Electronic Supplementary Information

The influence of secondary building linker geometry on photochromism of naphthalenediimide based metal-organic frameworks†

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1. Graphics

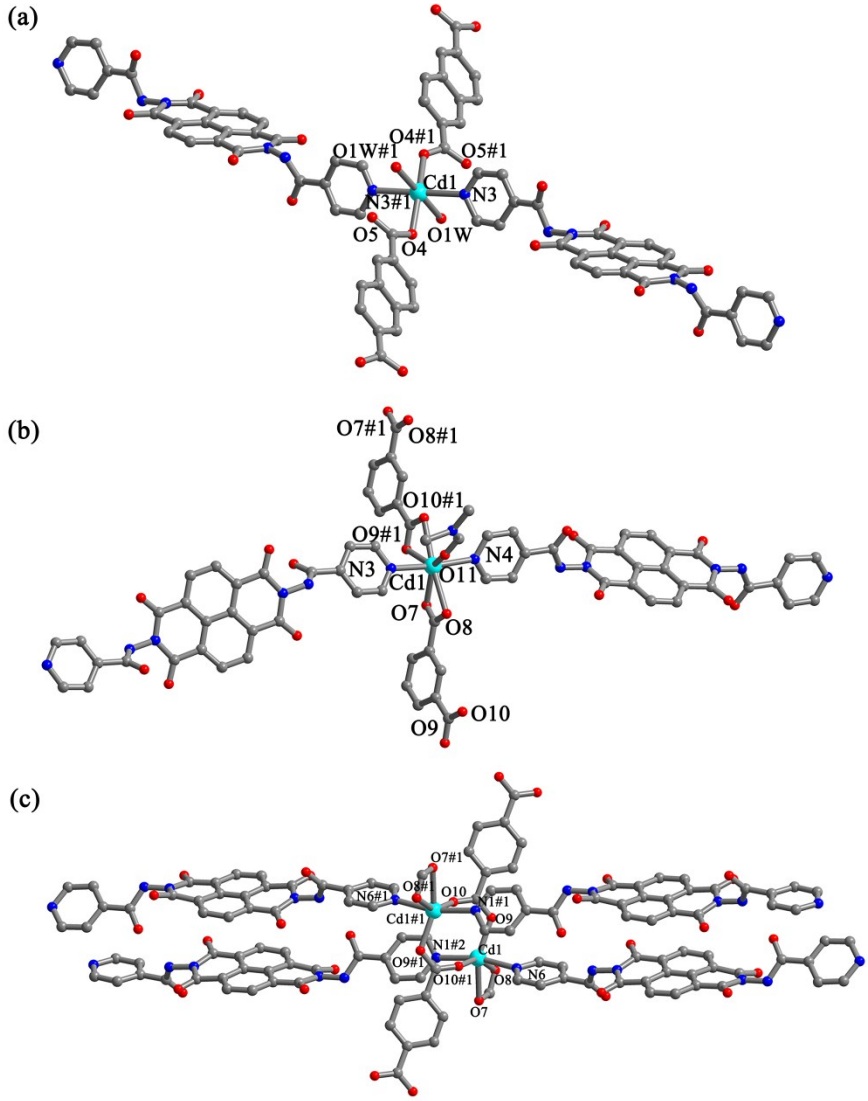

Fig. S1 Coordination environment of Cd^{2+} in **1** (a), **2** (b) and **3** (c).

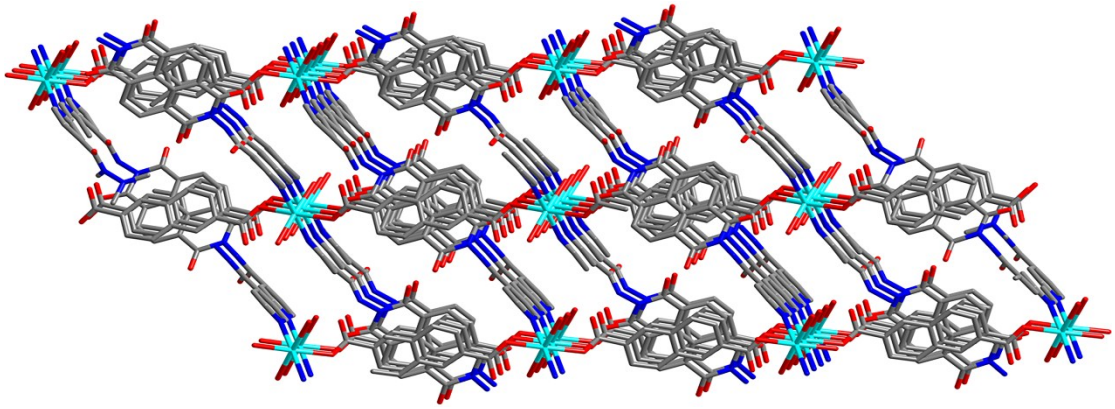

Fig. S2 The view of three-dimensional framework of **1**with 1-D channels.

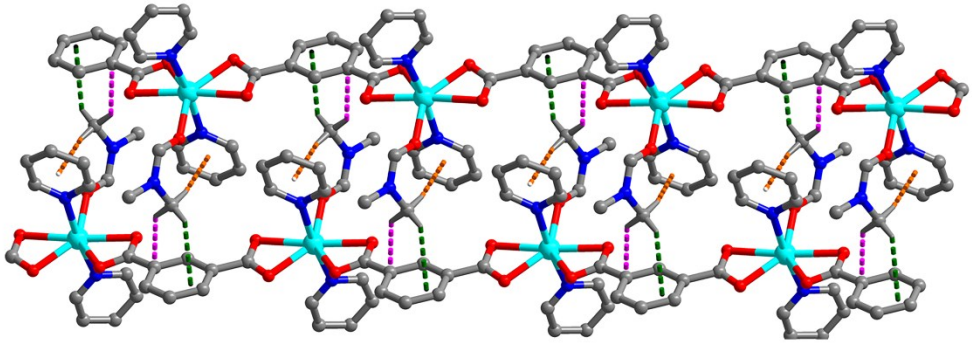

Fig. S3 The C-H···π interactions between DMF molecules and two kinds ligands in **2** (dashed orange bonds: 3.458 Å, dashed pink bonds: 2.795 Å, dashed green bonds: 2.987Å).

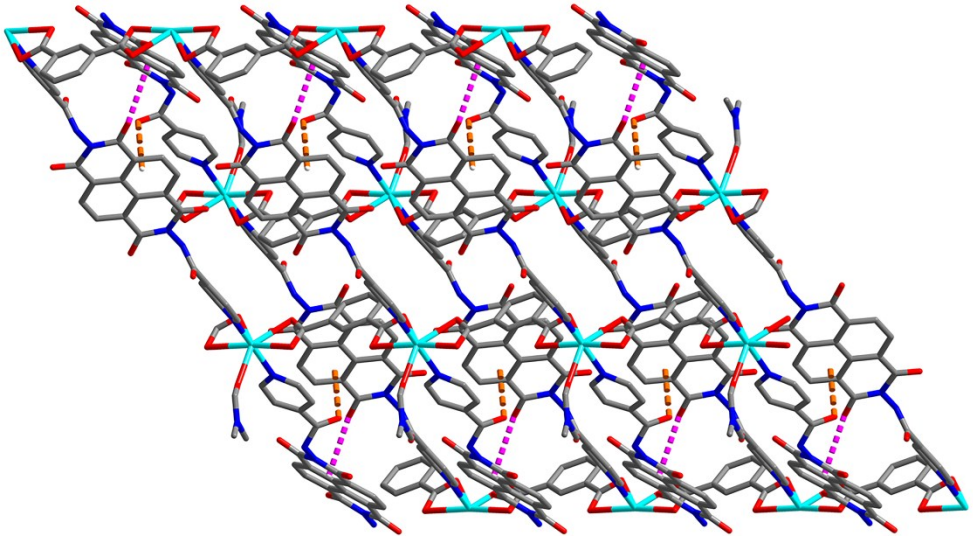

Fig. S4 The lone pair–π interactions in **2** (dashed orange bonds: 3.098 Å, dashed pink bonds: 3.146 Å).

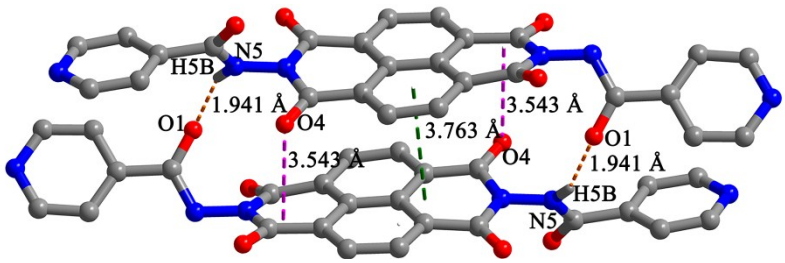

Fig. S5 Another N-H···O hydrogen bonds (dashed orange bonds: 1.941 Å), lone pair-π interactions (dashed pink bonds: 3.543 Å) and one kind π-π stacking interaction (dashed green bond: 3.763 Å) in neighbouring IsoNDI ligands in **3**.

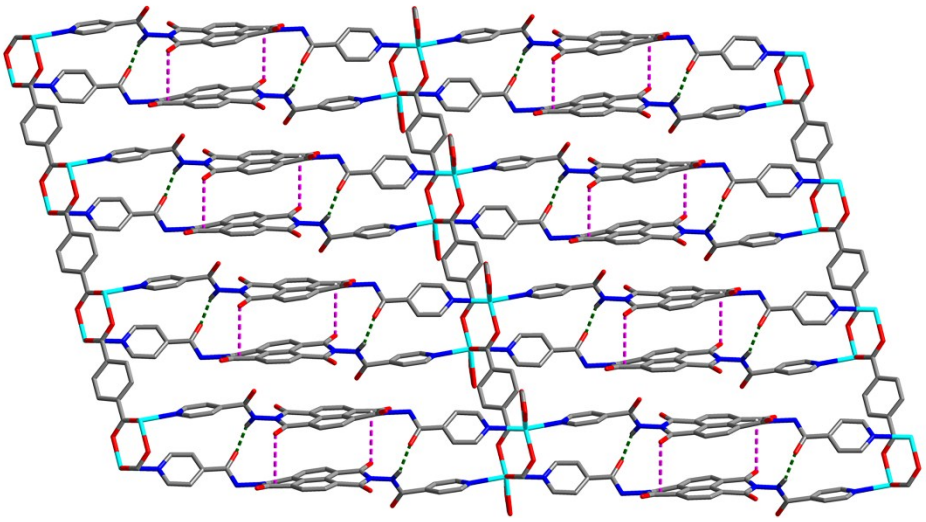

Fig. S6 The N-H···O hydrogen bonds and lone pair-π interactions showed in **3.**

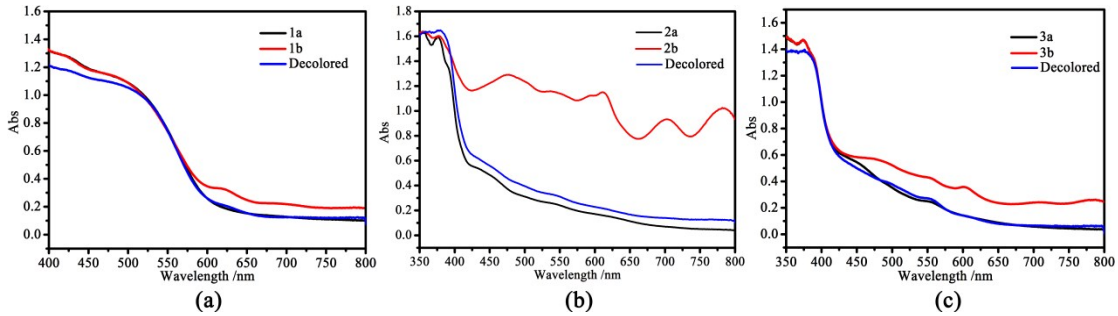

Fig. S7 The UV-Vis spectrums of **1-3** in the photochromic process. Lables: **1a**, **2a** and **3a**, before irradiation; **1b**, **2b** and **3b**, after irradiated by a 300W Xenon lamp in 10 min; **Decolored**: after dark treatment.

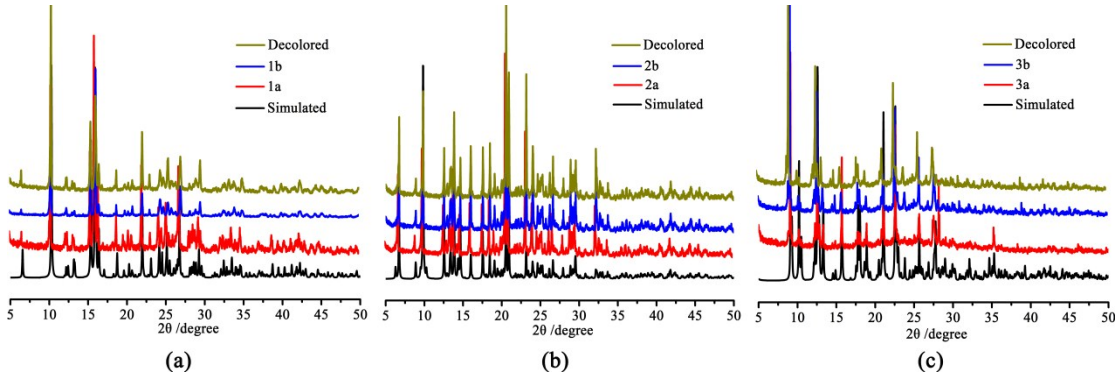

Fig. S8 PXRD patterns of **1-3**. Lables: **1a**, **2a** and **3a**, before irradiation; **1b**, **2b** and **3b**, after irradiation; **Decolored**: after dark treatment.

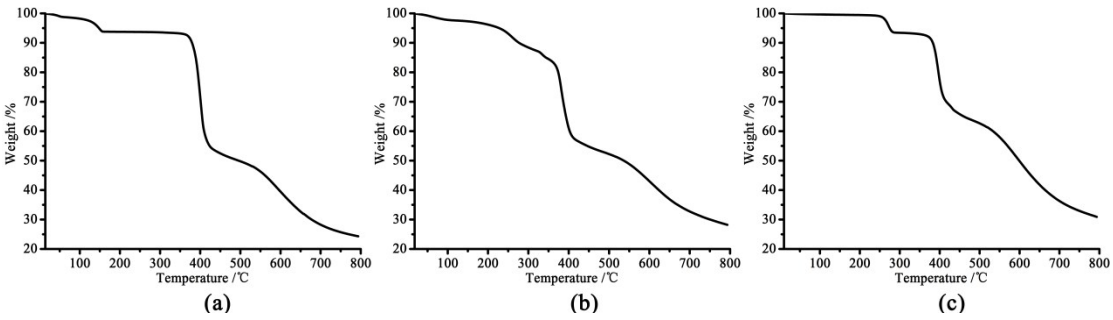

Fig. S9 Thermogravimetric analyses of **1** (a)**, 2** (b) and **3** (c) were carried out in powder states under N_2 atmosphere.

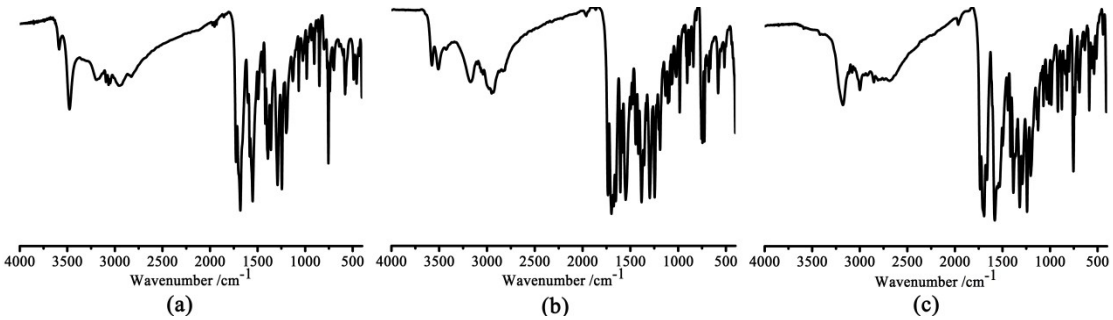

Fig. S10 FT-IR spectra of **1** (a)**, 2** (b) and **3** (c).

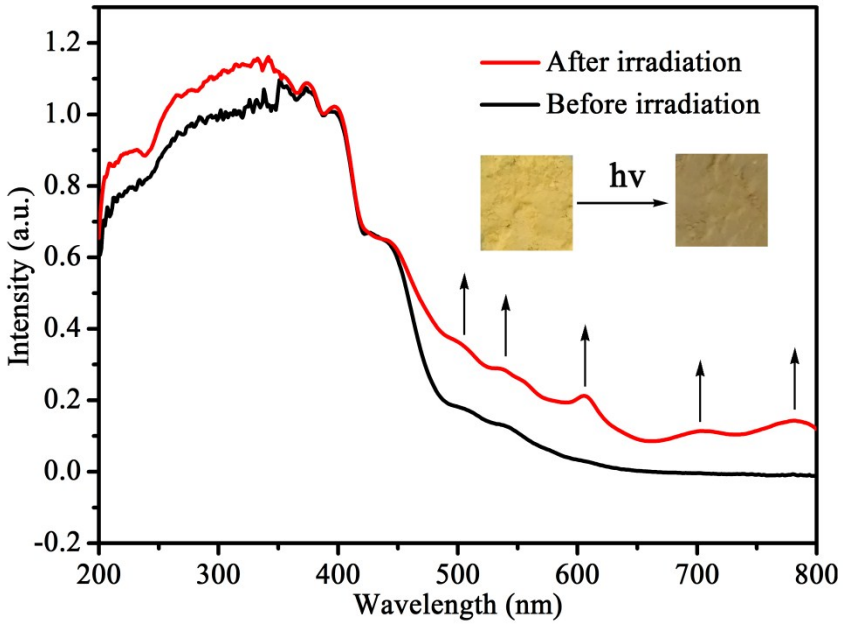

Fig. S11 The UV-Vis spectrum and photographic images of IsoNDI ligand in the photochromic process.

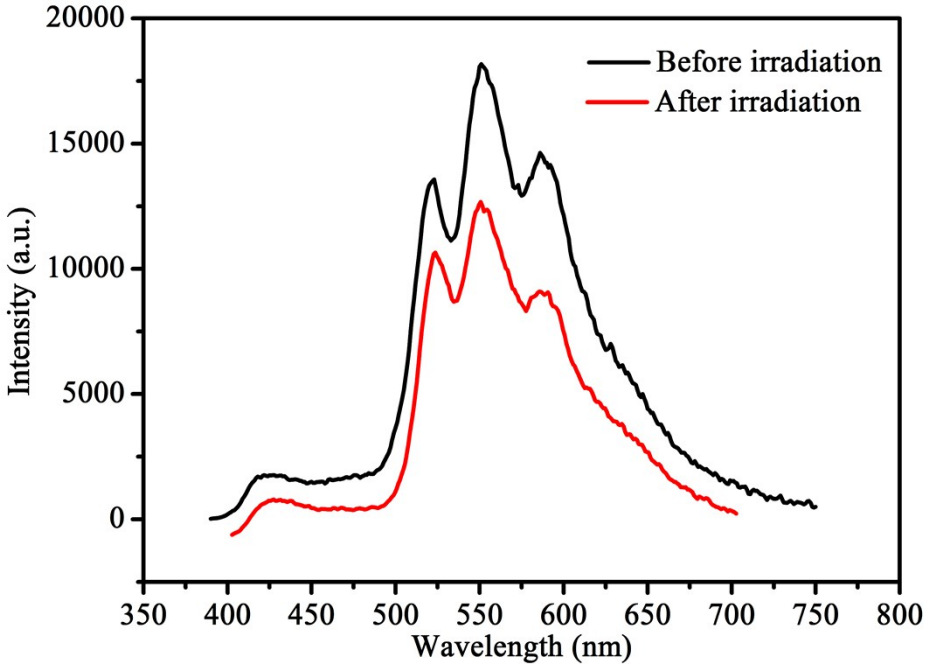

Fig. S12 Photo-controlled luminescence spectrum of IsoNDI ligand.

2. Tables

Table S1. Crystal data and structure refinement parameters for compounds **1-3**

Compound	**1**	**2**	**3**
Empirical formula	$C_{38}H_{24}N_6O_{12}Cd$	$C_{37}H_{26}N_7O_{11}Cd$	$C_{31}H_{15}N_6O_{10}Cd$
Formula weight	869.05	856.84	743.90
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	C 2c	Pī	Pī
a (Å)	26.906(4)	10.1261(7)	7.8706(10)
b(Å)	7.5367(9)	13.8772(9)	10.2356(13)
c (Å)	17.210(2)	14.7762(10)	19.467(3)
α (°)	90	88.202(1)	90.351(2)
β (°)	92.375(4)	72.861(1)	94.250(2)
γ (°)	90	71.667(1)	111.416(2)
V (Å^3)	3486.8(7)	1879.2(2)	1455.04(30)
Z	4	3	2
T (K)	296(2)	296(2)	296(2)
ρ_{calc} (g/cm^3)	1.655	1.737	1.698
F (000)	2940	948	1190
Absorption coefficient	0.704	1.756	0.823
Goodness-of-fit on F^2	0.990	1.339	1.141
$R_1{}^a$, $wR_2{}^b$ ($I > 2\sigma(I)$)	0.0440, 0.0873	0.0827, 0.2830	0.0277, 0.0858
$R_1{}^a$, $wR_2{}^b$ (*all data*)	0.0742, 0.0975	0.0890, 0.2959	0.0308, 0.0927

$^aR_1 = \sum \| F_0 | - | F_c \| / \sum | F_0 |$. $^bwR_2 = [\sum w(F_0^2 - F_c^2)^2 / \sum w(F_0^2)]^{1/2}$.

Table S2. Selected Bond lengths [Å] and angles [°] for compounds **1-3**

Compound 1			
Cd(1)-O(1W)	2.371(3)	Cd(1)-O(4)	2.238(2)
Cd(1)-O(1W)#1	2.371(3)	Cd(1)-O(4)#1	2.237(2)
Cd(1)-N(3)	2.362(3)	Cd(1)-N(3)#1	2.362(3)
O(1W)-Cd(1)-N(3)	80.977	O(1W)#1-Cd(1)-N(3)#1	80.977
O(1W)-Cd(1)-O(4)	89.263	O(1W)#1-Cd(1)-O(4)#1	89.263
O(1W)-Cd(1)- O(1W)#1	180.000	O(4)-Cd(1)-N(3)	83.502
O(4)#1-Cd(1)-N(3)#1	83.502	O(4)-Cd(1)-O(4)#1	180.000
N(3)-Cd(1)-N(3)#1	180.000		
Compound 2			
Cd(1)-O(7)	2.299(1)	Cd(1)-O(9)#1	2.371(0)
Cd(1)-O(10)#1	2.477(7)	Cd(1)-O(11)	2.267(6)
Cd(1)-N(3)	2.365(3)	Cd(1)-N(4)	2.317(8)
O(11)-Cd(1)-O(7)	135.8(42)	O(11)-Cd(1)-O(9)#1	139.8(40)
O(11)-Cd(1)-O(10)#1	89.5(42)	O(11)-Cd(1)-N(3)	79.0(89)
O(11)-Cd(1)-N(4)	96.2(66)	O(7)-Cd(1)-O(9)#1	80.8(71)
O(7)-Cd(1)-O(10)#1	134.2(87)	O(7)-Cd(1)-N(3)	94.1(27)
O(7)-Cd(1)-N(4)	92.4(53)	N(4)-Cd(1)-O(9)#1	97.6(82)
N(4)-Cd(1)-O(10)#1	86.2(24)	N(4)-Cd(1)-N(3)	173.418
N(3)-Cd(1)-O(9)#1	82.2(20)	N(3)-Cd(1)-O(10)#1	89.0(61)
O(9)#1-Cd(1)-O(10)#1	54.2(20)		
Compound 3			
Cd(1)-O(7)	2.379(8)	Cd(1)-O(8)	2.445(7)
Cd(1)-O(9)	2.208(4)	Cd(1)-O(10)#1	2.260(5)
Cd(1)-N(1)#2	2.357(7)	Cd(1)-N(6)	2.362(9)
O(9)-Cd(1)-O(10)#1	114.1(70)	O(9)-Cd(1)-O(7)	145.9(23)
O(9)-Cd(1)-O(8)	92.3(01)	O(9)-Cd(1)-N(1)#2	104.1(10)
O(9)-Cd(1)-N(6)	89.5(91)	O(10)#1-Cd(1)-O(7)	99.3(84)
O(10)#1-Cd(1)-O(8)	153.4(68)	O(10)#1-Cd(1)-N(1)#2	86.7(87)
O(10)#1-Cd(1)-N(6)	85.5(42)	O(7)-Cd(1)-O(8)	54.1(02)
N(1)#2-Cd(1)-O(7)	82.7(10)	N(1)#2-Cd(1)-O(8)	88.4(89)
N(1)#2-Cd(1)-N(6)	166.1(21)	N(6)-Cd(1)-O(7)	87.1(49)
N(6)-Cd(1)-O(8)	93.2(31)		

Symmetry codes: for **1:** #1, 1-x, -y, 1-z; for **2**: #1, 1+x, y, z; for **3**: #1, 1-x, 2-y, -z; #2, -1+x, 1+y, -1+z;