Supporting Information

Rapid and reliable triple-emissive detection of 2,6-dichloro-4-nitroaniline as a pesticide based on a high-nuclear Cd(II)-Sm(III) nanocluster

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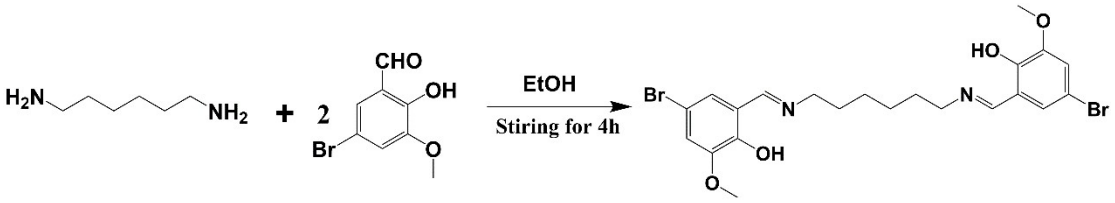
Contents

1. General Procedures

All chemical materials and solvents were purchased from commercial sources. The synthesis of lanthanide complex was carried out using Schlenk techniques. Powder XRD spectra were obtained using a D8 Advance; IR spectra were determined on a FTIR-650 spectrometer; Elemental analysis was performed on a EURO EA3000 with the solid sample after dried in the oven at 110°C for six hours; The thermogravimetric analyses were carried out on a Perking Elmer Diamond TG-DTA spectrum GX. The sample is under a N_2 flow of 200 mL min^{-1}, and heated from room temperature to 800 °C with a heating rate of 5°C min^{-1}; Dynamic light scattering (DLS) measurement was carried out on a Malvern Zetasizer Nano ZS using a solution of the nanocluster in EtOH (C = 10^{-5} M). The morphology of the sample was analyzed by Nova NanoSEM 200 scanning electron microscope (SEM) and an attached energy-dispersive X-ray spectrometer (EDX). The sample was installed on an aluminum sheet coated with Au.

Photophysical Studies. Absorption spectra were obtained on a UV-3600 spectrophotometer. Emission spectra were recorded on a FLS 980 fluorimeter. The light source for the spectra was a 450 W xenon arc lamp with continuous spectral distribution from 190 to 2600 nm. The temporal decay curves of the fluorescence signals were stored by using the attached storage digital oscilloscope. Systematic errors have been deducted through the standard instrument corrections. All the measurements were carried out at room temperature.

2. Synthesis of the ligand H_2L



Scheme S1. Synthetic approach to H_2L.

Synthesis of H_2L: 5-Bromo-2-hydroxy-3-methoxybenzaldehyde (6.0 mmol, 1.39 g) was dissolved in 10 mL of EtOH. The solution was heated to reflux, and 1,6-hexamethylenediamine (3.0 mmol, 0.35 g) in 20 mL of EtOH was added drop by drop with stirring. The mixture was heated to reflux for 4 hours with stirring, and then left to cool to give yellow solid precipitate. The solid was filtered, and then washed with 5 mL of ethanol for three times. Yield: 1.36 g (83%). ^{1}H NMR (500 MHz, DMSO) δ 14.07 (s, 2H), 8.48 (s, 2H), 7.18 (s, 2H), 7.06 (s, 2H), 3.77 (s, 6H), 3.58 (t, J = 6.5 Hz, 4H), 1.63 (s, 4H), 1.37 (s, 4H).

3. ^{1}H NMR spectra of the ligand H_2L

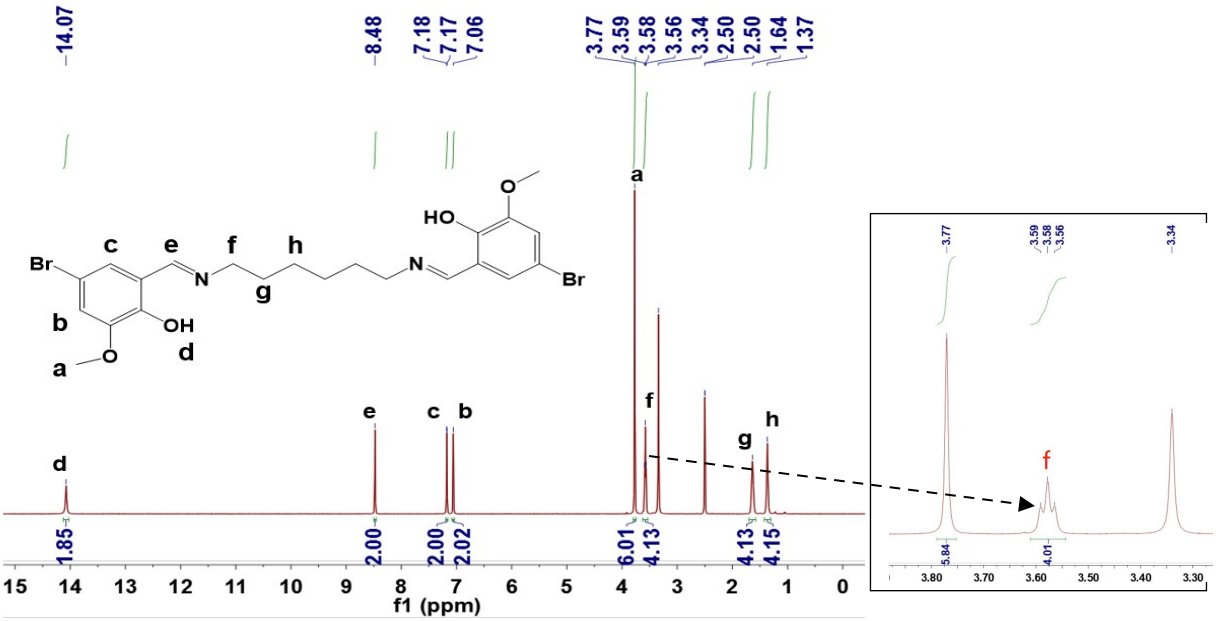


Figure S1. ^{1}H NMR of the ligand H_2L in DMSO.
(Right: an enlarged view of the triplet peak of the f proton)

4. IR spectra of the ligand H_2L and 1

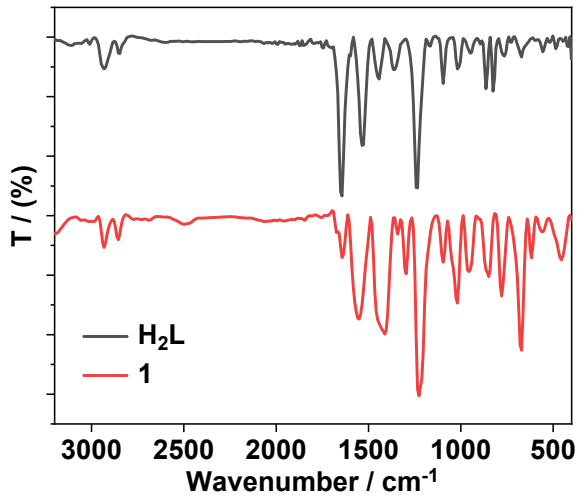


Figure S2. IR spectra of the ligand H_2L and **1**.

5. The coordination mode of the Schiff base ligand with metal ions in 1

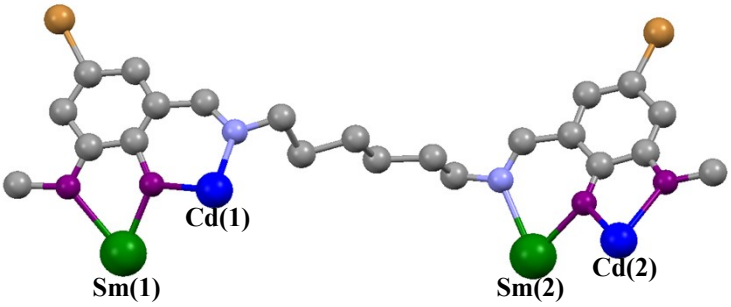


Figure S d with metal ions

6. The thermogravimetric analysis of 1

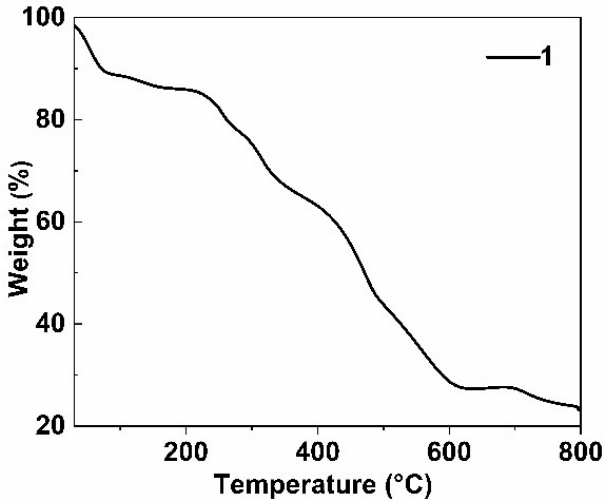


Figure S4. The thermogravimetric analysis of **1**.

7. UV-vis absorption spectra of the ligand $H_2L$and 1

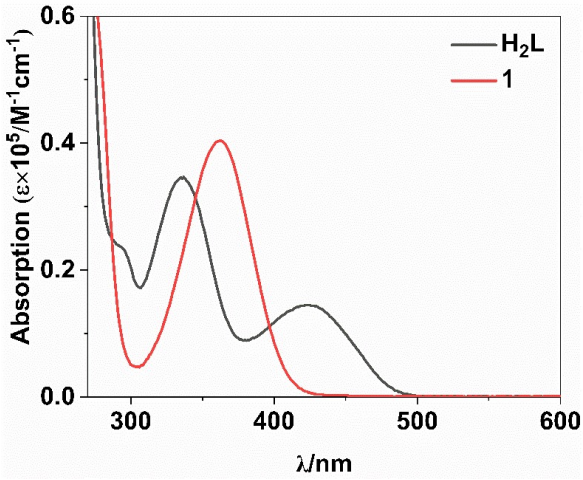


Figure S5. UV-vis absorption spectra of the ligand H_2L and **1** in CH_3CN.

8. The excitation and emission spectra of H_2L and 1

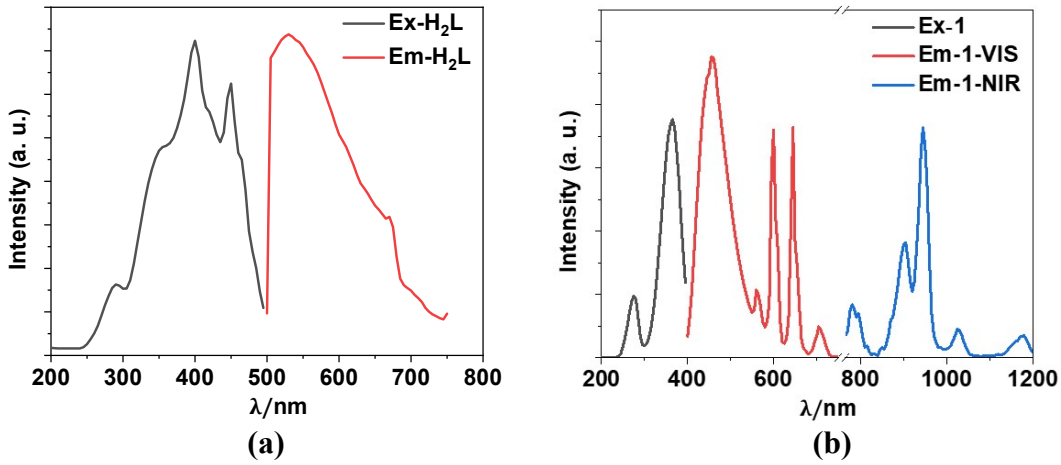
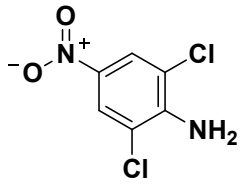
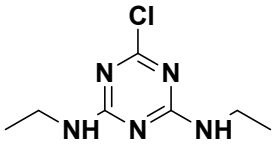


Figure S6. (a) The excitation (λ_{em} = 505 nm) and emission (λ_{ex} = 400 nm) spectra of **H_2L** in CH_3CN. (b) The excitation (λ_{em} = 645 nm) and emission (λ_{ex} = 365 nm) spectra of **1** (10 μM) in CH_3CN.

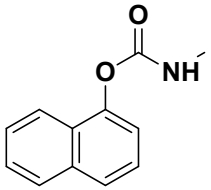
9. Chemical structures of pesticides



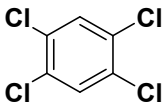
2,6-dichloro-4-nitroaniline (**DCN**)



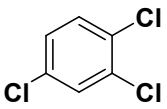
Atrazine



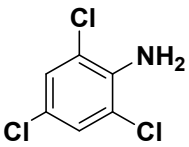
Carbaryl



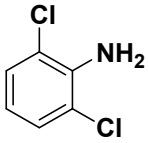
1,2,4,5-tetrachlorobenzene (**TetraCB**)



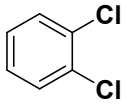
1,2,4-trichlorobenzene (**TriCB**)



2,4,6-trichloroaniline (**TCA**)



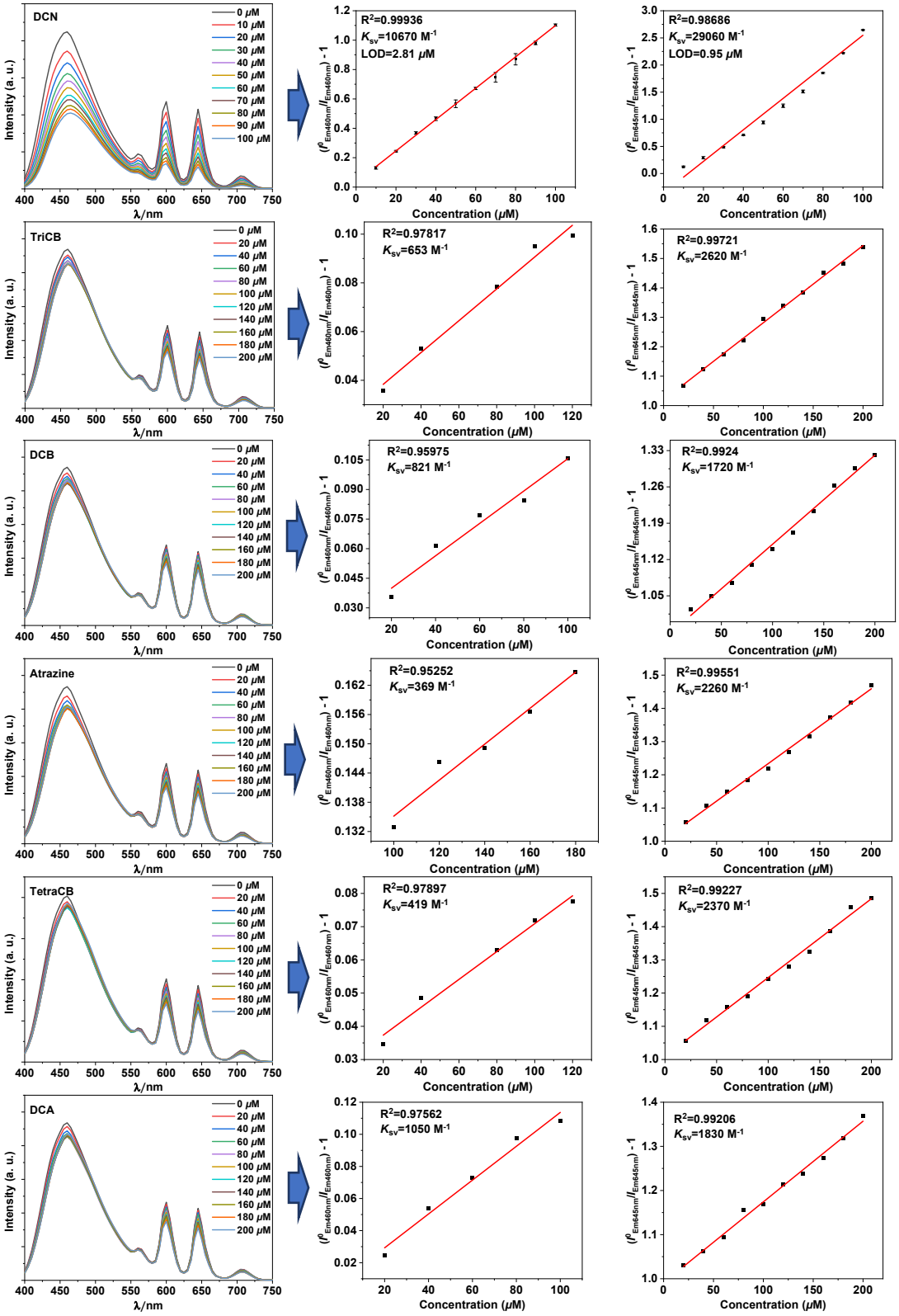
2,6-dichloroaniline (**DCA**)



1,2-dichlorobenzene (**DCB**)

Scheme S2. Chemical structures of DCN and other pesticides.

10. The visible fluorescence response of 1 to pesticides



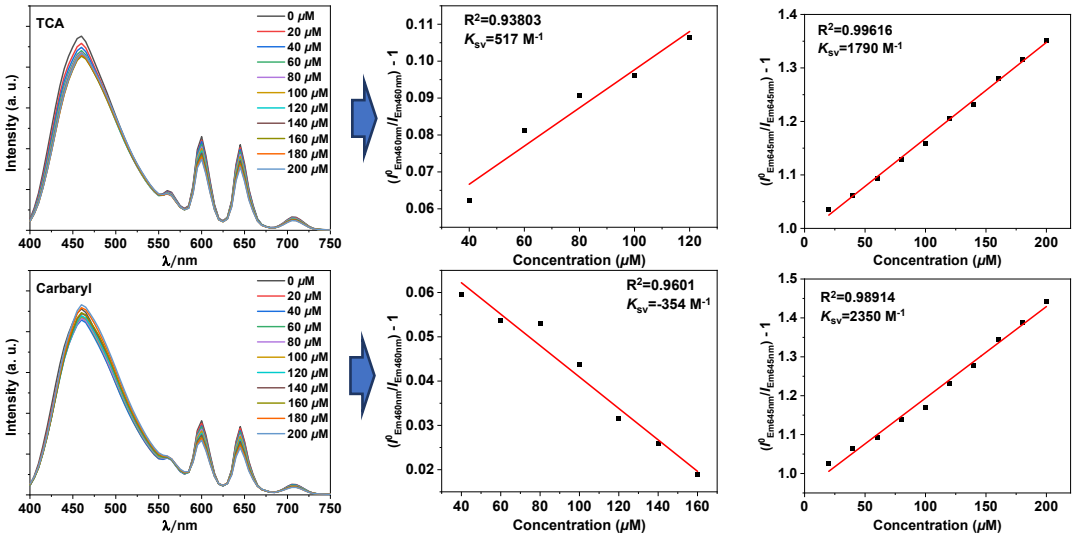
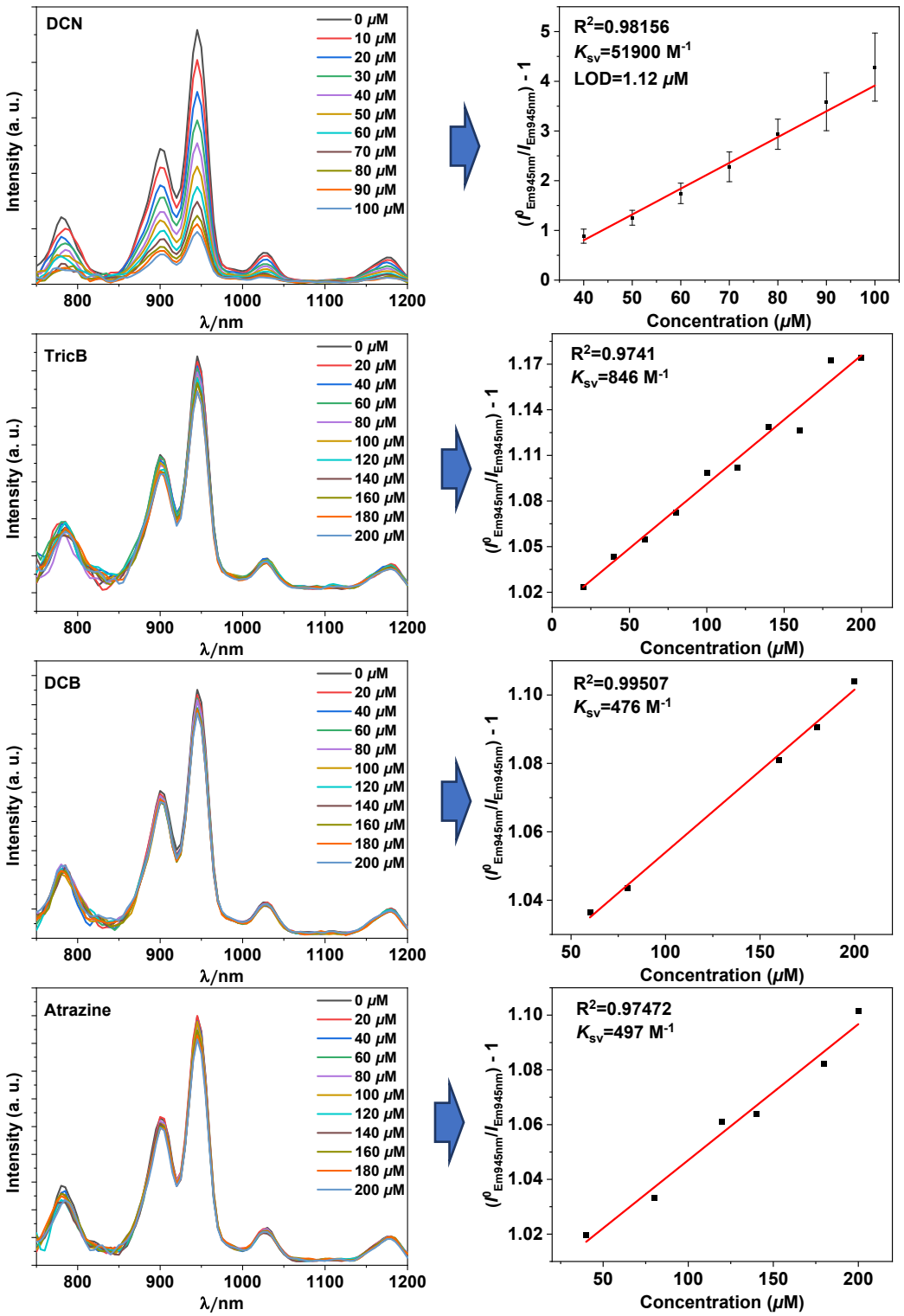


Figure S7. Left: The visible fluorescence response of **1** (10 μM) to the addition of DCN and other pesticides with different concentrations in CH_3CN (λ_{ex} = 365 nm). Right: K_{sv} values of DCN to the emissions of **1** at 460 nm and 645 nm.

11. The NIR luminescence response of 1 to pesticides



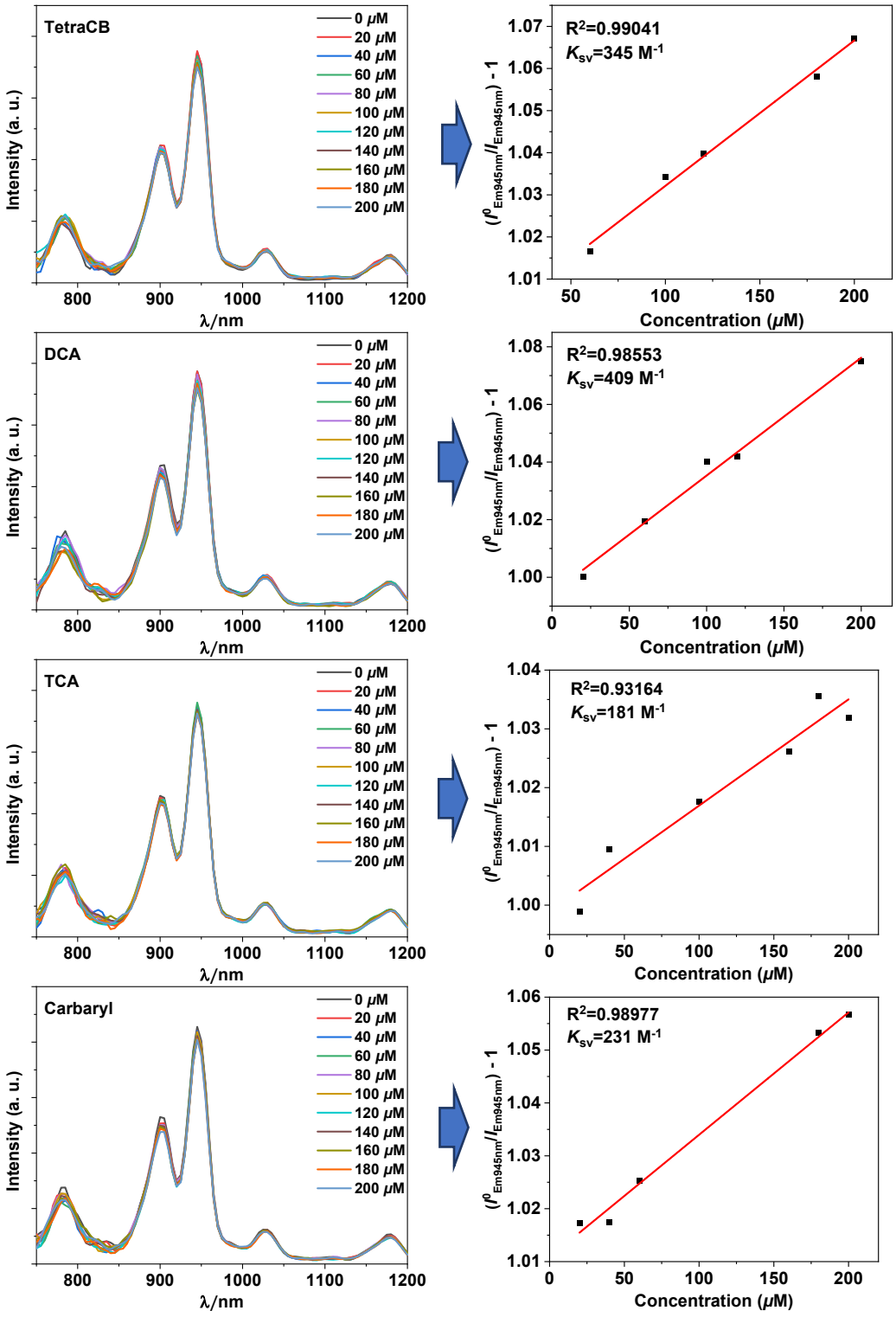


Figure S8. Left: The NIR luminescence response of **1** (10 μM) to the addition of DCN and other pesticides with different concentrations in CH_3CN (λ_{ex} = 365 nm). Right: The K_{sv} values of DCN to the lanthanide luminescence of **1** at 945 nm.

12. The emission quenching of 1 with the addition of pesticides

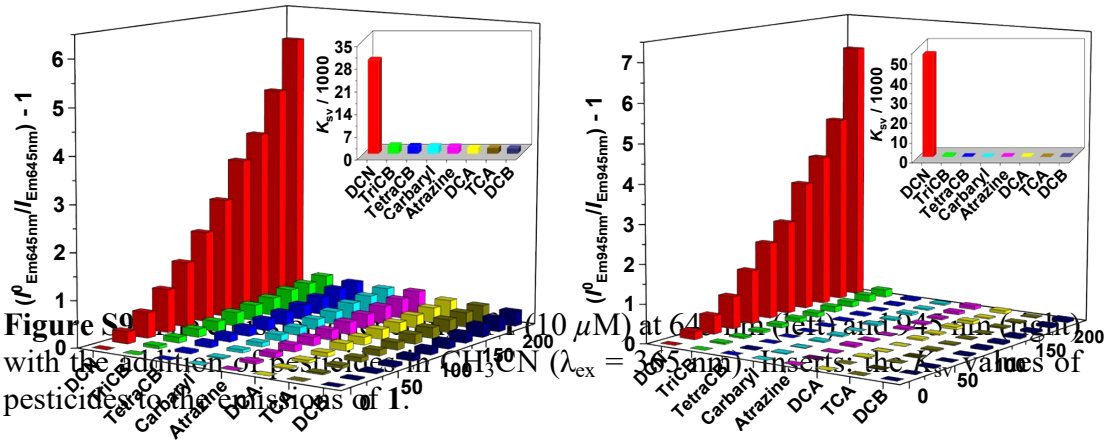


Figure S9. The emission intensities of **1** (10 μM) at 645 nm (left) and 945 nm (right) with the addition of pesticides in CH_3CN (λ_{ex} = 365 nm). Inserts: the K_{sv} values of pesticides to the emissions of **1**.

13. The fluorescence response of 1 to DCN with the existence of other pesticides

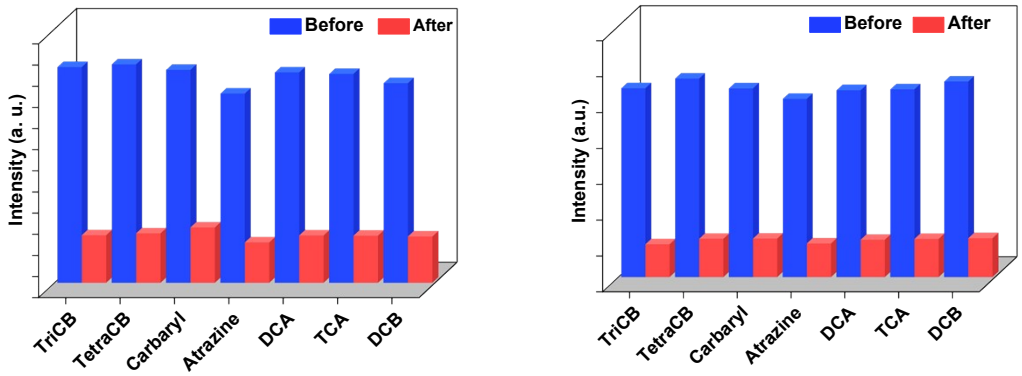


Figure S10. The emission intensities of **1** (10 μM) at 460 nm (left) and 945 nm (right) before and after the addition of DCN (c = 60 μM) with the existence of other pesticides (c = 300 μM) in CH_3CN. (λ_{ex} = 365 nm)

14. The fluorescence response of DCN in the extracts of grape and carrot skins

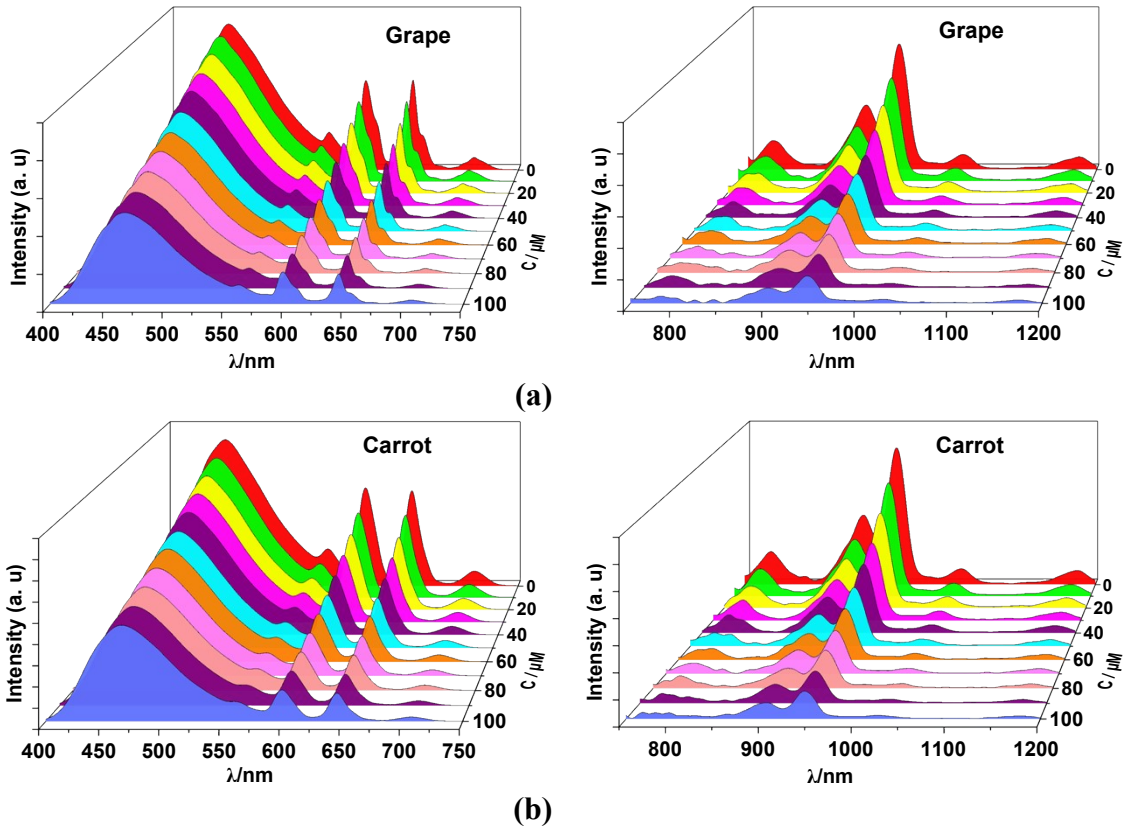


Figure S11. The fluorescence response of **1** (10 μM) to DCN in the extracts of grape (**a**) and carrot (**b**) skins.

15. Powder XRD patterns of 1 before and after treatment with DCN

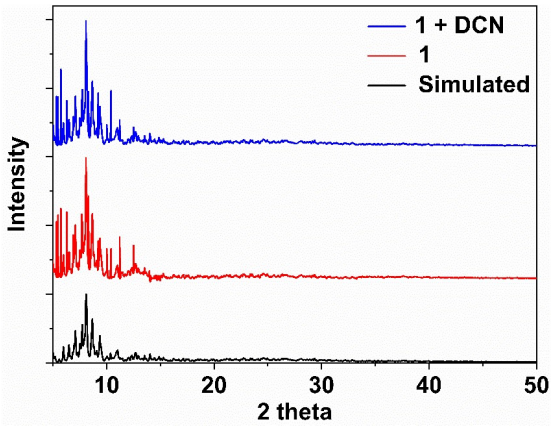


Figure S12. Powder XRD patterns of **1** before and after treatment with DCN.

16. UV-vis absorption spectra of pesticides

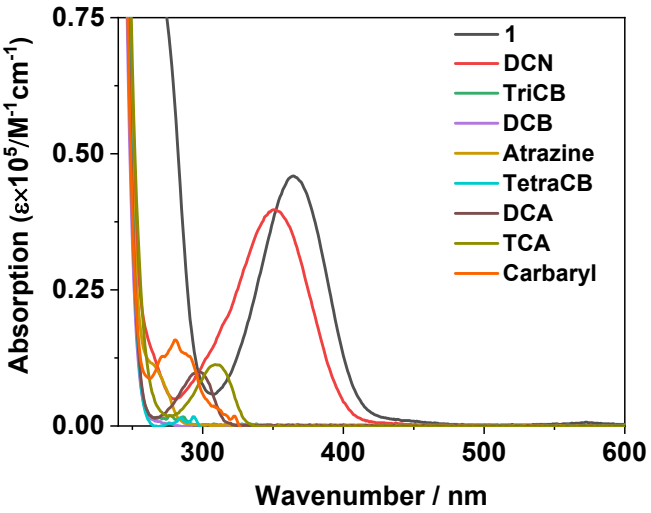


Figure S13. UV-vis absorption spectra of pesticides in CH_3CN (c = 10 μM).

17. Time scans of luminescence response of 1 to DCN

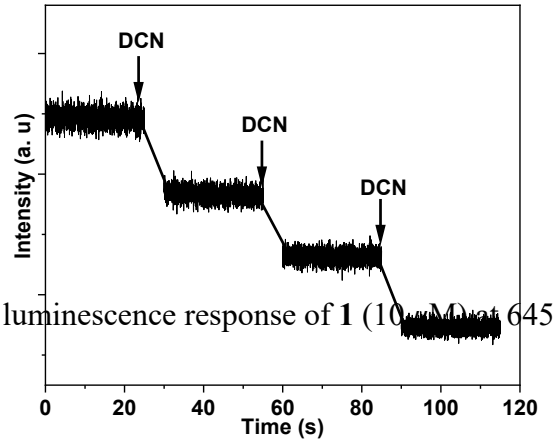


Figure S14. Time scans of luminescence response of **1** (10 μM) at 645 nm to DCN (20 μM added each time). (λ_{ex} = 365 nm)

18. The emission spectra of 1 with the addition of DCN

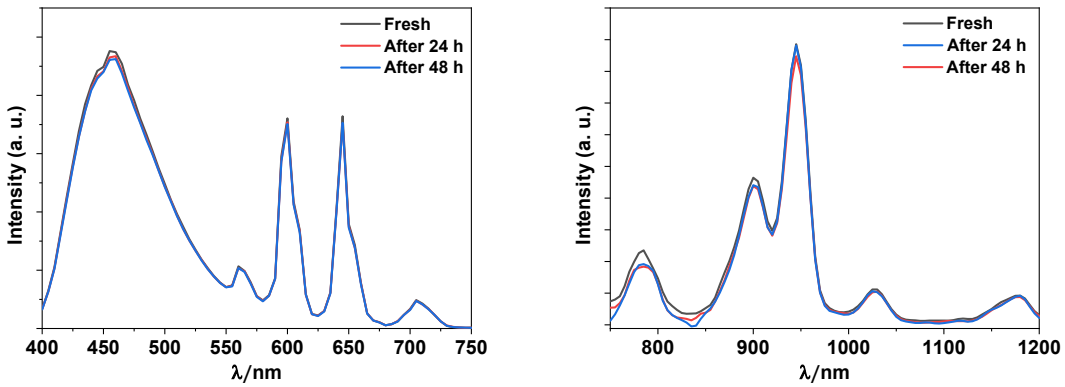


Figure S15. The visible and NIR emission spectra of **1** (10 μM) with the addition of DCN in CH_3CN.

19. X-ray crystallography

Table S1. Selected Bond Lengths (Å) and angles (◦) for **1**.

Sm(1)-O(168)	2.299(19)	Sm(2)-O(43)	2.27(2)
Sm(1)-O(71)	2.28(2)	Sm(2)-O(182)	2.38(3)
Sm(1)-O(161)	2.301(19)	Sm(2)-O(180)	2.37(2)
Sm(1)-O(188)	2.40(2)	Sm(2)-O(178)	2.38(2)
Sm(1)-O(160)	2.45(2)	Sm(2)-O(176)	2.49(2)
Sm(1)-O(75)	2.489(18)	Sm(2)-O(47)	2.50(2)
Sm(1)-N(36)	2.61(2)	Sm(2)-N(24)	2.52(3)
Sm(1)-O(72)	2.65(2)	Sm(2)-O(44)	2.539(19)

Sm(3)-O(171)	2.30(2)
Sm(3)-O(59)	2.32(2)
Sm(3)-O(63)	2.37(2)
Sm(3)-O(173)	2.40(2)
Sm(3)-O(170)	2.42(2)
Sm(3)-O(166)	2.404(18)
Sm(3)-O(60)	2.584(18)
Sm(3)-N(40)	2.61(3)
Sm(4)-O(150)	2.26(2)
Sm(4)-O(42)	2.30(2)
Sm(4)-O(152)	2.351(19)
Sm(4)-O(46)	2.42(2)
Sm(4)-O(157)	2.444(19)
Sm(4)-O(155)	2.46(2)
Sm(4)-O(45)	2.64(2)
Sm(4)-N(21)	2.70(3)
Sm(5)-O(142)	2.30(2)
Sm(5)-O(54)	2.35(2)
Sm(5)-O(144)	2.347(19)
Sm(5)-O(58)	2.37(2)
Sm(5)-O(148)	2.396(16)
Sm(5)-O(140)	2.464(19)
Sm(5)-N(27)	2.58(3)
Sm(5)-O(57)	2.56(2)
Sm(6)-O(154)	2.293(19)
Sm(6)-O(70)	2.326(19)
Sm(6)-O(74)	2.341(16)
Sm(6)-O(134)	2.35(2)
Sm(6)-O(135)	2.385(18)
Sm(6)-O(137)	2.485(18)
Sm(6)-N(33)	2.51(2)
Sm(6)-O(73)	2.64(2)
Sm(7)-O(191)	2.22(3)
Sm(7)-O(130)	2.29(2)
Sm(7)-O(39)	2.33(2)
Sm(7)-O(35)	2.37(3)
Sm(7)-O(111)	2.47(2)
Sm(7)-O(109)	2.50(2)
Sm(7)-N(20)	2.50(2)
Sm(7)-O(36)	2.56(3)
Sm(8)-O(118)	2.32(2)
Sm(8)-O(27)	2.32(2)
Sm(8)-O(23)	2.31(3)
Sm(8)-O(124)	2.37(2)
Sm(8)-O(127)	2.40(2)
Sm(8)-O(125)	2.44(2)
Sm(8)-O(24)	2.63(2)
Sm(8)-N(14)	2.62(3)
Sm(9)-O(15)	2.26(2)
Sm(9)-O(116)	2.293(19)
Sm(9)-O(11)	2.31(2)
Sm(9)-O(120)	2.38(2)
Sm(9)-O(121)	2.41(2)
Sm(9)-O(114)	2.46(3)
Sm(9)-N(8)	2.55(3)
Sm(9)-O(12)	2.68(2)
Sm(10)-O(89)	2.265(16)
Sm(10)-O(6)	2.349(18)
Sm(10)-O(10)	2.372(19)
Sm(10)-O(84)	2.39(2)
Sm(10)-O(86)	2.39(2)
Sm(10)-O(87)	2.394(19)
Sm(10)-O(9)	2.57(2)
Sm(10)-N(3)	2.66(3)
Sm(11)-O(103)	2.282(18)
Sm(11)-O(34)	2.302(19)
Sm(11)-O(105)	2.29(2)
Sm(11)-O(102)	2.318(19)
Sm(11)-O(38)	2.378(19)
Sm(11)-O(107)	2.395(19)
Sm(11)-N(17)	2.51(3)
Sm(11)-O(37)	2.58(2)
Sm(12)-O(93)	2.269(17)
Sm(12)-O(95)	2.289(18)
Sm(12)-O(26)	2.277(19)
Sm(12)-O(22)	2.365(19)
Sm(12)-O(99)	2.393(19)
Sm(12)-O(92)	2.42(2)
Sm(12)-O(25)	2.574(19)
Sm(12)-N(11)	2.60(3)
Cd(1)-O(79)	2.17(2)
Cd(1)-N(38)	2.25(3)
Cd(1)-O(160)	2.27(2)
Cd(1)-O(75)	2.290(19)
Cd(1)-O(192)	2.33(2)
Cd(1)-O(76)	2.52(3)
Cd(2)-O(184)	2.25(2)
Cd(2)-O(79)	2.24(2)
Cd(2)-O(192)	2.30(2)
Cd(2)-O(80)	2.39(3)
Cd(2)-Cl(10)	2.436(12)
Cd(2)-O(183)	2.53(2)
Cd(3)-O(181)	2.24(2)
Cd(3)-O(187)	2.30(2)
Cd(3)-N(22)	2.36(3)
Cd(3)-O(183)	2.38(2)
Cd(3)-O(43)	2.40(2)
Cd(3)-O(159)	2.52(2)
Cd(4)-N(26)	2.24(3)
Cd(4)-O(51)	2.25(2)
Cd(4)-O(176)	2.24(2)
Cd(4)-O(177)	2.28(2)
Cd(4)-O(47)	2.34(2)
Cd(4)-O(48)	2.44(3)
Cd(5)-O(51)	2.14(3)
Cd(5)-O(177)	2.29(2)
Cd(5)-Cl(9)	2.36(2)
Cd(5)-Cl(13)	2.439(14)
Cd(5)-O(52)	2.52(3)
Cd(6)-N(28)	2.23(3)
Cd(6)-O(55)	2.27(2)
Cd(6)-O(175)	2.31(2)

Cd(6)-Cl(11)	2.574(12)	Cd(16)-O(139)	2.290(18)
Cd(6)-Cl(15)	2.565(10)	Cd(16)-O(62)	2.35(2)
Cd(6)-Cl(13)	2.941(12)	Cd(16)-Cl(4)	2.462(10)
Cd(7)-O(55)	2.21(2)	Cd(16)-O(61)	2.49(2)
Cd(7)-O(174)	2.32(2)	Cd(16)-Cl(7)	2.568(9)
Cd(7)-Cl(12)	2.395(11)	Cd(16)-Cl(1)#1	2.568(9)
Cd(7)-O(56)	2.49(2)	Cd(17)-N(39)	2.25(2)
Cd(7)-Cl(11)	2.532(11)	Cd(17)-O(62)	2.29(2)
Cd(7)-Cl(8)	2.74(3)	Cd(17)-O(138)	2.361(19)
Cd(8)-N(30)	2.19(3)	Cd(17)-Cl(7)	2.525(9)
Cd(8)-O(174)	2.25(2)	Cd(17)-Cl(5)	2.587(9)
Cd(8)-O(172)	2.26(2)	Cd(18)-N(31)	2.18(3)
Cd(8)-O(59)	2.30(2)	Cd(18)-O(136)	2.248(19)
Cd(8)-Cl(15)	2.575(10)	Cd(18)-O(66)	2.26(2)
Cd(9)-O(166)	2.26(2)	Cd(18)-O(137)	2.267(18)
Cd(9)-N(32)	2.24(3)	Cd(18)-O(70)	2.35(2)
Cd(9)-O(169)	2.29(2)	Cd(18)-O(69)	2.49(2)
Cd(9)-O(67)	2.29(2)	Cd(19)-O(66)	2.18(2)
Cd(9)-O(63)	2.31(2)	Cd(19)-O(136)	2.337(18)
Cd(9)-O(64)	2.64(2)	Cd(19)-O(65)	2.42(2)
Cd(10)-O(163)	2.18(2)	Cd(19)-Cl(2)	2.488(10)
Cd(10)-O(67)	2.24(2)	Cd(19)-Cl(1)	2.541(10)
Cd(10)-O(169)	2.33(2)	Cd(19)-Cl(2)#1	2.678(9)
Cd(10)-Cl(14)	2.425(12)	Cd(20)-N(35)	2.25(2)
Cd(10)-O(68)	2.52(2)	Cd(20)-O(153)	2.286(19)
Cd(10)-O(164)	2.50(2)	Cd(20)-O(133)	2.31(2)
Cd(11)-O(162)	2.23(2)	Cd(20)-O(74)	2.339(16)
Cd(11)-N(34)	2.31(3)	Cd(20)-O(158)	2.353(19)
Cd(11)-O(167)	2.32(2)	Cd(20)-O(132)	2.489(19)
Cd(11)-O(71)	2.378(19)	Cd(20)-O(134)	2.588(18)
Cd(11)-O(164)	2.42(2)	Cd(21)-O(156)	2.202(18)
Cd(11)-O(165)	2.450(18)	Cd(21)-O(131)	2.22(2)
Cd(12)-O(46)	2.17(2)	Cd(21)-O(78)	2.27(2)
Cd(12)-O(149)	2.25(2)	Cd(21)-O(77)	2.44(2)
Cd(12)-O(151)	2.31(2)	Cd(21)-Cl(3)	2.459(12)
Cd(12)-N(23)	2.39(3)	Cd(21)-O(132)	2.532(19)
Cd(12)-O(147)	2.393(19)	Cd(22)-O(78)	2.20(2)
Cd(12)-O(146)	2.47(2)	Cd(22)-O(156)	2.234(19)
Cd(13)-O(50)	2.25(2)	Cd(22)-N(37)	2.27(2)
Cd(13)-O(145)	2.27(2)	Cd(22)-O(157)	2.286(17)
Cd(13)-O(143)	2.27(2)	Cd(22)-O(42)	2.29(2)
Cd(13)-O(146)	2.37(2)	Cd(22)-O(41)	2.48(2)
Cd(13)-Cl(6)	2.444(10)	Cd(23)-N(13)	2.29(2)
Cd(13)-O(49)	2.49(3)	Cd(23)-O(94)	2.289(17)
Cd(14)-O(50)	2.23(2)	Cd(23)-O(96)	2.286(19)
Cd(14)-N(25)	2.31(3)	Cd(23)-O(26)	2.342(19)
Cd(14)-O(148)	2.299(16)	Cd(23)-O(108)	2.366(19)
Cd(14)-O(143)	2.287(19)	Cd(23)-O(97)	2.394(18)
Cd(14)-O(54)	2.374(19)	Cd(24)-O(30)	2.241(19)
Cd(14)-O(53)	2.61(2)	Cd(24)-O(101)	2.316(18)
Cd(15)-O(141)	2.21(2)	Cd(24)-O(98)	2.39(3)
Cd(15)-N(29)	2.29(2)	Cd(24)-Cl(27)	2.405(10)
Cd(15)-O(139)	2.338(19)	Cd(24)-O(97)	2.449(18)
Cd(15)-O(58)	2.36(2)	Cd(24)-O(29)	2.48(3)
Cd(15)-Cl(5)	2.591(10)	Cd(25)-O(30)	2.16(2)
Cd(15)-O(140)	2.620(19)	Cd(25)-O(34)	2.247(19)

Cd(25)-O(107)	2.262(19)
Cd(25)-N(15)	2.28(2)
Cd(25)-O(101)	2.316(16)
Cd(25)-O(33)	2.571(19)
Cd(26)-O(104)	2.24(2)
Cd(26)-O(106)	2.268(19)
Cd(26)-O(38)	2.27(2)
Cd(26)-N(19)	2.29(2)
Cd(26)-O(83)	2.307(18)
Cd(26)-O(81)	2.55(2)
Cd(27)-O(2)	2.17(2)
Cd(27)-O(82)	2.24(3)
Cd(27)-O(85)	2.269(18)
Cd(27)-O(1)	2.40(2)
Cd(27)-Cl(25)	2.459(12)
Cd(27)-O(81)	2.48(2)
Cd(28)-O(84)	2.239(19)
Cd(28)-N(1)	2.26(3)
Cd(28)-O(85)	2.256(19)
Cd(28)-O(2)	2.264(19)
Cd(28)-O(6)	2.34(2)
Cd(28)-O(5)	2.54(2)
Cd(29)-O(90)	2.19(2)
Cd(29)-N(5)	2.24(2)
Cd(29)-O(88)	2.30(2)
Cd(29)-O(10)	2.42(2)
Cd(29)-Cl(28)	2.563(9)
Cd(29)-O(87)	2.611(18)
Cd(30)-O(88)	2.30(2)
Cd(30)-O(14)	2.356(19)
Cd(30)-Cl(31)	2.444(10)
Cd(30)-O(13)	2.59(2)
Cd(30)-Cl(29)	2.613(9)
Cd(30)-Cl(26)#2	2.623(9)
Cd(31)-N(7)	2.26(2)
Cd(31)-O(14)	2.29(2)
Cd(31)-O(91)	2.306(19)
Cd(31)-Cl(29)	2.552(9)
Cd(31)-Cl(28)	2.583(9)
Cd(32)-O(18)	2.26(2)
Cd(32)-O(100)	2.304(19)
Cd(32)-Cl(19)	2.387(10)
Cd(32)-Cl(26)	2.426(10)
Cd(32)-O(17)	2.50(2)
Cd(33)-N(9)	2.25(3)
Cd(33)-O(100)	2.244(19)
Cd(33)-O(18)	2.28(2)
Cd(33)-O(92)	2.292(19)
Cd(33)-O(22)	2.30(2)
Cd(33)-O(21)	2.54(2)
Cd(34)-O(31)	2.13(2)
Cd(34)-N(16)	2.23(3)
Cd(34)-O(27)	2.27(2)
Cd(34)-O(128)	2.31(2)
Cd(34)-O(125)	2.40(2)
Cd(34)-O(126)	2.50(2)
Cd(34)-O(28)	2.41(3)
Cd(35)-O(32)	2.03(3)
Cd(35)-O(185)	2.394(17)
Cd(35)-O(190)	2.370(18)
Cd(36)-N(18)	2.23(3)
Cd(36)-O(129)	2.28(2)
Cd(36)-O(35)	2.32(3)
Cd(36)-O(126)	2.30(3)
Cd(36)-O(189)	2.45(3)
Cd(36)-O(185)	2.526(14)
Cd(37)-O(110)	2.21(3)
Cd(37)-O(111)	2.22(2)
Cd(37)-N(2)	2.27(3)
Cd(37)-O(3)	2.34(4)
Cd(37)-O(39)	2.35(2)
Cd(37)-O(40)	2.58(3)
Cd(38)-O(3)	2.23(3)
Cd(38)-Cl(24)	2.344(16)
Cd(38)-O(110)	2.46(3)
Cd(38)-Cl(21)	2.51(3)
Cd(38)-O(4)	2.61(4)
Cd(39)-O(112)	2.27(2)
Cd(39)-N(4)	2.26(3)
Cd(39)-O(7)	2.29(3)
Cd(39)-Cl(30)	2.564(11)
Cd(39)-Cl(23)	2.622(10)
Cd(39)-Cl(24)	2.850(17)
Cd(40)-O(7)	2.23(3)
Cd(40)-O(113)	2.35(2)
Cd(40)-Cl(17)	2.426(13)
Cd(40)-O(8)	2.52(3)
Cd(40)-Cl(30)	2.573(10)
Cd(40)-Cl(16)	2.75(4)
Cd(41)-O(115)	2.18(2)
Cd(41)-N(6)	2.29(3)
Cd(41)-O(11)	2.28(2)
Cd(41)-O(113)	2.323(19)
Cd(41)-O(114)	2.53(3)
Cd(41)-Cl(23)	2.585(9)
Cd(42)-O(119)	2.19(2)
Cd(42)-N(10)	2.30(3)
Cd(42)-O(121)	2.31(2)
Cd(42)-O(19)	2.34(3)
Cd(42)-O(15)	2.37(2)
Cd(42)-O(16)	2.56(3)
Cd(43)-O(19)	2.21(3)
Cd(43)-O(119)	2.28(2)
Cd(43)-O(20)	2.39(4)
Cd(43)-Cl(18)	2.376(19)
Cd(43)-Cl(20)	2.57(2)
Cd(44)-O(117)	2.32(3)
Cd(44)-N(12)	2.34(3)
Cd(44)-O(123)	2.31(2)
Cd(44)-O(23)	2.36(3)
Cd(44)-O(122)	2.42(2)
Cd(44)-Cl(20)	2.66(2)

O(168)-Sm(1)-O(71)	90.4(7)	O(171)-Sm(3)-O(59)	85.8(7)
O(168)-Sm(1)-O(161)	75.1(7)	O(171)-Sm(3)-O(63)	117.0(7)
O(71)-Sm(1)-O(161)	75.5(7)	O(59)-Sm(3)-O(63)	135.7(7)
O(168)-Sm(1)-O(188)	143.2(7)	O(171)-Sm(3)-O(173)	77.3(7)
O(71)-Sm(1)-O(188)	104.0(7)	O(59)-Sm(3)-O(173)	74.4(7)
O(161)-Sm(1)-O(188)	76.0(7)	O(63)-Sm(3)-O(173)	144.1(7)
O(168)-Sm(1)-O(160)	78.0(7)	O(171)-Sm(3)-O(170)	148.2(7)
O(71)-Sm(1)-O(160)	158.8(7)	O(59)-Sm(3)-O(170)	104.3(7)
O(161)-Sm(1)-O(160)	84.3(7)	O(63)-Sm(3)-O(170)	76.7(7)
O(188)-Sm(1)-O(160)	76.8(7)	O(173)-Sm(3)-O(170)	76.6(7)
O(168)-Sm(1)-O(75)	111.1(6)	O(171)-Sm(3)-O(166)	79.8(7)
O(71)-Sm(1)-O(75)	130.1(7)	O(59)-Sm(3)-O(166)	155.0(7)
O(161)-Sm(1)-O(75)	152.0(7)	O(63)-Sm(3)-O(166)	69.2(7)
O(188)-Sm(1)-O(75)	85.4(6)	O(173)-Sm(3)-O(166)	82.5(7)
O(160)-Sm(1)-O(75)	71.0(7)	O(170)-Sm(3)-O(166)	79.0(6)
O(168)-Sm(1)-N(36)	77.1(7)	O(171)-Sm(3)-O(60)	135.8(7)
O(71)-Sm(1)-N(36)	73.6(7)	O(59)-Sm(3)-O(60)	62.3(7)
O(161)-Sm(1)-N(36)	137.8(7)	O(63)-Sm(3)-O(60)	76.4(7)
O(188)-Sm(1)-N(36)	139.3(8)	O(173)-Sm(3)-O(60)	117.6(7)
O(160)-Sm(1)-N(36)	119.8(8)	O(170)-Sm(3)-O(60)	73.5(6)
O(75)-Sm(1)-N(36)	68.7(7)	O(166)-Sm(3)-O(60)	140.0(7)
O(168)-Sm(1)-O(72)	146.6(7)	O(171)-Sm(3)-N(40)	74.1(8)
O(71)-Sm(1)-O(72)	61.2(7)	O(59)-Sm(3)-N(40)	80.0(8)
O(161)-Sm(1)-O(72)	110.8(7)	O(63)-Sm(3)-N(40)	71.9(9)
O(188)-Sm(1)-O(72)	66.5(7)	O(173)-Sm(3)-N(40)	142.7(9)
O(160)-Sm(1)-O(72)	134.4(7)	O(170)-Sm(3)-N(40)	136.9(8)
O(75)-Sm(1)-O(72)	79.6(7)	O(166)-Sm(3)-N(40)	115.0(8)
N(36)-Sm(1)-O(72)	78.0(7)	O(60)-Sm(3)-N(40)	71.0(7)
O(43)-Sm(2)-O(182)	77.3(9)	O(150)-Sm(4)-O(42)	151.9(8)
O(43)-Sm(2)-O(180)	85.3(7)	O(150)-Sm(4)-O(152)	74.2(7)
O(182)-Sm(2)-O(180)	78.3(9)	O(42)-Sm(4)-O(152)	117.7(8)
O(43)-Sm(2)-O(178)	106.5(7)	O(150)-Sm(4)-O(46)	74.7(8)
O(182)-Sm(2)-O(178)	73.1(9)	O(42)-Sm(4)-O(46)	128.0(8)
O(180)-Sm(2)-O(178)	145.4(8)	O(152)-Sm(4)-O(46)	88.6(7)
O(43)-Sm(2)-O(176)	159.2(7)	O(150)-Sm(4)-O(157)	88.6(7)
O(182)-Sm(2)-O(176)	84.0(9)	O(42)-Sm(4)-O(157)	68.8(7)
O(180)-Sm(2)-O(176)	82.1(7)	O(152)-Sm(4)-O(157)	83.7(7)
O(178)-Sm(2)-O(176)	76.0(7)	O(46)-Sm(4)-O(157)	163.1(6)
O(43)-Sm(2)-O(47)	132.2(8)	O(150)-Sm(4)-O(155)	73.5(7)
O(182)-Sm(2)-O(47)	146.7(9)	O(42)-Sm(4)-O(155)	84.2(8)
O(180)-Sm(2)-O(47)	114.2(8)	O(152)-Sm(4)-O(155)	141.5(7)
O(178)-Sm(2)-O(47)	82.2(8)	O(46)-Sm(4)-O(155)	102.5(7)
O(176)-Sm(2)-O(47)	68.4(7)	O(157)-Sm(4)-O(155)	75.2(6)
O(43)-Sm(2)-N(24)	74.5(9)	O(150)-Sm(4)-O(45)	111.3(8)
O(182)-Sm(2)-N(24)	142.2(10)	O(42)-Sm(4)-O(45)	74.3(8)
O(180)-Sm(2)-N(24)	74.9(9)	O(152)-Sm(4)-O(45)	145.3(7)
O(178)-Sm(2)-N(24)	139.3(9)	O(46)-Sm(4)-O(45)	61.8(7)
O(176)-Sm(2)-N(24)	117.5(9)	O(157)-Sm(4)-O(45)	129.5(6)
O(47)-Sm(2)-N(24)	70.1(9)	O(155)-Sm(4)-O(45)	67.8(7)
O(43)-Sm(2)-O(44)	62.6(6)	O(150)-Sm(4)-N(21)	136.1(8)
O(182)-Sm(2)-O(44)	112.8(8)	O(42)-Sm(4)-N(21)	71.5(8)
O(180)-Sm(2)-O(44)	140.8(7)	O(152)-Sm(4)-N(21)	75.2(8)
O(178)-Sm(2)-O(44)	70.3(7)	O(46)-Sm(4)-N(21)	73.9(8)
O(176)-Sm(2)-O(44)	134.8(6)	O(157)-Sm(4)-N(21)	118.2(8)
O(47)-Sm(2)-O(44)	77.9(7)	O(155)-Sm(4)-N(21)	143.2(8)
N(24)-Sm(2)-O(44)	75.1(8)	O(45)-Sm(4)-N(21)	79.1(8)

O(142)-Sm(5)-O(54)	112.6(7)	O(191)-Sm(7)-O(130)	79.4(8)
O(142)-Sm(5)-O(144)	147.8(7)	O(191)-Sm(7)-O(39)	148.4(8)
O(54)-Sm(5)-O(144)	81.8(7)	O(130)-Sm(7)-O(39)	115.6(8)
O(142)-Sm(5)-O(58)	89.2(8)	O(191)-Sm(7)-O(35)	75.3(9)
O(54)-Sm(5)-O(58)	135.1(7)	O(130)-Sm(7)-O(35)	84.7(8)
O(144)-Sm(5)-O(58)	100.5(7)	O(39)-Sm(7)-O(35)	131.2(8)
O(142)-Sm(5)-O(148)	77.7(6)	O(191)-Sm(7)-O(111)	85.9(8)
O(54)-Sm(5)-O(148)	70.5(6)	O(130)-Sm(7)-O(111)	76.3(7)
O(144)-Sm(5)-O(148)	80.9(6)	O(39)-Sm(7)-O(111)	72.1(8)
O(58)-Sm(5)-O(148)	154.4(7)	O(35)-Sm(7)-O(111)	155.4(8)
O(142)-Sm(5)-O(140)	78.3(6)	O(191)-Sm(7)-O(109)	75.7(9)
O(54)-Sm(5)-O(140)	146.5(6)	O(130)-Sm(7)-O(109)	142.7(7)
O(144)-Sm(5)-O(140)	75.1(6)	O(39)-Sm(7)-O(109)	76.7(8)
O(58)-Sm(5)-O(140)	73.9(7)	O(35)-Sm(7)-O(109)	114.5(8)
O(148)-Sm(5)-O(140)	81.9(6)	O(111)-Sm(7)-O(109)	74.8(7)
O(142)-Sm(5)-N(27)	75.5(8)	O(191)-Sm(7)-N(20)	141.4(9)
O(54)-Sm(5)-N(27)	73.3(8)	O(130)-Sm(7)-N(20)	76.0(8)
O(144)-Sm(5)-N(27)	136.6(8)	O(39)-Sm(7)-N(20)	70.0(8)
O(58)-Sm(5)-N(27)	75.3(8)	O(35)-Sm(7)-N(20)	73.3(8)
O(148)-Sm(5)-N(27)	121.1(7)	O(111)-Sm(7)-N(20)	115.9(7)
O(140)-Sm(5)-N(27)	139.4(7)	O(109)-Sm(7)-N(20)	138.5(8)
O(142)-Sm(5)-O(57)	140.4(7)	O(191)-Sm(7)-O(36)	106.5(9)
O(54)-Sm(5)-O(57)	79.3(6)	O(130)-Sm(7)-O(36)	140.9(7)
O(144)-Sm(5)-O(57)	68.6(7)	O(39)-Sm(7)-O(36)	80.0(8)
O(58)-Sm(5)-O(57)	60.9(7)	O(35)-Sm(7)-O(36)	60.9(9)
O(148)-Sm(5)-O(57)	139.6(6)	O(111)-Sm(7)-O(36)	141.7(8)
O(140)-Sm(5)-O(57)	113.3(6)	O(109)-Sm(7)-O(36)	73.6(8)
N(27)-Sm(5)-O(57)	72.3(8)	N(20)-Sm(7)-O(36)	76.7(8)
O(154)-Sm(6)-O(70)	109.0(7)	O(118)-Sm(8)-O(27)	145.8(9)
O(154)-Sm(6)-O(74)	87.4(6)	O(118)-Sm(8)-O(23)	76.2(9)
O(70)-Sm(6)-O(74)	135.2(6)	O(27)-Sm(8)-O(23)	134.2(9)
O(154)-Sm(6)-O(134)	79.6(7)	O(118)-Sm(8)-O(124)	75.6(8)
O(70)-Sm(6)-O(134)	149.7(7)	O(27)-Sm(8)-O(124)	116.7(8)
O(74)-Sm(6)-O(134)	72.5(6)	O(23)-Sm(8)-O(124)	84.1(8)
O(154)-Sm(6)-O(135)	149.2(7)	O(118)-Sm(8)-O(127)	76.2(8)
O(70)-Sm(6)-O(135)	82.1(6)	O(27)-Sm(8)-O(127)	78.6(8)
O(74)-Sm(6)-O(135)	105.0(5)	O(23)-Sm(8)-O(127)	107.7(9)
O(134)-Sm(6)-O(135)	77.7(6)	O(124)-Sm(8)-O(127)	145.6(9)
O(154)-Sm(6)-O(137)	79.2(7)	O(118)-Sm(8)-O(125)	82.7(9)
O(70)-Sm(6)-O(137)	71.3(6)	O(27)-Sm(8)-O(125)	70.9(8)
O(74)-Sm(6)-O(137)	153.4(6)	O(23)-Sm(8)-O(125)	153.9(9)
O(134)-Sm(6)-O(137)	82.4(6)	O(124)-Sm(8)-O(125)	75.8(8)
O(135)-Sm(6)-O(137)	77.5(6)	O(127)-Sm(8)-O(125)	81.5(8)
O(154)-Sm(6)-N(33)	74.1(7)	O(118)-Sm(8)-O(24)	114.1(8)
O(70)-Sm(6)-N(33)	73.0(7)	O(27)-Sm(8)-O(24)	79.4(7)
O(74)-Sm(6)-N(33)	72.3(7)	O(23)-Sm(8)-O(24)	60.8(8)
O(134)-Sm(6)-N(33)	136.4(7)	O(124)-Sm(8)-O(24)	137.5(8)
O(135)-Sm(6)-N(33)	136.3(7)	O(127)-Sm(8)-O(24)	73.0(8)
O(137)-Sm(6)-N(33)	124.5(7)	O(125)-Sm(8)-O(24)	144.1(8)
O(154)-Sm(6)-O(73)	141.5(7)	O(118)-Sm(8)-N(14)	144.2(9)
O(70)-Sm(6)-O(73)	79.6(6)	O(27)-Sm(8)-N(14)	68.9(8)
O(74)-Sm(6)-O(73)	63.9(6)	O(23)-Sm(8)-N(14)	77.1(9)
O(134)-Sm(6)-O(73)	112.2(6)	O(124)-Sm(8)-N(14)	78.3(9)
O(135)-Sm(6)-O(73)	67.6(6)	O(127)-Sm(8)-N(14)	135.3(8)
O(137)-Sm(6)-O(73)	137.1(6)	O(125)-Sm(8)-N(14)	114.1(9)
N(33)-Sm(6)-O(73)	73.0(7)	O(24)-Sm(8)-N(14)	71.5(8)

O(15)-Sm(9)-O(116)	116.0(8)	O(103)-Sm(11)-O(34)	151.2(7)
O(15)-Sm(9)-O(11)	138.0(7)	O(103)-Sm(11)-O(105)	77.8(7)
O(116)-Sm(9)-O(11)	84.4(7)	O(34)-Sm(11)-O(105)	113.3(7)
O(15)-Sm(9)-O(120)	80.8(8)	O(103)-Sm(11)-O(102)	76.5(7)
O(116)-Sm(9)-O(120)	147.2(7)	O(34)-Sm(11)-O(102)	79.7(7)
O(11)-Sm(9)-O(120)	101.8(8)	O(105)-Sm(11)-O(102)	141.9(7)
O(15)-Sm(9)-O(121)	70.0(8)	O(103)-Sm(11)-O(38)	75.8(6)
O(116)-Sm(9)-O(121)	81.1(8)	O(34)-Sm(11)-O(38)	129.0(6)
O(11)-Sm(9)-O(121)	152.0(7)	O(105)-Sm(11)-O(38)	88.0(7)
O(120)-Sm(9)-O(121)	78.9(8)	O(102)-Sm(11)-O(38)	112.1(7)
O(15)-Sm(9)-O(114)	144.4(8)	O(103)-Sm(11)-O(107)	88.2(6)
O(116)-Sm(9)-O(114)	75.8(8)	O(34)-Sm(11)-O(107)	69.6(6)
O(11)-Sm(9)-O(114)	73.6(8)	O(105)-Sm(11)-O(107)	77.8(7)
O(120)-Sm(9)-O(114)	75.3(8)	O(102)-Sm(11)-O(107)	73.7(7)
O(121)-Sm(9)-O(114)	79.7(8)	O(38)-Sm(11)-O(107)	160.6(6)
O(15)-Sm(9)-N(8)	71.4(8)	O(103)-Sm(11)-N(17)	135.6(8)
O(116)-Sm(9)-N(8)	78.0(8)	O(34)-Sm(11)-N(17)	72.9(8)
O(11)-Sm(9)-N(8)	78.4(8)	O(105)-Sm(11)-N(17)	75.6(9)
O(120)-Sm(9)-N(8)	134.7(8)	O(102)-Sm(11)-N(17)	141.1(9)
O(121)-Sm(9)-N(8)	121.2(8)	O(38)-Sm(11)-N(17)	68.4(8)
O(114)-Sm(9)-N(8)	143.1(9)	O(107)-Sm(11)-N(17)	119.5(8)
O(15)-Sm(9)-O(12)	78.6(8)	O(103)-Sm(11)-O(37)	110.6(7)
O(116)-Sm(9)-O(12)	139.2(7)	O(34)-Sm(11)-O(37)	75.8(7)
O(11)-Sm(9)-O(12)	64.1(7)	O(105)-Sm(11)-O(37)	145.9(7)
O(120)-Sm(9)-O(12)	69.0(7)	O(102)-Sm(11)-O(37)	70.6(7)
O(121)-Sm(9)-O(12)	137.9(7)	O(38)-Sm(11)-O(37)	63.9(7)
O(114)-Sm(9)-O(12)	115.6(8)	O(107)-Sm(11)-O(37)	133.7(7)
N(8)-Sm(9)-O(12)	71.0(8)	N(17)-Sm(11)-O(37)	76.2(8)
O(89)-Sm(10)-O(6)	113.0(6)	O(93)-Sm(12)-O(95)	78.1(7)
O(89)-Sm(10)-O(10)	93.3(6)	O(93)-Sm(12)-O(26)	85.0(7)
O(6)-Sm(10)-O(10)	130.9(7)	O(95)-Sm(12)-O(26)	73.3(7)
O(89)-Sm(10)-O(84)	79.7(6)	O(93)-Sm(12)-O(22)	115.3(7)
O(6)-Sm(10)-O(84)	69.4(7)	O(95)-Sm(12)-O(22)	147.1(7)
O(10)-Sm(10)-O(84)	159.2(7)	O(26)-Sm(12)-O(22)	134.8(7)
O(89)-Sm(10)-O(86)	144.2(7)	O(93)-Sm(12)-O(99)	145.7(7)
O(6)-Sm(10)-O(86)	81.8(7)	O(95)-Sm(12)-O(99)	76.8(6)
O(10)-Sm(10)-O(86)	100.9(7)	O(26)-Sm(12)-O(99)	109.5(7)
O(84)-Sm(10)-O(86)	75.4(7)	O(22)-Sm(12)-O(99)	77.0(6)
O(89)-Sm(10)-O(87)	77.4(6)	O(93)-Sm(12)-O(92)	76.5(7)
O(6)-Sm(10)-O(87)	148.4(7)	O(95)-Sm(12)-O(92)	84.6(7)
O(10)-Sm(10)-O(87)	75.2(6)	O(26)-Sm(12)-O(92)	153.7(7)
O(84)-Sm(10)-O(87)	84.1(6)	O(22)-Sm(12)-O(92)	70.9(6)
O(86)-Sm(10)-O(87)	74.8(7)	O(99)-Sm(12)-O(92)	78.2(7)
O(89)-Sm(10)-O(9)	142.7(7)	O(93)-Sm(12)-O(25)	140.9(6)
O(6)-Sm(10)-O(9)	75.2(6)	O(95)-Sm(12)-O(25)	108.8(7)
O(10)-Sm(10)-O(9)	60.2(6)	O(26)-Sm(12)-O(25)	62.1(6)
O(84)-Sm(10)-O(9)	134.0(6)	O(22)-Sm(12)-O(25)	80.3(6)
O(86)-Sm(10)-O(9)	71.2(7)	O(99)-Sm(12)-O(25)	70.3(6)
O(87)-Sm(10)-O(9)	115.5(6)	O(92)-Sm(12)-O(25)	141.2(6)
O(89)-Sm(10)-N(3)	75.7(7)	O(93)-Sm(12)-N(11)	75.9(8)
O(6)-Sm(10)-N(3)	72.2(7)	O(95)-Sm(12)-N(11)	140.0(8)
O(10)-Sm(10)-N(3)	75.6(7)	O(26)-Sm(12)-N(11)	74.6(8)
O(84)-Sm(10)-N(3)	120.6(7)	O(22)-Sm(12)-N(11)	72.5(8)
O(86)-Sm(10)-N(3)	139.7(7)	O(99)-Sm(12)-N(11)	137.2(8)
O(87)-Sm(10)-N(3)	138.6(6)	O(92)-Sm(12)-N(11)	117.6(8)
O(9)-Sm(10)-N(3)	72.7(8)	O(25)-Sm(12)-N(11)	75.5(8)