |
| Nd(3)-O(11) | 2.293(10) | O(17)-Nd(2)-O(6) | 74.4(4) |
| Nd(3)-O(9) | 2.309(13) | O(31)-Nd(2)-O(6) | 141.1(4) |
| Nd(3)-O(8) | 2.405(11) | O(30)-Nd(2)-O(21) | 143.7(4) |
| Nd(3)-O(21) | 2.522(10) | O(17)-Nd(2)-O(21) | 109.3(4) |
| Nd(3)-O(1) | 2.541(11) | O(31)-Nd(2)-O(21) | 77.9(3) |
| Zn(1)-O(18) | 1.991(9) | O(6)-Nd(2)-O(21) | 85.0(4) |
| Zn(1)-O(3) | 2.049(10) | O(30)-Nd(2)-O(19) | 77.8(4) |
| Zn(1)-O(20) | 2.066(12) | O(17)-Nd(2)-O(19) | 81.3(4) |
| Zn(1)-N(2) | 2.114(13) | O(31)-Nd(2)-O(19) | 68.6(4) |
| Zn(1)-O(22) | 2.167(12) | O(6)-Nd(2)-O(19) | 143.8(4) |
| Zn(1)-O(23) | 2.387(12) | O(21)-Nd(2)-O(19) | 128.8(4) |
| Zn(2)-O(31) | 1.934(9) | O(30)-Nd(2)-O(22) | 143.4(4) |
| Zn(2)-O(29) | 1.939(14) | O(17)-Nd(2)-O(22) | 75.6(4) |
| Zn(2)-O(15) | 1.952(14) | O(31)-Nd(2)-O(22) | 74.7(3) |
| Zn(2)-O(10) | 1.982(17) | O(6)-Nd(2)-O(22) | 130.6(4) |
| Zn(3)-O(7) | 2.009(11) | O(21)-Nd(2)-O(22) | 69.1(4) |
| Zn(3)-O(5) | 2.026(10) | O(19)-Nd(2)-O(22) | 65.6(4) |
| Zn(3)-N(1) | 2.079(12) | O(30)-Nd(2)-O(8) | 79.5(4) |
| Zn(3)-O(2) | 2.080(10) | O(17)-Nd(2)-O(8) | 148.2(4) |
| Zn(3)-O(21) | 2.096(11) | O(31)-Nd(2)-O(8) | 67.2(4) |
| O(31)-Nd(1)-O(14) | 97.6(4) | O(6)-Nd(2)-O(8) | 73.9(4) |
| O(31)-Nd(1)-O(12) | 81.0(4) | O(21)-Nd(2)-O(8) | 64.7(4) |
| O(14)-Nd(1)-O(12) | 78.9(4) | O(19)-Nd(2)-O(8) | 128.0(4) |
| O(31)-Nd(1)-O(16) | 95.8(4) | O(22)-Nd(2)-O(8) | 124.5(4) |
| O(14)-Nd(1)-O(16) | 149.2(4) | O(31)-Nd(3)-O(13) | 98.1(4) |
| O(12)-Nd(1)-O(16) | 76.0(5) | O(31)-Nd(3)-O(2) | 138.9(3) |
| O(31)-Nd(1)-O(3) | 142.7(3) | O(13)-Nd(3)-O(2) | 89.1(4) |
| O(14)-Nd(1)-O(3) | 90.4(4) | O(31)-Nd(3)-O(11) | 82.1(3) |
| O(12)-Nd(1)-O(3) | 136.3(4) | O(13)-Nd(3)-O(11) | 77.0(4) |
| O(16)-Nd(1)-O(3) | 95.5(4) | O(2)-Nd(3)-O(11) | 138.7(4) |
| O(31)-Nd(1)-O(22) | 76.4(3) | O(31)-Nd(3)-O(9) | 96.5(4) |
| O(14)-Nd(1)-O(22) | 75.5(4) | O(13)-Nd(3)-O(9) | 146.4(4) |
| O(12)-Nd(1)-O(22) | 142.9(4) | O(2)-Nd(3)-O(9) | 99.4(4) |

| | | | |
|---|---|---|---|
| O(11)-Nd(3)-O(9) | 75.3(4) | O(9)-Nd(3)-O(21) | 135.7(4) |
| O(31)-Nd(3)-O(8) | 69.6(4) | O(8)-Nd(3)-O(21) | 62.9(3) |
| O(13)-Nd(3)-O(8) | 140.2(4) | O(31)-Nd(3)-O(1) | 157.2(3) |
| O(2)-Nd(3)-O(8) | 79.1(4) | O(13)-Nd(3)-O(1) | 83.6(4) |
| O(11)-Nd(3)-O(8) | 134.4(4) | O(2)-Nd(3)-O(1) | 63.7(4) |
| O(9)-Nd(3)-O(8) | 73.3(4) | O(11)-Nd(3)-O(1) | 76.1(4) |
| O(31)-Nd(3)-O(21) | 75.5(3) | O(9)-Nd(3)-O(1) | 71.6(4) |
| O(13)-Nd(3)-O(21) | 77.4(4) | O(8)-Nd(3)-O(1) | 122.5(4) |
| O(2)-Nd(3)-O(21) | 66.7(4) | O(21)-Nd(3)-O(1) | 126.7(4) |
| O(11)-Nd(3)-O(21) | 142.9(4) | | |

**Table S3**. Selected Bond Lengths (Å) and Angles (°) for **3**.

| | | | |
|---|---|---|---|
| Sm(1)-O(31) | 2.299(11) | O(3)-Sm(1)-O(22) | 69.6(4) |
| Sm(1)-O(12) | 2.356(15) | O(14)-Sm(1)-O(22) | 75.9(5) |
| Sm(1)-O(16) | 2.361(15) | O(31)-Sm(1)-O(19) | 66.7(4) |
| Sm(1)-O(3) | 2.367(12) | O(12)-Sm(1)-O(19) | 133.3(5) |
| Sm(1)-O(14) | 2.379(19) | O(16)-Sm(1)-O(19) | 72.6(5) |
| Sm(1)-O(22) | 2.483(12) | O(3)-Sm(1)-O(19) | 81.2(4) |
| Sm(1)-O(19) | 2.541(13) | O(14)-Sm(1)-O(19) | 141.1(5) |
| Sm(1)-O(4) | 2.639(11) | O(22)-Sm(1)-O(19) | 65.3(4) |
| Sm(2)-O(17) | 2.322(15) | O(31)-Sm(1)-O(4) | 156.3(4) |
| Sm(2)-O(31) | 2.356(12) | O(12)-Sm(1)-O(4) | 78.8(5) |
| Sm(2)-O(6) | 2.363(12) | O(16)-Sm(1)-O(4) | 70.8(5) |
| Sm(2)-O(30) | 2.368(14) | O(3)-Sm(1)-O(4) | 60.6(4) |
| Sm(2)-O(19) | 2.436(12) | O(14)-Sm(1)-O(4) | 85.1(6) |
| Sm(2)-O(21) | 2.457(12) | O(22)-Sm(1)-O(4) | 127.0(4) |
| Sm(2)-O(8) | 2.505(12) | O(19)-Sm(1)-O(4) | 120.0(4) |
| Sm(2)-O(22) | 2.516(12) | O(17)-Sm(2)-O(31) | 143.5(4) |
| Sm(3)-O(31) | 2.282(12) | O(17)-Sm(2)-O(6) | 76.6(5) |
| Sm(3)-O(13) | 2.322(18) | O(31)-Sm(2)-O(6) | 139.7(4) |
| Sm(3)-O(9) | 2.359(17) | O(17)-Sm(2)-O(30) | 96.8(5) |
| Sm(3)-O(11) | 2.368(15) | O(31)-Sm(2)-O(30) | 91.8(4) |
| Sm(3)-O(2) | 2.387(12) | O(6)-Sm(2)-O(30) | 84.8(5) |
| Sm(3)-O(1) | 2.546(16) | O(17)-Sm(2)-O(19) | 79.8(5) |
| Sm(3)-O(8) | 2.553(12) | O(31)-Sm(2)-O(19) | 67.6(4) |
| Sm(3)-O(21) | 2.582(12) | O(6)-Sm(2)-O(19) | 148.2(5) |
| Zn(1)-O(18) | 1.977(13) | O(30)-Sm(2)-O(19) | 76.9(5) |
| Zn(1)-O(3) | 2.054(12) | O(17)-Sm(2)-O(21) | 111.1(5) |
| Zn(1)-O(20) | 2.073(16) | O(31)-Sm(2)-O(21) | 77.5(4) |
| Zn(1)-N(2) | 2.113(15) | O(6)-Sm(2)-O(21) | 83.1(4) |
| Zn(1)-O(22) | 2.199(12) | O(30)-Sm(2)-O(21) | 145.9(5) |
| Zn(1)-O(23) | 2.336(15) | O(19)-Sm(2)-O(21) | 125.8(4) |
| Zn(2)-O(15) | 1.895(19) | O(17)-Sm(2)-O(8) | 148.7(4) |
| Zn(2)-O(29) | 1.930(19) | O(31)-Sm(2)-O(8) | 67.7(4) |
| Zn(2)-O(31) | 1.938(12) | O(6)-Sm(2)-O(8) | 72.1(4) |
| Zn(2)-O(10) | 1.999(17) | O(30)-Sm(2)-O(8) | 80.3(5) |
| Zn(3)-O(5) | 1.991(13) | O(19)-Sm(2)-O(8) | 128.6(4) |
| Zn(3)-O(7) | 2.023(13) | O(21)-Sm(2)-O(8) | 65.7(4) |
| Zn(3)-O(2) | 2.072(14) | O(17)-Sm(2)-O(22) | 77.0(4) |
| Zn(3)-N(1) | 2.084(15) | O(31)-Sm(2)-O(22) | 75.1(4) |
| Zn(3)-O(21) | 2.139(11) | O(6)-Sm(2)-O(22) | 127.2(4) |
| O(31)-Sm(1)-O(12) | 81.3(5) | O(30)-Sm(2)-O(22) | 143.2(5) |
| O(31)-Sm(1)-O(16) | 91.8(5) | O(19)-Sm(2)-O(22) | 66.3(4) |
| O(12)-Sm(1)-O(16) | 75.5(5) | O(21)-Sm(2)-O(22) | 65.4(4) |
| O(31)-Sm(1)-O(3) | 140.9(4) | O(8)-Sm(2)-O(22) | 123.1(4) |
| O(12)-Sm(1)-O(3) | 137.7(4) | O(31)-Sm(3)-O(13) | 99.8(7) |
| O(16)-Sm(1)-O(3) | 99.6(5) | O(31)-Sm(3)-O(9) | 92.1(5) |
| O(31)-Sm(1)-O(14) | 102.9(6) | O(13)-Sm(3)-O(9) | 147.4(6) |
| O(12)-Sm(1)-O(14) | 77.0(6) | O(31)-Sm(3)-O(11) | 82.6(5) |
| O(16)-Sm(1)-O(14) | 146.3(6) | O(13)-Sm(3)-O(11) | 78.5(6) |
| O(3)-Sm(1)-O(14) | 87.9(6) | O(9)-Sm(3)-O(11) | 73.1(5) |
| O(31)-Sm(1)-O(22) | 76.7(4) | O(31)-Sm(3)-O(2) | 138.1(5) |
| O(12)-Sm(1)-O(22) | 140.0(4) | O(13)-Sm(3)-O(2) | 89.9(6) |
| O(16)-Sm(1)-O(22) | 137.5(5) | O(9)-Sm(3)-O(2) | 101.2(5) |

| | | | |
|---|---|---|---|
| O(11)-Sm(3)-O(2) | 139.2(5) | O(2)-Sm(3)-O(8) | 78.1(4) |
| O(31)-Sm(3)-O(1) | 159.1(4) | O(1)-Sm(3)-O(8) | 119.9(4) |
| O(13)-Sm(3)-O(1) | 85.7(7) | O(31)-Sm(3)-O(21) | 76.3(4) |
| O(9)-Sm(3)-O(1) | 73.5(5) | O(13)-Sm(3)-O(21) | 76.2(5) |
| O(11)-Sm(3)-O(1) | 78.8(5) | O(9)-Sm(3)-O(21) | 136.4(5) |
| O(2)-Sm(3)-O(1) | 61.3(5) | O(11)-Sm(3)-O(21) | 143.4(5) |
| O(31)-Sm(3)-O(8) | 68.0(4) | O(2)-Sm(3)-O(21) | 66.6(4) |
| O(13)-Sm(3)-O(8) | 139.2(6) | O(1)-Sm(3)-O(21) | 124.5(4) |
| O(9)-Sm(3)-O(8) | 73.4(5) | O(8)-Sm(3)-O(21) | 63.2(4) |
| O(11)-Sm(3)-O(8) | 133.9(5) | | |