Supporting information

The first 2D trinuclear Cd(II)-complex with adenine nucleobase: hydrothermal synthesis, crystal structure and fluorescent properties

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Table S1. Crystal Data and Structure Refinement of **1**

Formula	$C_{11}H_{15.5}Cd_{1.5}N_5O_{5.75}$
Fw(g mol^{-1})	478.38
Wavelength (Å)	0.71073
Crystal size(mm)	0.35×0.24×0.20
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	9.250(2)
b (Å)	12.011(3)
c (Å)	14.326(4)
β (°)	92.618(3)
V (Å^3)	1590.0(7)
Z	4
θ range (°)	2.21 – 25.00
Index ranges	$-10 \le h \le 11$, $-14 \le k \le 14$, $-17 \le l \le 9$
ρ (g cm^{-3})	1.998
μ (mm^{-1})	2.061
Reflections collected/ Unique	8203/2788 (R_{int} = 0.0347)
Data/restraints/parameters	2788 / 0 / 224
GoF	1.034
F(000)	938
T/K	293(2)
R_1[a]/wR_2 [b](I>2σ(I))	0.0362 / 0.0836
R_1/wR_2 (all data)	0.0511 / 0.0917
Largest diff. peak and hole (e.Å^{-3})	0.595 and –0.889

[a] $R_1 = \Sigma||F_o|-|F_c||/|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

Table S2. Selected Bond Distances (Å) and Angles (°)

Cd(1)–N(7)$^{\#1}$	2.282(4)	Cd(2)–N(9)$^{\#2}$	2.195(4)
Cd(1)–N(3)	2.326(5)	Cd(2)–N(9)	2.195(5)
Cd(1)–O(4)$^{\#2}$	2.389(4)	Cd(2)–O(1)$^{\#2}$	2.350(4)
Cd(1)–O(1)	2.392(4)	Cd(2)–O(1)	2.350(4)
Cd(1)–O(5)	2.405(5)	Cd(2)–O(4)	2.383(4)
Cd(1)–O(2)	2.462(5)	Cd(2)–O(4)$^{\#2}$	2.383(4)
Cd(1)–O(3)$^{\#2}$	2.536(5)		
N(7)$^{\#1}$–Cd(1)–N(3)	104.52(16)	O(1)–Cd(1)–O(3)$^{\#2}$	125.56(15)
N(7)$^{\#1}$–Cd(1)–O(4)$^{\#2}$	133.37(16)	O(5)–Cd(1)–O(3)$^{\#2}$	101.7(2)
N(3)–Cd(1)–O(4)$^{\#2}$	93.28(16)	O(2)–Cd(1)–O(3)$^{\#2}$	176.62(19)
N(7)$^{\#1}$–Cd(1)–O(1)	147.62(15)	N(9)$^{\#2}$–Cd(2)–N(9)	180.0(2)
N(3)–Cd(1)–O(1)	86.87(15)	N(9)$^{\#2}$–Cd(2)–O(1)$^{\#2}$	90.48(15)
O(4)$^{\#2}$–Cd(1)–O(1)	74.48(14)	N(9)–Cd(2)–O(1)$^{\#2}$	89.52(15)
N(7)$^{\#1}$–Cd(1)–O(5)	84.69(18)	N(9)$^{\#2}$–Cd(2)–O(1)	89.52(15)
N(3)–Cd(1)–O(5)	167.84(18)	N(9)–Cd(2)–O(1)	90.48(15)
O(4)$^{\#2}$–Cd(1)–O(5)	85.77(19)	O(1)$^{\#2}$–Cd(2)–O(1)	180.000(1)
O(1)–Cd(1)–O(5)	81.19(18)	N(9)$^{\#2}$–Cd(2)–O(4)	89.93(17)
N(7)$^{\#1}$–Cd(1)–O(2)	95.88(16)	N(9)–Cd(2)–O(4)	90.07(17)
N(3)–Cd(1)–O(2)	89.61(16)	O(1)$^{\#2}$–Cd(2)–O(4)	75.35(15)
O(4)$^{\#2}$–Cd(1)–O(2)	127.49(14)	O(1)–Cd(2)–O(4)	104.65(15)
O(1)–Cd(1)–O(2)	53.33(14)	N(9)$^{\#2}$–Cd(2)–O(4)$^{\#2}$	90.07(17)
O(5)–Cd(1)–O(2)	81.4(2)	N(9)–Cd(2)–O(4)$^{\#2}$	89.93(17)
N(7)$^{\#1}$–Cd(1)–O(3)$^{\#2}$	85.77(16)	O(1)$^{\#2}$–Cd(2)–O(4)$^{\#2}$	104.65(15)
N(3)–Cd(1)–O(3)$^{\#2}$	87.1(2)	O(1)–Cd(2)–O(4)$^{\#2}$	75.35(15)
O(4)$^{\#2}$–Cd(1)–O(3)$^{\#2}$	51.97(15)	O(4)–Cd(2)–O(4)$^{\#2}$	180.000(1)

Symmetry Codes: #1: x, $-y + 3/2$, z + 1/2; #2: $-x + 2$, $-y + 1$, $-z + 2$.

Table S3. Selected Hydrogen Bond Lengths (Å) and Bond Angles (°) [a]

D–H···A	*d* (D–H)	*d* (H···.A)	*d* (D···A)	∠DHA
O5–H5'···O6[a]	0.853	1.791	2.627(3)	166.18
O5–H5"···O3[b]	0.851	2.007	2.848(5)	169.29
N6–H6'···N1[c]	0.860	2.082	2.932(1)	169.70
N6–H6"···O2[d]	0.860	1.966	2.813(2)	167.81

[a] $x + 1, y, z + 1$; [b] $x, -y + 1/2, z + 1/2$; [c] $-x + 1, -y + 2, -z + 2$; [d] $x, -y + 3/2, z - 1/2$.

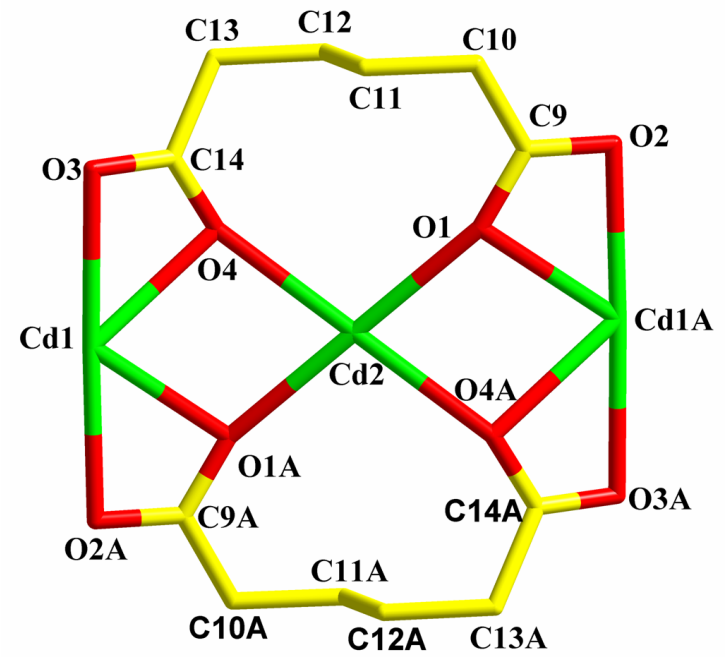
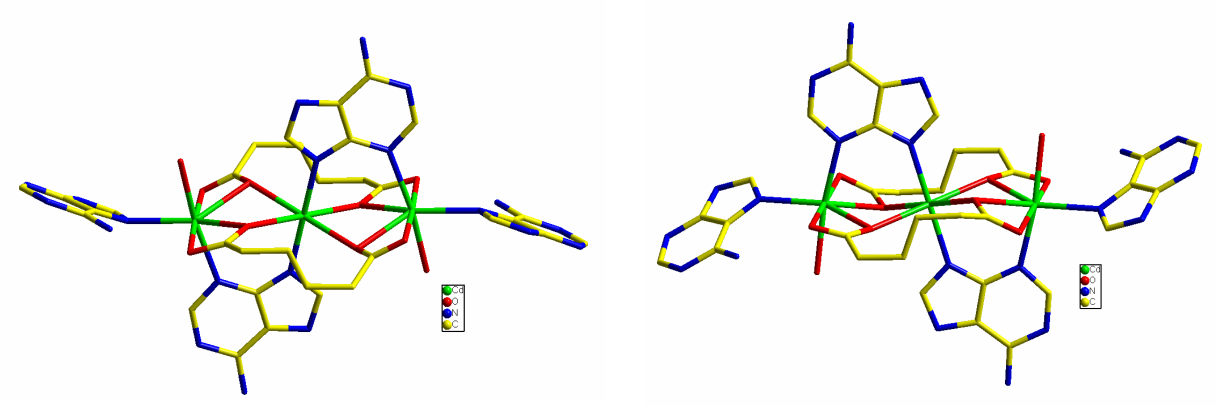


Figure S1. The unique plane formed by three Cd(II) centers and two ap ligands



(a) (b)

Figure S2. A local view of neighboring trinuclear Cd(II)-Ade-ap clusters by rotation exhibiting different geometries

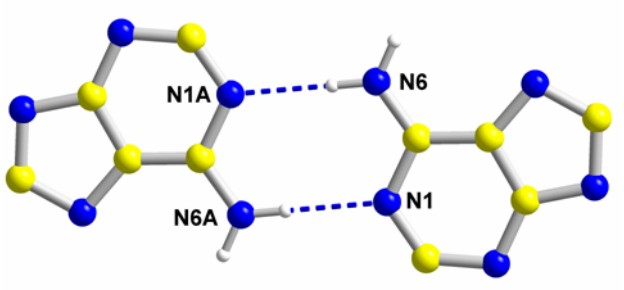


Figure S3. Pairs of "head to tail" N6–H6′···N1A base pair interactions

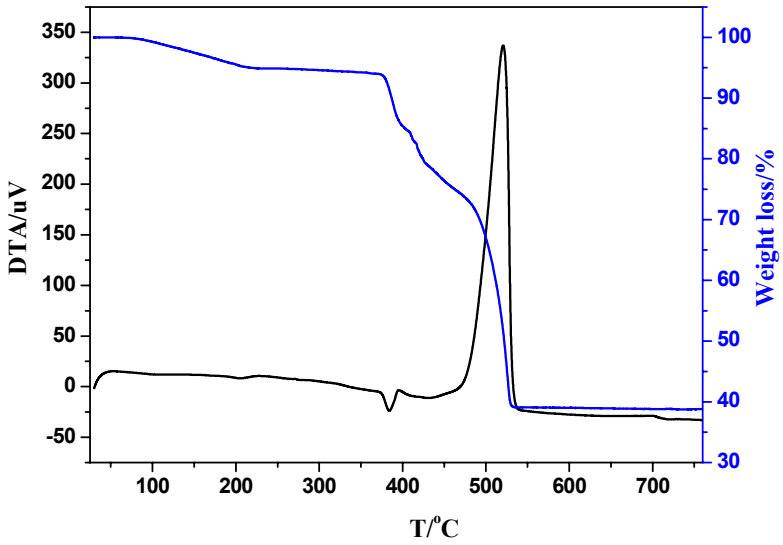


Figure S4. TGA and DTA curve of **1**