Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

A 24-Metal Cd(II)-Sm(III) Nanocage with Rapid Triple-Emissive Response of 2,6-Dichloro-4-Nitroaniline

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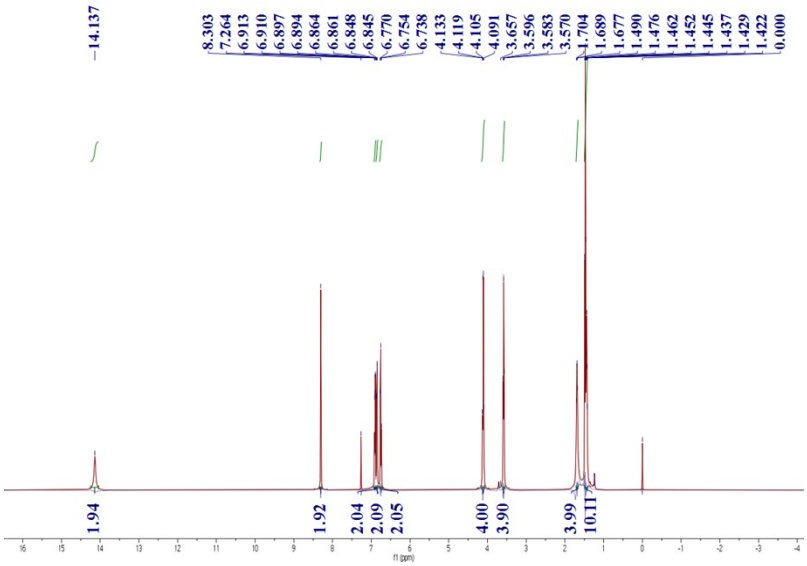
Contents

1. General Procedures

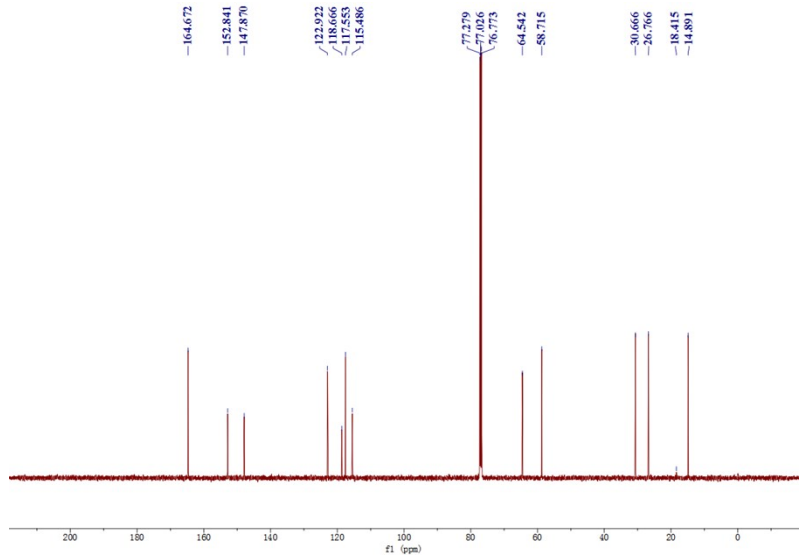
All chemical materials and solvents were purchased from commercial sources. The synthesis of lanthanide complex was carried out using Schlenk techniques. Powder XRD spectra were obtained using a D8 Advance; IR spectra were determined on a FTIR-650 spectrometer; Elemental analysis was performed on a EURO 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, and heated from room temperature to 800°C with a heating rate of 5°C/min; 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. Visible and NIR emission and excitation 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 visible emission from 400 nm to 800 nm were collected by R928 detector. 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. Systematic errors have been deducted through the standard instrument corrections. All the measurements were carried out at room temperature.

2. ^{1}H NMR and ^{13}C NMR spectra of H_2L



(**a**)



(**b**)

Figure S1. (**a**) ^{1}H NMR of the ligand H_2L in $CDCl_3$; (**b**) ^{13}C NMR of the ligand H_2L in $CDCl_3$.

3. IR spectra and thermogravimetric analysis

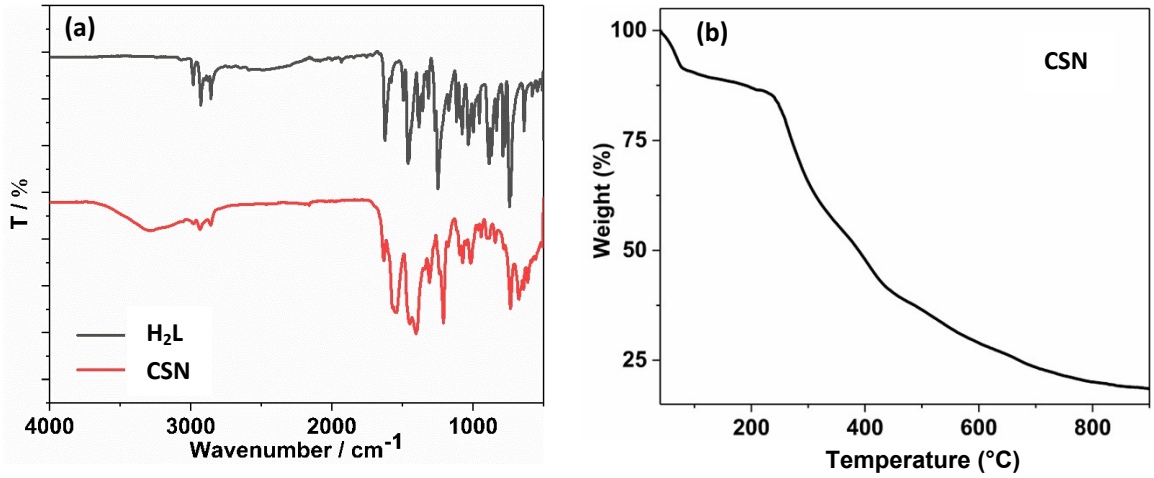


Figure S2. (**a**) IR spectra of the ligand H_2L and **CSN**; (**b**) The thermogravimetric analysis of **CSN**.

4. The coordination modes of Cd(II) and Sm(III) ions

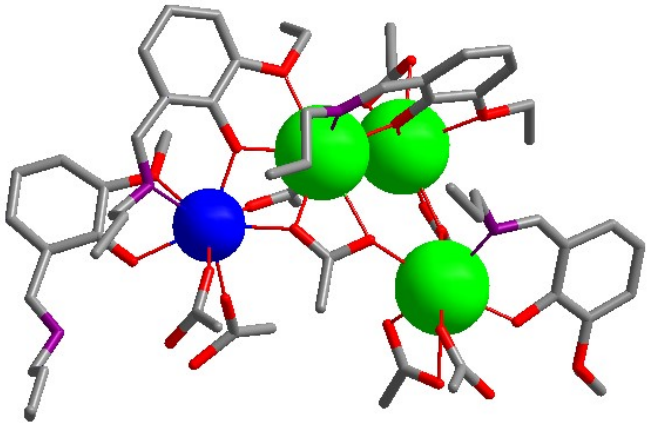


Figure S3. The coordination modes of Cd(II) (green) and Sm(III) (blue) ions in **CSN**.

5. UV-vis absorption spectra of H_2L and CSN

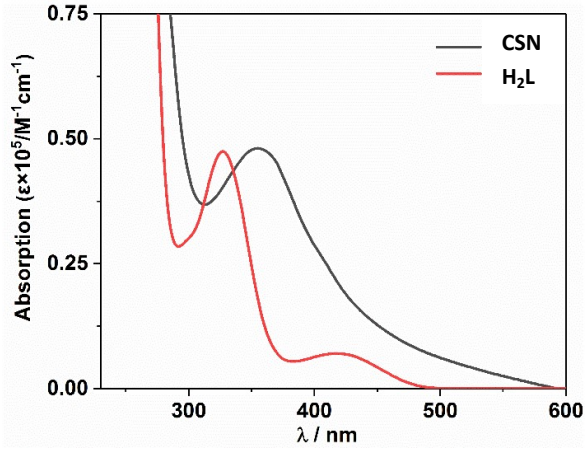


Figure S4. UV-vis absorption spectra of the ligand H_2L and **CSN** in CH_3CN.

6. The excitation and emission spectra of the ligand H_2L

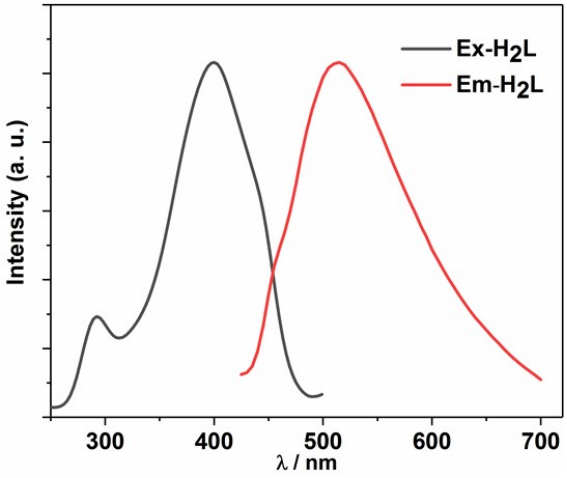


Figure S5.The excitation (λ_{ex} = 400 nm) and emission (λ_{em} = 515 nm) spectra of the free ligand H_2L (10 μM) in CH_3CN.

7. The excitation and emission spectra of CSN

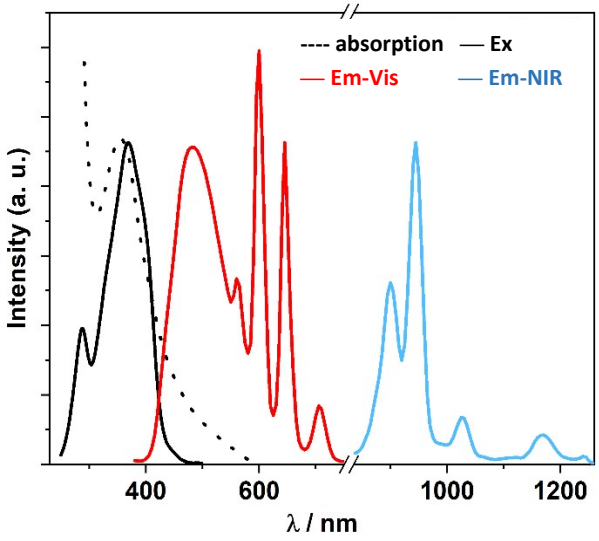


Figure S6. The excitation (λ_{em} = 945 nm) and emission (λ_{ex} = 365 nm) spectra of **CSN** (10 μM) in CH_3CN, with the insert of the absorption spectrum of **CSN** (- - - -).

8. The K_{sv} values of DCN to the emissions of CSN in CH_3CN

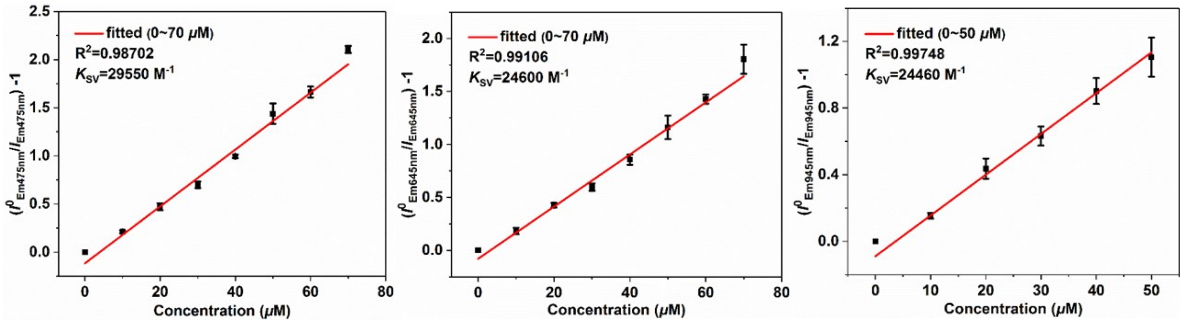
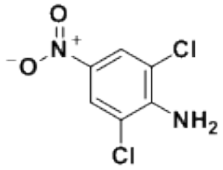
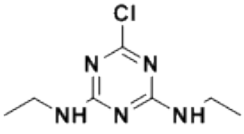


Figure S7. The K_{sv} values of DCN to the emissions of **CSN** (10 μM) at 475 nm, 645 nm and 945 nm in CH_3CN. (λ_{ex} = 365 nm)

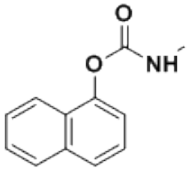
9. Chemical structures of pesticides



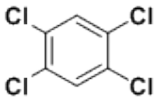
2,6-dichloro-4-nitroanine
(**DCN**)



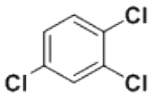
Atrazine



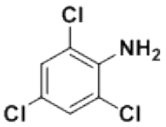
Carbaryl



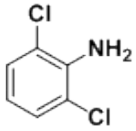
1,2,4,5-tetrachlorobenzene
(**TetraCB**)



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



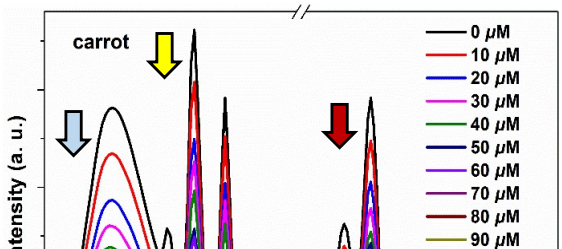
2,4,6-trichloroaniline
(**TCA**)



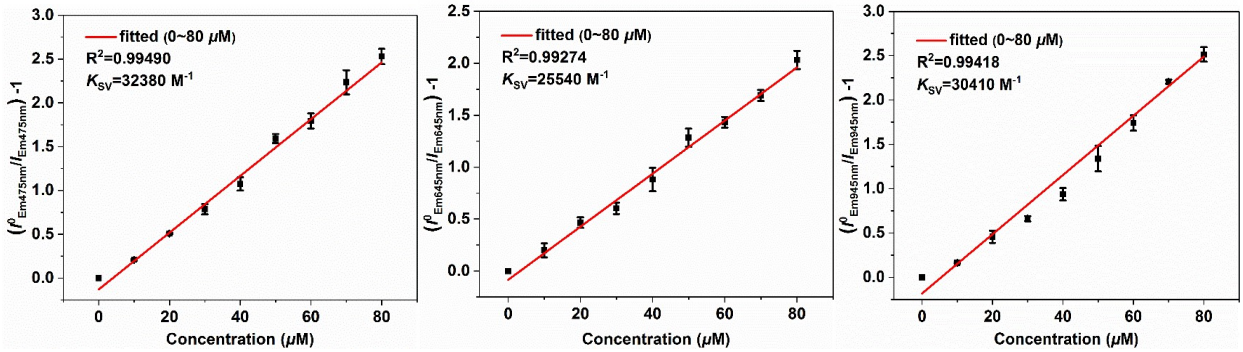
2,6-dichloroaniline
(**DCA**)

Scheme S1. Chemical structures of pesticides.

10. The fluorescence response of CSN to DCN in the extract of carrot



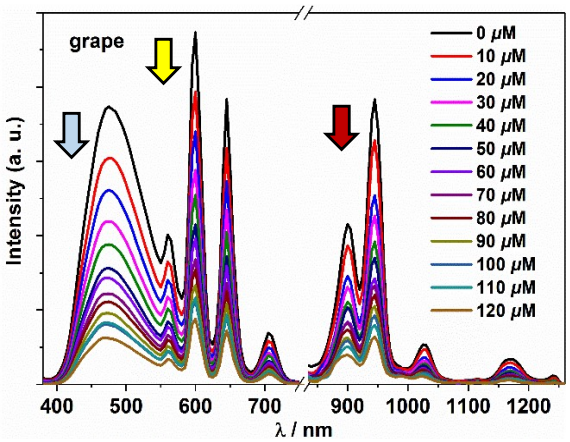
(a)



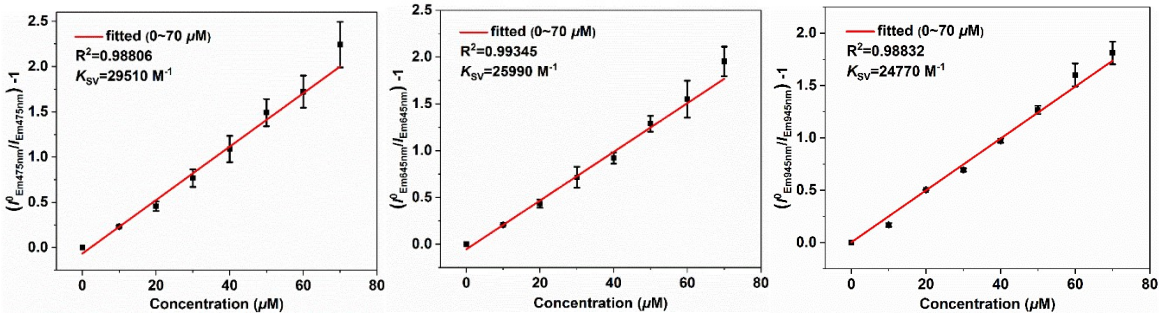
(b)

Figure S8. (a) The fluorescence response of **CSN** (10 μM) to DCN in the extract of carrot. (b) The K_{sv} values of DCN to the emissions of **CSN** at 475 nm, 645 nm and 945 nm. (λ_{ex} = 365 nm)

11. The fluorescence response of CSN to DCN in the extract of grape



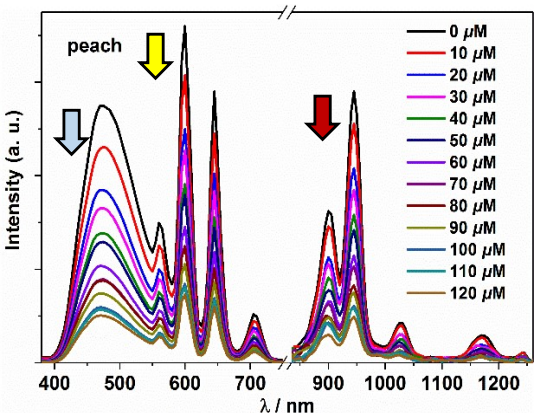
(a)



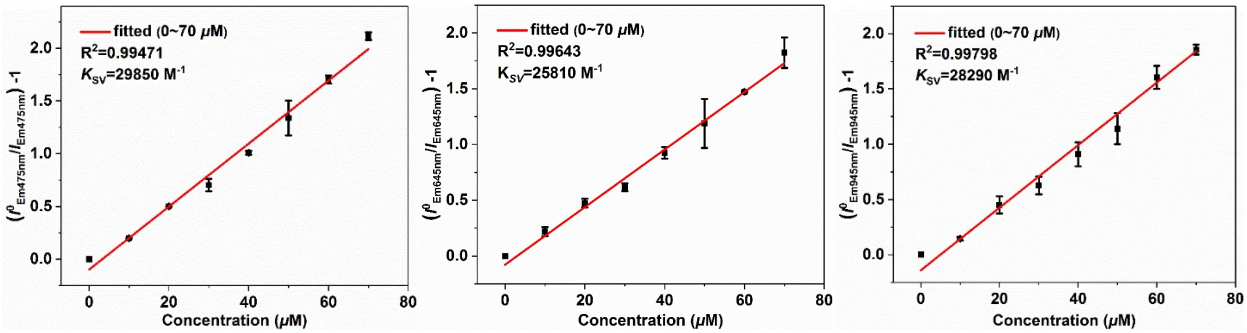
(b)

Figure S9. (a) The fluorescence response of **CSN** (10 μM) to DCN in the extract of grape. (b) The K_{sv} values of DCN to the emissions of **CSN** at 475 nm, 645 nm and 945 nm. (λ_{ex} = 365 nm)

12. The fluorescence response of CSN to DCN in the extract of peach



(a)



(b)

Figure S10. (a) The fluorescence response of **CSN** (10 μM) to DCN in the extract of peach. (b) The K_{sv} values of DCN to the emissions of **CSN** at 475 nm, 645 nm and 945 nm. (λ_{ex} = 365 nm)

13. Powder XRD patterns of CSN before and after treated with DCN

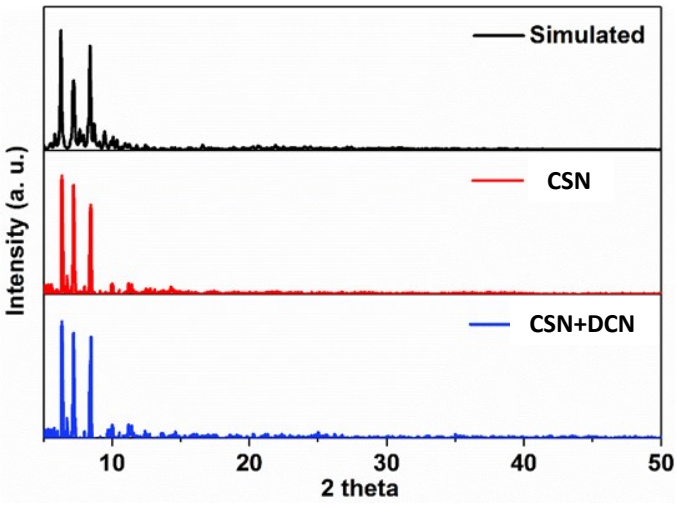


Figure S11. Powder XRD patterns of **CSN** before and after treated with DCN.

14. UV-vis absorption spectra of pesticides

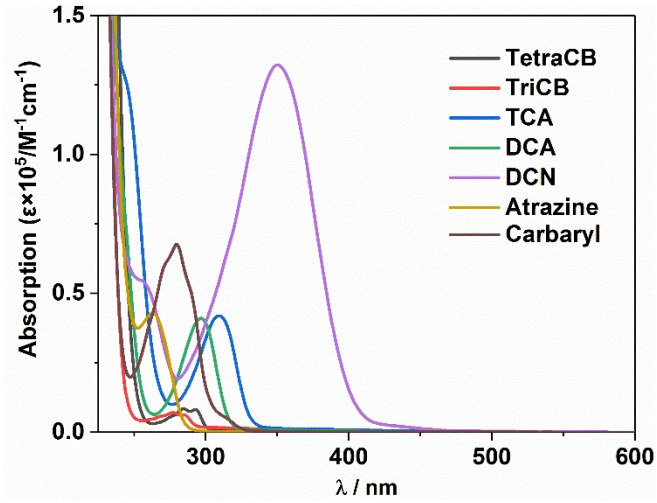


Figure S12. UV-vis absorption spectra of pesticides in CH_3CN. (c = 10 μM)

15. X-Ray Crystallography

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

Sm(1)-O(53)	2.194(10)	Cd(1)-O(71)	2.314(11)
Sm(1)-O(70)	2.205(8)	Cd(1)-O(2)	2.320(11)
Sm(1)-O(10)	2.249(9)	Cd(1)-O(45)	2.395(11)
Sm(1)-O(14)	2.329(9)	Cd(1)-O(51)	2.441(11)
Sm(1)-O(50)	2.368(8)	Cd(2)-O(46)	2.232(14)
Sm(1)-O(52)	2.399(8)	Cd(2)-O(6)	2.248(9)
Sm(1)-N(5)	2.473(10)	Cd(2)-O(49)	2.323(9)
Sm(1)-O(13)	2.500(8)	Cd(2)-O(48)	2.43(2)
Sm(2)-O(68)	2.213(15)	Cd(2)-O(47)	2.449(19)
Sm(2)-O(64)	2.225(9)	Cd(2)-O(5)	2.517(12)
Sm(2)-O(26)	2.261(11)	Cd(2)-O(45)	2.592(11)
Sm(2)-O(22)	2.288(9)	Cd(3)-O(52)	2.251(8)
Sm(2)-O(60)	2.321(13)	Cd(3)-N(3)	2.257(12)
Sm(2)-O(65)	2.361(9)	Cd(3)-O(49)	2.260(9)
Sm(2)-N(11)	2.519(11)	Cd(3)-O(6)	2.275(9)
Sm(2)-O(25)	2.553(12)	Cd(3)-O(10)	2.343(9)
Sm(3)-O(43)	2.215(10)	Cd(3)-O(9)	2.511(10)
Sm(3)-O(34)	2.266(11)	Cd(4)-O(54)	2.187(11)
Sm(3)-O(72)	2.271(10)	Cd(4)-N(7)	2.263(11)
Sm(3)-O(2)	2.277(10)	Cd(4)-O(69)	2.287(9)
Sm(3)-O(61)	2.352(12)	Cd(4)-O(14)	2.329(8)
Sm(3)-O(42)	2.359(13)	Cd(4)-O(66)	2.370(10)
Sm(3)-N(17)	2.550(15)	Cd(4)-O(55)	2.432(10)
Sm(3)-O(1)	2.549(11)	Cd(5)-O(18)	2.250(9)
Sm(4)-O(103)	2.208(9)	Cd(5)-O(56)	2.253(11)
Sm(4)-O(106)	2.237(9)	Cd(5)-O(58)	2.302(17)
Sm(4)-O(11)	2.264(9)	Cd(5)-O(59)	2.305(11)
Sm(4)-O(15)	2.264(9)	Cd(5)-O(17)	2.402(12)
Sm(4)-O(86)	2.359(9)	Cd(5)-O(55)	2.522(10)
Sm(4)-O(90)	2.370(9)	Cd(5)-O(57)	2.54(2)
Sm(4)-N(8)	2.529(10)	Cd(6)-N(9)	2.196(11)
Sm(4)-O(12)	2.554(9)	Cd(6)-O(59)	2.236(11)
Sm(5)-O(94)	2.194(15)	Cd(6)-O(18)	2.266(9)
Sm(5)-O(96)	2.235(10)	Cd(6)-O(65)	2.299(8)
Sm(5)-O(3)	2.258(10)	Cd(6)-O(22)	2.341(8)
Sm(5)-O(35)	2.268(11)	Cd(6)-O(21)	2.473(10)
Sm(5)-O(99)	2.299(10)	Cd(7)-O(67)	2.179(13)
Sm(5)-O(101)	2.363(10)	Cd(7)-N(13)	2.258(13)
Sm(5)-N(2)	2.490(14)	Cd(7)-O(26)	2.321(11)
Sm(5)-O(36)	2.617(12)	Cd(7)-O(40)	2.347(16)
Sm(6)-O(82)	2.224(9)	Cd(7)-O(63)	2.361(11)
Sm(6)-O(79)	2.229(14)	Cd(7)-O(62)	2.438(11)
Sm(6)-O(27)	2.235(11)	Cd(8)-O(39)	2.170(17)
Sm(6)-O(23)	2.284(10)	Cd(8)-O(30)	2.281(12)
Sm(6)-O(78)	2.297(12)	Cd(8)-O(38)	2.36(2)
Sm(6)-O(75)	2.391(11)	Cd(8)-O(41)	2.366(11)
Sm(6)-N(14)	2.541(14)	Cd(8)-O(37)	2.52(2)
Sm(6)-O(24)	2.571(13)	Cd(8)-O(29)	2.561(17)
Cd(1)-O(44)	2.267(11)	Cd(8)-O(40)	2.605(16)
Cd(1)-N(1)	2.301(12)	Cd(9)-O(61)	2.230(11)

Cd(9)-O(30)	2.265(11)
Cd(9)-N(15)	2.269(18)
Cd(9)-O(41)	2.268(12)
Cd(9)-O(34)	2.369(12)
Cd(9)-O(33)	2.460(14)
Cd(10)-O(7)	2.216(10)
Cd(10)-O(101)	2.262(10)
Cd(10)-O(100)	2.275(12)
Cd(10)-N(4)	2.297(14)
Cd(10)-O(3)	2.303(10)
Cd(10)-O(4)	2.492(10)
Cd(11)-O(108)	2.172(13)
Cd(11)-O(100)	2.281(11)
Cd(11)-O(7)	2.296(11)
Cd(11)-O(98)	2.342(14)
Cd(11)-O(8)	2.498(12)
Cd(11)-O(107)	2.507(9)
Cd(11)-O(97)	2.57(2)
Cd(12)-O(104)	2.282(9)
Cd(12)-N(6)	2.291(12)
Cd(12)-O(105)	2.347(13)
Cd(12)-O(11)	2.353(8)
Cd(12)-O(107)	2.381(9)
Cd(12)-O(102)	2.421(10)
Cd(12)-O(106)	2.638(10)
Cd(13)-O(19)	2.237(8)
Cd(13)-O(85)	2.253(8)
Cd(13)-O(90)	2.288(9)
Cd(13)-N(10)	2.302(10)
Cd(13)-O(15)	2.373(8)
Cd(13)-O(16)	2.476(9)
Cd(14)-O(84)	2.172(10)
Cd(14)-O(19)	2.244(8)
Cd(14)-O(88)	2.286(11)
Cd(14)-O(85)	2.333(9)
Cd(14)-O(20)	2.494(10)
Cd(14)-O(87)	2.50(2)
Cd(15)-O(81)	2.280(11)
Cd(15)-O(23)	2.298(10)
Cd(15)-N(12)	2.312(13)
Cd(15)-O(80)	2.322(13)
Cd(15)-O(83)	2.390(12)
Cd(15)-O(89)	2.426(10)
Cd(16)-O(77)	2.171(14)
Cd(16)-N(16)	2.230(15)
Cd(16)-O(75)	2.263(10)
Cd(16)-O(31)	2.278(14)
Cd(16)-O(27)	2.347(12)
Cd(16)-O(28)	2.464(12)
Cd(17)-O(91)	2.246(18)
Cd(17)-O(31)	2.265(14)
Cd(17)-O(77)	2.358(14)
Cd(17)-O(74)	2.44(2)
Cd(17)-O(73)	2.48(2)
Cd(17)-O(32)	2.501(17)
Cd(18)-O(93)	2.21(3)
Cd(18)-N(18)	2.247(13)
Cd(18)-O(35)	2.264(11)
Cd(18)-O(95)	2.369(10)
Cd(18)-O(92)	2.384(13)
Cd(18)-O(76)	2.395(12)
O(53)-Sm(1)-O(70)	78.1(3)
O(53)-Sm(1)-O(10)	146.8(4)
O(70)-Sm(1)-O(10)	112.0(3)
O(53)-Sm(1)-O(14)	74.6(3)
O(70)-Sm(1)-O(14)	86.4(3)
O(10)-Sm(1)-O(14)	135.4(3)
O(53)-Sm(1)-O(50)	77.3(3)
O(70)-Sm(1)-O(50)	145.9(3)
O(10)-Sm(1)-O(50)	78.4(3)
O(14)-Sm(1)-O(50)	109.3(3)
O(53)-Sm(1)-O(52)	81.5(3)
O(70)-Sm(1)-O(52)	76.4(3)
O(10)-Sm(1)-O(52)	71.2(3)
O(14)-Sm(1)-O(52)	153.0(3)
O(50)-Sm(1)-O(52)	76.8(3)
O(53)-Sm(1)-N(5)	139.3(3)
O(70)-Sm(1)-N(5)	74.9(3)
O(10)-Sm(1)-N(5)	72.7(3)
O(14)-Sm(1)-N(5)	73.9(3)
O(50)-Sm(1)-N(5)	137.8(3)
O(52)-Sm(1)-N(5)	120.1(3)
O(53)-Sm(1)-O(13)	112.9(3)
O(70)-Sm(1)-O(13)	142.5(3)
O(10)-Sm(1)-O(13)	79.0(3)
O(14)-Sm(1)-O(13)	64.3(3)
O(50)-Sm(1)-O(13)	70.0(3)
O(52)-Sm(1)-O(13)	139.0(3)
N(5)-Sm(1)-O(13)	74.7(3)
O(68)-Sm(2)-O(64)	76.1(5)
O(68)-Sm(2)-O(26)	81.7(5)
O(64)-Sm(2)-O(26)	86.3(4)
O(68)-Sm(2)-O(22)	142.6(4)
O(64)-Sm(2)-O(22)	116.4(4)
O(26)-Sm(2)-O(22)	131.6(3)
O(68)-Sm(2)-O(60)	73.9(5)
O(64)-Sm(2)-O(60)	145.6(4)
O(26)-Sm(2)-O(60)	105.5(4)
O(22)-Sm(2)-O(60)	79.9(4)
O(68)-Sm(2)-O(65)	79.0(5)
O(64)-Sm(2)-O(65)	79.2(3)
O(26)-Sm(2)-O(65)	158.2(3)
O(22)-Sm(2)-O(65)	70.0(3)
O(60)-Sm(2)-O(65)	78.9(4)
O(68)-Sm(2)-N(11)	141.8(5)
O(64)-Sm(2)-N(11)	73.0(3)
O(26)-Sm(2)-N(11)	74.5(4)
O(22)-Sm(2)-N(11)	72.9(3)

O(60)-Sm(2)-N(11)	141.0(4)	O(11)-Sm(4)-N(8)	76.2(3)
O(65)-Sm(2)-N(11)	115.8(4)	O(15)-Sm(4)-N(8)	71.5(3)
O(68)-Sm(2)-O(25)	117.7(5)	O(86)-Sm(4)-N(8)	135.4(4)
O(64)-Sm(2)-O(25)	141.4(4)	O(90)-Sm(4)-N(8)	119.7(3)
O(26)-Sm(2)-O(25)	62.6(4)	O(103)-Sm(4)-O(12)	139.5(3)
O(22)-Sm(2)-O(25)	75.7(3)	O(106)-Sm(4)-O(12)	109.5(3)
O(60)-Sm(2)-O(25)	69.6(4)	O(11)-Sm(4)-O(12)	63.0(3)
O(65)-Sm(2)-O(25)	136.6(3)	O(15)-Sm(4)-O(12)	81.6(3)
N(11)-Sm(2)-O(25)	76.9(4)	O(86)-Sm(4)-O(12)	70.3(3)
O(43)-Sm(3)-O(34)	144.2(4)	O(90)-Sm(4)-O(12)	142.9(3)
O(43)-Sm(3)-O(72)	77.1(4)	N(8)-Sm(4)-O(12)	73.4(3)
O(34)-Sm(3)-O(72)	114.5(4)	O(94)-Sm(5)-O(96)	76.1(5)
O(43)-Sm(3)-O(2)	74.1(4)	O(94)-Sm(5)-O(3)	148.5(5)
O(34)-Sm(3)-O(2)	137.6(4)	O(96)-Sm(5)-O(3)	113.9(4)
O(72)-Sm(3)-O(2)	85.6(4)	O(94)-Sm(5)-O(35)	75.2(5)
O(43)-Sm(3)-O(61)	80.4(4)	O(96)-Sm(5)-O(35)	89.1(4)
O(34)-Sm(3)-O(61)	70.2(4)	O(3)-Sm(5)-O(35)	132.1(4)
O(72)-Sm(3)-O(61)	77.9(4)	O(94)-Sm(5)-O(99)	75.3(5)
O(2)-Sm(3)-O(61)	152.2(4)	O(96)-Sm(5)-O(99)	144.9(4)
O(43)-Sm(3)-O(42)	78.6(4)	O(3)-Sm(5)-O(99)	82.2(4)
O(34)-Sm(3)-O(42)	76.9(4)	O(35)-Sm(5)-O(99)	102.8(4)
O(72)-Sm(3)-O(42)	149.7(4)	O(94)-Sm(5)-O(101)	83.4(5)
O(2)-Sm(3)-O(42)	104.8(4)	O(96)-Sm(5)-O(101)	80.3(4)
O(61)-Sm(3)-O(42)	80.5(4)	O(3)-Sm(5)-O(101)	70.0(3)
O(43)-Sm(3)-N(17)	139.4(5)	O(35)-Sm(5)-O(101)	157.9(4)
O(34)-Sm(3)-N(17)	74.8(5)	O(99)-Sm(5)-O(101)	76.5(4)
O(72)-Sm(3)-N(17)	73.5(5)	O(94)-Sm(5)-N(2)	137.8(6)
O(2)-Sm(3)-N(17)	76.2(4)	O(96)-Sm(5)-N(2)	74.3(4)
O(61)-Sm(3)-N(17)	119.1(5)	O(3)-Sm(5)-N(2)	72.4(4)
O(42)-Sm(3)-N(17)	136.3(5)	O(35)-Sm(5)-N(2)	75.0(4)
O(43)-Sm(3)-O(1)	115.2(4)	O(99)-Sm(5)-N(2)	140.6(4)
O(34)-Sm(3)-O(1)	79.4(4)	O(101)-Sm(5)-N(2)	119.9(4)
O(72)-Sm(3)-O(1)	138.6(4)	O(94)-Sm(5)-O(36)	115.9(5)
O(2)-Sm(3)-O(1)	62.9(4)	O(96)-Sm(5)-O(36)	144.3(4)
O(61)-Sm(3)-O(1)	141.0(4)	O(3)-Sm(5)-O(36)	74.3(4)
O(42)-Sm(3)-O(1)	69.1(4)	O(35)-Sm(5)-O(36)	64.4(4)
N(17)-Sm(3)-O(1)	73.4(5)	O(99)-Sm(5)-O(36)	68.4(4)
O(103)-Sm(4)-O(106)	82.0(3)	O(101)-Sm(5)-O(36)	132.4(4)
O(103)-Sm(4)-O(11)	85.8(3)	N(2)-Sm(5)-O(36)	75.9(4)
O(106)-Sm(4)-O(11)	72.2(3)	O(82)-Sm(6)-O(79)	77.7(5)
O(103)-Sm(4)-O(15)	110.6(3)	O(82)-Sm(6)-O(27)	113.9(4)
O(106)-Sm(4)-O(15)	146.3(3)	O(79)-Sm(6)-O(27)	143.1(5)
O(11)-Sm(4)-O(15)	137.6(3)	O(82)-Sm(6)-O(23)	84.8(4)
O(103)-Sm(4)-O(86)	148.6(3)	O(79)-Sm(6)-O(23)	75.2(5)
O(106)-Sm(4)-O(86)	76.2(3)	O(27)-Sm(6)-O(23)	138.2(4)
O(11)-Sm(4)-O(86)	108.2(3)	O(82)-Sm(6)-O(78)	148.4(4)
O(15)-Sm(4)-O(86)	78.2(3)	O(79)-Sm(6)-O(78)	75.4(5)
O(103)-Sm(4)-O(90)	75.7(3)	O(27)-Sm(6)-O(78)	79.9(4)
O(106)-Sm(4)-O(90)	81.9(3)	O(23)-Sm(6)-O(78)	103.9(4)
O(11)-Sm(4)-O(90)	150.0(3)	O(82)-Sm(6)-O(75)	78.2(4)
O(15)-Sm(4)-O(90)	72.0(3)	O(79)-Sm(6)-O(75)	80.8(5)
O(86)-Sm(4)-O(90)	79.0(3)	O(27)-Sm(6)-O(75)	68.5(4)
O(103)-Sm(4)-N(8)	74.5(3)	O(23)-Sm(6)-O(75)	153.1(3)
O(106)-Sm(4)-N(8)	141.7(4)	O(78)-Sm(6)-O(75)	81.4(4)

O(82)-Sm(6)-N(14)	73.9(4)	O(49)-Cd(3)-O(6)	76.2(3)
O(79)-Sm(6)-N(14)	140.7(5)	O(52)-Cd(3)-O(10)	72.2(3)
O(27)-Sm(6)-N(14)	74.6(4)	N(3)-Cd(3)-O(10)	95.3(4)
O(23)-Sm(6)-N(14)	75.6(4)	O(49)-Cd(3)-O(10)	97.7(3)
O(78)-Sm(6)-N(14)	137.5(4)	O(6)-Cd(3)-O(10)	153.9(3)
O(75)-Sm(6)-N(14)	118.4(4)	O(52)-Cd(3)-O(9)	136.0(3)
O(82)-Sm(6)-O(24)	139.0(4)	N(3)-Cd(3)-O(9)	83.9(4)
O(79)-Sm(6)-O(24)	115.2(5)	O(49)-Cd(3)-O(9)	84.7(3)
O(27)-Sm(6)-O(24)	79.9(4)	O(6)-Cd(3)-O(9)	88.9(3)
O(23)-Sm(6)-O(24)	63.7(4)	O(10)-Cd(3)-O(9)	65.1(3)
O(78)-Sm(6)-O(24)	69.2(5)	O(54)-Cd(4)-N(7)	157.7(4)
O(75)-Sm(6)-O(24)	140.1(4)	O(54)-Cd(4)-O(69)	107.7(4)
N(14)-Sm(6)-O(24)	73.3(4)	N(7)-Cd(4)-O(69)	94.5(4)
O(44)-Cd(1)-N(1)	160.7(4)	O(54)-Cd(4)-O(14)	102.6(4)
O(44)-Cd(1)-O(71)	108.1(4)	N(7)-Cd(4)-O(14)	79.0(4)
N(1)-Cd(1)-O(71)	90.5(4)	O(69)-Cd(4)-O(14)	90.4(3)
O(44)-Cd(1)-O(2)	103.0(4)	O(54)-Cd(4)-O(66)	85.6(4)
N(1)-Cd(1)-O(2)	80.6(4)	N(7)-Cd(4)-O(66)	92.4(4)
O(71)-Cd(1)-O(2)	92.8(4)	O(69)-Cd(4)-O(66)	89.7(3)
O(44)-Cd(1)-O(45)	78.4(4)	O(14)-Cd(4)-O(66)	171.4(4)
N(1)-Cd(1)-O(45)	82.5(4)	O(54)-Cd(4)-O(55)	77.2(4)
O(71)-Cd(1)-O(45)	169.4(4)	N(7)-Cd(4)-O(55)	80.5(4)
O(2)-Cd(1)-O(45)	93.8(4)	O(69)-Cd(4)-O(55)	174.5(4)
O(44)-Cd(1)-O(51)	84.6(4)	O(14)-Cd(4)-O(55)	90.9(3)
N(1)-Cd(1)-O(51)	90.7(4)	O(66)-Cd(4)-O(55)	88.2(3)
O(71)-Cd(1)-O(51)	89.2(4)	O(18)-Cd(5)-O(56)	150.2(4)
O(2)-Cd(1)-O(51)	171.0(3)	O(18)-Cd(5)-O(58)	102.4(6)
O(45)-Cd(1)-O(51)	83.0(4)	O(56)-Cd(5)-O(58)	101.9(6)
O(46)-Cd(2)-O(6)	146.5(5)	O(18)-Cd(5)-O(59)	74.1(4)
O(46)-Cd(2)-O(49)	103.3(5)	O(56)-Cd(5)-O(59)	106.6(4)
O(6)-Cd(2)-O(49)	75.5(3)	O(58)-Cd(5)-O(59)	122.3(6)
O(46)-Cd(2)-O(48)	119.3(7)	O(18)-Cd(5)-O(17)	68.3(4)
O(6)-Cd(2)-O(48)	89.7(7)	O(56)-Cd(5)-O(17)	100.3(4)
O(49)-Cd(2)-O(48)	115.2(6)	O(58)-Cd(5)-O(17)	78.4(6)
O(46)-Cd(2)-O(47)	86.9(6)	O(59)-Cd(5)-O(17)	140.4(4)
O(6)-Cd(2)-O(47)	126.2(6)	O(18)-Cd(5)-O(55)	96.3(3)
O(49)-Cd(2)-O(47)	89.0(6)	O(56)-Cd(5)-O(55)	54.0(4)
O(48)-Cd(2)-O(47)	51.0(7)	O(58)-Cd(5)-O(55)	143.4(6)
O(46)-Cd(2)-O(5)	104.6(5)	O(59)-Cd(5)-O(55)	92.9(4)
O(6)-Cd(2)-O(5)	66.7(4)	O(17)-Cd(5)-O(55)	79.7(4)
O(49)-Cd(2)-O(5)	141.6(4)	O(18)-Cd(5)-O(57)	122.9(7)
O(48)-Cd(2)-O(5)	72.0(6)	O(56)-Cd(5)-O(57)	85.4(7)
O(47)-Cd(2)-O(5)	118.3(6)	O(58)-Cd(5)-O(57)	55.0(4)
O(46)-Cd(2)-O(45)	56.0(5)	O(59)-Cd(5)-O(57)	78.4(6)
O(6)-Cd(2)-O(45)	90.5(4)	O(17)-Cd(5)-O(57)	133.1(6)
O(49)-Cd(2)-O(45)	93.9(3)	O(55)-Cd(5)-O(57)	134.5(7)
O(48)-Cd(2)-O(45)	150.0(6)	N(9)-Cd(6)-O(59)	158.3(4)
O(47)-Cd(2)-O(45)	142.5(6)	N(9)-Cd(6)-O(18)	83.3(4)
O(5)-Cd(2)-O(45)	80.6(4)	O(59)-Cd(6)-O(18)	75.1(4)
O(52)-Cd(3)-N(3)	110.7(4)	N(9)-Cd(6)-O(65)	101.2(4)
O(52)-Cd(3)-O(49)	91.2(3)	O(59)-Cd(6)-O(65)	95.9(4)
N(3)-Cd(3)-O(49)	157.1(4)	O(18)-Cd(6)-O(65)	135.1(3)
O(52)-Cd(3)-O(6)	132.5(3)	N(9)-Cd(6)-O(22)	97.0(3)
N(3)-Cd(3)-O(6)	83.8(4)	O(59)-Cd(6)-O(22)	101.3(4)

O(18)-Cd(6)-O(22)	154.3(3)	O(30)-Cd(9)-O(33)	89.4(5)
O(65)-Cd(6)-O(22)	70.2(3)	N(15)-Cd(9)-O(33)	80.2(6)
N(9)-Cd(6)-O(21)	86.4(4)	O(41)-Cd(9)-O(33)	86.1(5)
O(59)-Cd(6)-O(21)	90.6(4)	O(34)-Cd(9)-O(33)	63.5(4)
O(18)-Cd(6)-O(21)	88.5(3)	O(7)-Cd(10)-O(101)	134.8(4)
O(65)-Cd(6)-O(21)	136.1(3)	O(7)-Cd(10)-O(100)	75.8(4)
O(22)-Cd(6)-O(21)	65.9(3)	O(101)-Cd(10)-O(100)	92.0(4)
O(67)-Cd(7)-N(13)	173.8(5)	O(7)-Cd(10)-N(4)	82.3(5)
O(67)-Cd(7)-O(26)	104.0(5)	O(101)-Cd(10)-N(4)	106.6(5)
N(13)-Cd(7)-O(26)	82.2(4)	O(100)-Cd(10)-N(4)	157.7(5)
O(67)-Cd(7)-O(40)	92.7(6)	O(7)-Cd(10)-O(3)	153.3(4)
N(13)-Cd(7)-O(40)	86.1(5)	O(101)-Cd(10)-O(3)	71.0(3)
O(26)-Cd(7)-O(40)	93.3(5)	O(100)-Cd(10)-O(3)	99.9(4)
O(67)-Cd(7)-O(63)	86.9(5)	N(4)-Cd(10)-O(3)	97.7(5)
N(13)-Cd(7)-O(63)	94.0(4)	O(7)-Cd(10)-O(4)	87.7(4)
O(26)-Cd(7)-O(63)	90.2(4)	O(101)-Cd(10)-O(4)	136.5(4)
O(40)-Cd(7)-O(63)	176.4(5)	O(100)-Cd(10)-O(4)	90.1(4)
O(67)-Cd(7)-O(62)	81.7(5)	N(4)-Cd(10)-O(4)	84.8(4)
N(13)-Cd(7)-O(62)	92.1(4)	O(3)-Cd(10)-O(4)	65.8(4)
O(26)-Cd(7)-O(62)	173.0(4)	O(108)-Cd(11)-O(100)	120.2(5)
O(40)-Cd(7)-O(62)	82.2(5)	O(108)-Cd(11)-O(7)	142.0(4)
O(63)-Cd(7)-O(62)	94.3(4)	O(100)-Cd(11)-O(7)	74.1(4)
O(39)-Cd(8)-O(30)	143.9(6)	O(108)-Cd(11)-O(98)	106.7(5)
O(39)-Cd(8)-O(38)	86.5(8)	O(100)-Cd(11)-O(98)	106.8(5)
O(30)-Cd(8)-O(38)	128.8(7)	O(7)-Cd(11)-O(98)	101.1(5)
O(39)-Cd(8)-O(41)	99.8(6)	O(108)-Cd(11)-O(8)	89.5(5)
O(30)-Cd(8)-O(41)	75.9(4)	O(100)-Cd(11)-O(8)	141.0(4)
O(38)-Cd(8)-O(41)	90.0(6)	O(7)-Cd(11)-O(8)	67.1(4)
O(39)-Cd(8)-O(37)	119.3(7)	O(98)-Cd(11)-O(8)	85.6(5)
O(30)-Cd(8)-O(37)	91.6(6)	O(108)-Cd(11)-O(107)	53.2(4)
O(38)-Cd(8)-O(37)	54.7(4)	O(100)-Cd(11)-O(107)	94.0(4)
O(41)-Cd(8)-O(37)	121.8(6)	O(7)-Cd(11)-O(107)	93.3(3)
O(39)-Cd(8)-O(29)	107.2(7)	O(98)-Cd(11)-O(107)	157.2(5)
O(30)-Cd(8)-O(29)	65.0(5)	O(8)-Cd(11)-O(107)	83.9(4)
O(38)-Cd(8)-O(29)	119.9(7)	O(108)-Cd(11)-O(97)	82.4(6)
O(41)-Cd(8)-O(29)	140.2(5)	O(100)-Cd(11)-O(97)	81.6(6)
O(37)-Cd(8)-O(29)	68.4(7)	O(7)-Cd(11)-O(97)	135.6(6)
O(39)-Cd(8)-O(40)	54.2(6)	O(98)-Cd(11)-O(97)	51.4(6)
O(30)-Cd(8)-O(40)	89.7(5)	O(8)-Cd(11)-O(97)	130.5(6)
O(38)-Cd(8)-O(40)	140.0(7)	O(107)-Cd(11)-O(97)	125.5(6)
O(41)-Cd(8)-O(40)	89.9(5)	O(104)-Cd(12)-N(6)	92.9(4)
O(37)-Cd(8)-O(40)	147.6(6)	O(104)-Cd(12)-O(105)	106.2(4)
O(29)-Cd(8)-O(40)	82.9(5)	N(6)-Cd(12)-O(105)	158.5(4)
O(61)-Cd(9)-O(30)	136.0(5)	O(104)-Cd(12)-O(11)	91.3(3)
O(61)-Cd(9)-N(15)	109.9(6)	N(6)-Cd(12)-O(11)	80.5(4)
O(30)-Cd(9)-N(15)	81.4(6)	O(105)-Cd(12)-O(11)	108.3(4)
O(61)-Cd(9)-O(41)	94.3(4)	O(104)-Cd(12)-O(107)	176.2(3)
O(30)-Cd(9)-O(41)	78.2(4)	N(6)-Cd(12)-O(107)	84.8(4)
N(15)-Cd(9)-O(41)	155.5(6)	O(105)-Cd(12)-O(107)	75.6(4)
O(61)-Cd(9)-O(34)	70.5(4)	O(11)-Cd(12)-O(107)	91.3(3)
O(30)-Cd(9)-O(34)	152.6(4)	O(104)-Cd(12)-O(102)	86.0(3)
N(15)-Cd(9)-O(34)	96.4(6)	N(6)-Cd(12)-O(102)	88.9(4)
O(41)-Cd(9)-O(34)	95.5(4)	O(105)-Cd(12)-O(102)	82.7(4)
O(61)-Cd(9)-O(33)	133.8(4)	O(11)-Cd(12)-O(102)	168.9(3)

O(107)-Cd(12)-O(102)	90.9(3)	N(12)-Cd(15)-O(89)	90.5(4)
O(104)-Cd(12)-O(106)	82.8(3)	O(80)-Cd(15)-O(89)	83.3(4)
N(6)-Cd(12)-O(106)	143.9(4)	O(83)-Cd(15)-O(89)	82.4(4)
O(105)-Cd(12)-O(106)	51.3(4)	O(77)-Cd(16)-N(16)	155.2(5)
O(11)-Cd(12)-O(106)	63.9(3)	O(77)-Cd(16)-O(75)	97.4(5)
O(107)-Cd(12)-O(106)	100.9(3)	N(16)-Cd(16)-O(75)	105.9(4)
O(102)-Cd(12)-O(106)	126.2(3)	O(77)-Cd(16)-O(31)	76.2(5)
O(19)-Cd(13)-O(85)	76.2(3)	N(16)-Cd(16)-O(31)	81.1(5)
O(19)-Cd(13)-O(90)	133.1(3)	O(75)-Cd(16)-O(31)	136.4(4)
O(85)-Cd(13)-O(90)	92.5(3)	O(77)-Cd(16)-O(27)	97.7(5)
O(19)-Cd(13)-N(10)	83.4(4)	N(16)-Cd(16)-O(27)	98.6(5)
O(85)-Cd(13)-N(10)	158.0(4)	O(75)-Cd(16)-O(27)	68.9(4)
O(90)-Cd(13)-N(10)	107.7(4)	O(31)-Cd(16)-O(27)	154.1(4)
O(19)-Cd(13)-O(15)	154.6(3)	O(77)-Cd(16)-O(28)	86.0(5)
O(85)-Cd(13)-O(15)	99.8(3)	N(16)-Cd(16)-O(28)	83.9(5)
O(90)-Cd(13)-O(15)	71.5(3)	O(75)-Cd(16)-O(28)	134.3(4)
N(10)-Cd(13)-O(15)	95.0(4)	O(31)-Cd(16)-O(28)	88.8(5)
O(19)-Cd(13)-O(16)	90.4(3)	O(27)-Cd(16)-O(28)	65.5(4)
O(85)-Cd(13)-O(16)	86.6(3)	O(91)-Cd(17)-O(31)	144.6(6)
O(90)-Cd(13)-O(16)	134.9(3)	O(91)-Cd(17)-O(77)	102.2(6)
N(10)-Cd(13)-O(16)	85.3(3)	O(31)-Cd(17)-O(77)	72.9(5)
O(15)-Cd(13)-O(16)	64.3(3)	O(91)-Cd(17)-O(74)	83.0(8)
O(84)-Cd(14)-O(19)	139.0(4)	O(31)-Cd(17)-O(74)	131.8(7)
O(84)-Cd(14)-O(88)	123.5(4)	O(77)-Cd(17)-O(74)	95.0(7)
O(19)-Cd(14)-O(88)	94.8(4)	O(91)-Cd(17)-O(73)	120.6(7)
O(84)-Cd(14)-O(85)	101.2(4)	O(31)-Cd(17)-O(73)	90.5(6)
O(19)-Cd(14)-O(85)	74.5(3)	O(77)-Cd(17)-O(73)	118.8(6)
O(88)-Cd(14)-O(85)	110.7(4)	O(74)-Cd(17)-O(73)	54.1(4)
O(84)-Cd(14)-O(20)	106.5(4)	O(91)-Cd(17)-O(32)	104.6(7)
O(19)-Cd(14)-O(20)	66.7(3)	O(31)-Cd(17)-O(32)	68.5(5)
O(88)-Cd(14)-O(20)	75.4(4)	O(77)-Cd(17)-O(32)	140.5(5)
O(85)-Cd(14)-O(20)	141.2(3)	O(74)-Cd(17)-O(32)	116.5(7)
O(84)-Cd(14)-O(87)	81.5(5)	O(73)-Cd(17)-O(32)	69.9(6)
O(19)-Cd(14)-O(87)	138.9(5)	O(93)-Cd(18)-N(18)	162.2(6)
O(88)-Cd(14)-O(87)	51.9(5)	O(93)-Cd(18)-O(35)	115.6(6)
O(85)-Cd(14)-O(87)	93.8(5)	N(18)-Cd(18)-O(35)	81.1(4)
O(20)-Cd(14)-O(87)	116.5(5)	O(93)-Cd(18)-O(95)	92.5(7)
O(81)-Cd(15)-O(23)	92.5(4)	N(18)-Cd(18)-O(95)	92.7(4)
O(81)-Cd(15)-N(12)	94.2(4)	O(35)-Cd(18)-O(95)	93.3(4)
O(23)-Cd(15)-N(12)	79.6(4)	O(93)-Cd(18)-O(92)	84.4(7)
O(81)-Cd(15)-O(80)	102.6(5)	N(18)-Cd(18)-O(92)	89.5(5)
O(23)-Cd(15)-O(80)	104.8(4)	O(35)-Cd(18)-O(92)	90.1(4)
N(12)-Cd(15)-O(80)	162.3(5)	O(95)-Cd(18)-O(92)	176.2(4)
O(81)-Cd(15)-O(83)	174.4(4)	O(93)-Cd(18)-O(76)	72.2(6)
O(23)-Cd(15)-O(83)	91.6(4)	N(18)-Cd(18)-O(76)	90.6(4)
N(12)-Cd(15)-O(83)	82.9(4)	O(35)-Cd(18)-O(76)	170.0(4)
O(80)-Cd(15)-O(83)	79.9(5)	O(95)-Cd(18)-O(76)	92.6(4)
O(81)-Cd(15)-O(89)	92.9(3)	O(92)-Cd(18)-O(76)	84.2(4)
O(23)-Cd(15)-O(89)	169.0(3)		