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Poly[bis[μ_2-2-(2-pyridylmethylamino)-ethanesulfonato]cadmium(II)]

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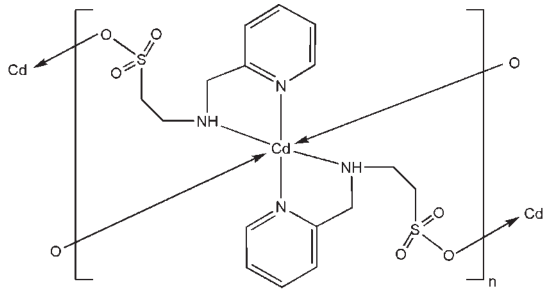
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.019; wR factor = 0.049; data-to-parameter ratio = 16.4.

The title compound $[Cd(C_8H_{11}N_2O_3S)_2]_n$, is a two-dimensional coordination polymer based on a Cd^{2+} atom and deprotonated 2-(2-pyridylmethylamino)ethanesulfonic acid (Hpmt). The complex has molecular symmetry C_i as a consequence of the Cd^{II} being located on an inversion centre. Two N atoms of each pmt$^-$ ligand coordinate to the Cd^{2+} ion and its sulfonate O atom bonds to an adjacent Cd^{2+} ion. 24-membered (–Cd—N—C—C—S—O–)$_4$ rings are formed between neighbouring Cd^{2+} ions; these are interconnected, forming a two-dimensional layer structure. In respect to stereogenic amino N atom and the inversion symmetry of the complex, the compound is a 1:1 racemate. The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds and further connected by π–π stacking interactions between the pyridyl rings [average interplanar distance and centroid–centroid separation = 3.582 (1) and 3.634 (1)Å, respectively], forming a three-dimensional supramolecular architecture.

Related literature

For different coordination modes of the pmt$^-$ ligand in complexes derived from Hpmt, see: Du & Zhang (2009); Li *et al.* (2006, 2007*a*,*b*, 2008*a*,*b*); Liao *et al.* (2007).



Experimental

Crystal data

$[Cd(C_8H_{11}N_2O_3S)_2]$
M_r = 542.90
Monoclinic, $P2_1/c$
a = 8.8982 (8) Å
b = 14.0206 (12) Å
c = 7.9040 (7) Å
β = 103.579 (1)°
V = 958.52 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.40 mm^{-1}
T = 291 K
0.22 × 0.16 × 0.12 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.749, T_{max} = 0.849
5691 measured reflections
2178 independent reflections
2008 reflections with $I > 2\sigma(I)$
R_{int} = 0.011

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.049
S = 1.03
2178 reflections
133 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N1	2.2853 (14)	Cd1—N2	2.3979 (15)
Cd1—O2^i	2.3496 (14)		

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3^{ii}	0.91	2.26	3.089 (2)	152

Symmetry code: (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2239).

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supplementary materials

Acta Cryst. (2009). E**65**, m1655   [**doi:10.1107/S1600536809049162**]

Poly[bis[μ_2-2-(2-pyridylmethylamino)ethanesulfonato]cadmium(II)]

Z.-X. Du and **X.-H. Chang**

Comment

In the previous literatures, several complexes derived from Hpmt have been reported. Among them, pmt$^-$ ligand displays different coordination modes, such as tridentate chelate (Du & Zhang, 2009; Li *et al.*, 2006, 2008*a*; Liao *et al.*, 2007), μ_2 bridge(Li *et al.*, 2007*a*, 2008*b*) and μ_3 bridge (Li *et al.*, 2007*b*). In this paper, we describe another new complex of pmt$^-$, (I), Figure 1.

Compound 1 is a two-dimensional coordination polymer and the repeating unit comprises one Cd^{2+} ion and two pmt$^-$ ligands(Fig. 1, Table 1). Cd^{2+} ion situates on a centre of symmetry and is six-coordinated with four N atoms from two pmt$^-$ ligands along with two sulfonate O atoms belonging to another two ligands, showing a distorted octahedral geometry (Table 1). The four N atoms from two pmt$^-$ ligands define the equatorial plane with the Cd centre located in the plane, and two O atoms are at the axial positions with O2A—Cd1—O2B angle of just 180°[Symmetry codes: (A)1 - *x*, -1/2 + *y*, 0.5 - *z*; (B)*x*, 0.5 - *y*, -1/2 + *z*]. Each pmt$^-$ plays as a μ_2 bridge to connect two Cd^{2+} ions and each Cd^{2+} ion links four pmt$^-$ ligands, forming an infinite two-dimensional layer structure with (4, 4) topology (Figure 2). The network is based on (Cd(pmt))$_4$ rhombus, a 24-membered metal-ligand ring (–Cd—N—C—C—S—O–)$_4$ formed by four pmt$^-$ and four quadruply connected Cd^{2+} ions. The edge Cd···Cd distance of the rhombus is 8.048 (3)Å and the Cd···Cd separations through the diagonal of the rhombus are 7.904 (2)Å and 14.021 (1) Å, respectively (Figure 2).

The two-dimensional layer is stabilized by intermolecular N—H···O hydrogen bonds (Figure 3 & Table 2). The interlayers are further connected by π-π stacking interactions of parallel pyridine rings of adjacent layers. The interplanar average distance and ringcentroid separation distance are 3.582 (1)Å and 3.634 (1) Å, respectively. Thus, the three-dimensional supramolecular architecture of (I) is formed (Figure 4).

Experimental

The ligand Hpmt was prepared according to the method of Li *et al.*, 2006. A water solution (5 ml) of ligand Hpmt (2 mmol, 0.432 g) was added dropwise to a solution of $CdCl_2$. $2.5H_2O$ (0.228 g, 1.0 mmol) in methanol (8 ml), then the obtained mixture was stirred at 333 K for 3 h. After that, the mixture was basified with KOH (1 mol/l) to a pH of 7.5–8.0 and continued stirring for another 4 h, filtrated. Two weeks later, colourless claviform crystals were grown from the filtrate by slow evaporation. Analysis, found: C 35.40, H 4.02, N 10.36, S 11.36%; $C_{16}H_{22}CdN_4O_6S_2$ requires: C 35.36, H 4.05, N 10.31, S 11.42%. IR (KBr, ν, cm^{-1}): 771.2[γ(CC—H)], 745.7(γCH_2); 1188.3, 1157.4, 1040.6(ν SO_3^-); 1607.7, 1571.7(ν CC + ν CN); 3266.2(ν N—H). CCDC 614219.

Refinement

H atoms bonded to C were positioned geometrically with C—H distance of 0.93–0.97 Å, and treated as riding atoms, with U_{iso}(H)=1.2U_{eq}(C). The N—H hydrogen atom was located in a difference Fourier map and refined isotropically.

Figures

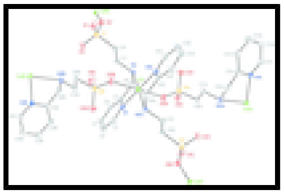

Fig. 1. The coordination of Cd^{2+} ion of (I) with the atom-numbering scheme. Displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted. [Symmetry codes: (A)1 - *x*, -1/2 + *y*, 0.5 - *z*; (B)*x*, 0.5 - *y*, -1/2 + *z*; (C)1 - *x*, -*y*, -*z*; (D)1 - *x*, 1/2 + *y*, 0.5 - *z*]

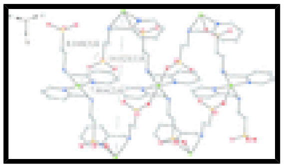

Fig. 2. The two-dimensional layer structure of (I). H atoms have been omitted.

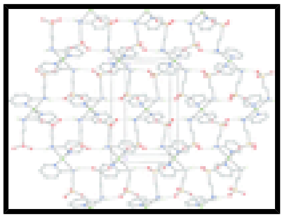

Fig. 3. The hydrogen bonding interactions in (I)(dashed lines) projected in the plane *bc*. H atoms on C atoms have been omitted.

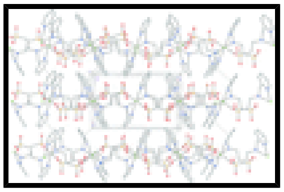

Fig. 4. Packing diagram for (I), showing π-π stacking as dashed lines in the plane *ab*. H atoms on C have been deleted.

Poly[bis[μ_2-2-(2-pyridylmethylamino)ethanesulfonato]cadmium(II)]

Crystal data

$[Cd(C_8H_{11}N_2O_3S)_2]$	F_{000} = 548
M_r = 542.90	D_x = 1.881 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3852 reflections
a = 8.8982 (8) Å	θ = 2.4–28.2°
b = 14.0206 (12) Å	μ = 1.40 mm^{-1}
c = 7.9040 (7) Å	*T* = 291 K
β = 103.5790 (10)°	Claviform, colourless
V = 958.52 (15) Å^3	0.22 × 0.16 × 0.12 mm
Z = 2	

Data collection

Bruker APEXII CCD area-detector diffractometer	2178 independent reflections
Radiation source: fine-focus sealed tube	2008 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.011$
$T = 291$ K	$\theta_{\text{max}} = 27.5°$
φ and ω scans	$\theta_{\text{min}} = 2.4°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -7 \rightarrow 11$
$T_{\text{min}} = 0.749$, $T_{\text{max}} = 0.849$	$k = -18 \rightarrow 15$
5691 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.019$	H-atom parameters constrained
$wR(F^2) = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 0.5977P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2178 reflections	$\Delta\rho_{\text{max}} = 0.48$ e Å^{-3}
133 parameters	$\Delta\rho_{\text{min}} = -0.38$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes)

are estimated using the full covariance matrix. The cell e.s.d.'s are taken

into account individually in the estimation of e.s.d.'s in distances, angles

and torsion angles; correlations between e.s.d.'s in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)

treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\text{iso}}*/U_{\text{eq}}$

Cd1	0.5000	0.0000	0.0000	0.02456 (7)
S1	0.33469 (5)	0.35013 (3)	0.12343 (6)	0.02701 (10)
O1	0.17221 (17)	0.35246 (12)	0.0384 (2)	0.0474 (4)
O2	0.36412 (18)	0.38778 (10)	0.30088 (18)	0.0382 (3)
O3	0.43417 (19)	0.39430 (11)	0.0247 (2)	0.0446 (4)
N1	0.72897 (17)	0.05064 (11)	−0.05239 (19)	0.0265 (3)
N2	0.60386 (17)	0.11240 (10)	0.22587 (19)	0.0260 (3)
H2	0.5777	0.0929	0.3250	0.031*
C1	0.7692 (2)	0.04398 (15)	−0.2058 (2)	0.0342 (4)
H1	0.7061	0.0096	−0.2957	0.041*
C2	0.9010 (2)	0.08650 (17)	−0.2341 (3)	0.0409 (5)
H2A	0.9275	0.0800	−0.3406	0.049*
C3	0.9923 (2)	0.13852 (18)	−0.1025 (3)	0.0456 (5)
H3	1.0805	0.1688	−0.1196	0.055*
C4	0.9522 (2)	0.14571 (16)	0.0561 (3)	0.0393 (5)
H4	1.0134	0.1805	0.1468	0.047*
C5	0.8193 (2)	0.10009 (13)	0.0778 (2)	0.0270 (4)
C6	0.7732 (2)	0.10068 (13)	0.2504 (2)	0.0289 (4)
H6A	0.8052	0.0413	0.3111	0.035*
H6B	0.8260	0.1525	0.3217	0.035*
C7	0.5616 (2)	0.21429 (13)	0.1977 (2)	0.0301 (4)
H7A	0.6054	0.2395	0.1055	0.036*
H7B	0.6048	0.2499	0.3031	0.036*
C8	0.3876 (2)	0.22747 (12)	0.1489 (2)	0.0289 (4)
H8A	0.3435	0.1996	0.2386	0.035*
H8B	0.3451	0.1940	0.0409	0.035*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02285 (10)	0.02064 (10)	0.03077 (10)	−0.00396 (6)	0.00747 (7)	−0.00131 (7)
S1	0.0320 (2)	0.0237 (2)	0.0260 (2)	0.00119 (16)	0.00802 (17)	−0.00138 (16)
O1	0.0355 (8)	0.0447 (9)	0.0561 (10)	0.0066 (6)	−0.0011 (7)	−0.0040 (7)
O2	0.0547 (9)	0.0275 (7)	0.0328 (7)	−0.0018 (6)	0.0109 (6)	−0.0074 (6)
O3	0.0567 (9)	0.0389 (8)	0.0447 (8)	0.0005 (7)	0.0249 (7)	0.0101 (7)
N1	0.0246 (7)	0.0267 (8)	0.0287 (7)	−0.0016 (6)	0.0071 (6)	0.0000 (6)
N2	0.0295 (7)	0.0237 (7)	0.0263 (7)	−0.0002 (6)	0.0098 (6)	0.0002 (6)
C1	0.0332 (10)	0.0393 (11)	0.0309 (9)	0.0007 (8)	0.0092 (8)	−0.0007 (8)
C2	0.0353 (10)	0.0545 (13)	0.0375 (10)	0.0039 (9)	0.0178 (9)	0.0075 (10)
C3	0.0289 (10)	0.0554 (14)	0.0563 (14)	−0.0057 (9)	0.0176 (9)	0.0085 (11)
C4	0.0274 (9)	0.0428 (11)	0.0468 (12)	−0.0094 (8)	0.0071 (8)	−0.0037 (9)
C5	0.0234 (8)	0.0245 (8)	0.0324 (9)	0.0015 (6)	0.0052 (7)	0.0018 (7)
C6	0.0271 (9)	0.0294 (9)	0.0277 (8)	−0.0013 (7)	0.0018 (7)	−0.0015 (7)
C7	0.0336 (9)	0.0217 (8)	0.0361 (9)	−0.0005 (7)	0.0103 (8)	−0.0035 (7)
C8	0.0332 (9)	0.0226 (8)	0.0316 (9)	−0.0006 (7)	0.0089 (7)	−0.0056 (7)

Geometric parameters (Å, °)

Cd1—N1	2.2853 (14)	C1—C2	1.380 (3)

Cd1—N1^{i}	2.2853 (14)	C1—H1	0.9300
Cd1—O2^{ii}	2.3496 (14)	C2—C3	1.370 (3)
Cd1—O2^{iii}	2.3497 (14)	C2—H2A	0.9300
Cd1—N2	2.3979 (15)	C3—C4	1.385 (3)
Cd1—N2^{i}	2.3979 (15)	C3—H3	0.9300
S1—O1	1.4447 (15)	C4—C5	1.390 (3)
S1—O3	1.4496 (15)	C4—H4	0.9300
S1—O2	1.4635 (14)	C5—C6	1.514 (2)
S1—C8	1.7821 (18)	C6—H6A	0.9700
O2—Cd1^{iv}	2.3497 (14)	C6—H6B	0.9700
N1—C5	1.341 (2)	C7—C8	1.516 (3)
N1—C1	1.346 (2)	C7—H7A	0.9700
N2—C7	1.481 (2)	C7—H7B	0.9700
N2—C6	1.483 (2)	C8—H8A	0.9700
N2—H2	0.9100	C8—H8B	0.9700

N1—Cd1—N1^{i}	180	N1—C1—H1	118.9
N1—Cd1—O2^{ii}	89.37 (5)	C2—C1—H1	118.9
N1^{i}—Cd1—O2^{ii}	90.63 (5)	C3—C2—C1	118.77 (19)
N1—Cd1—O2^{iii}	90.63 (5)	C3—C2—H2A	120.6
N1^{i}—Cd1—O2^{iii}	89.37 (5)	C1—C2—H2A	120.6
O2^{ii}—Cd1—O2^{iii}	179.999 (1)	C2—C3—C4	119.59 (19)
N1—Cd1—N2	74.13 (5)	C2—C3—H3	120.2
N1^{i}—Cd1—N2	105.87 (5)	C4—C3—H3	120.2
O2^{ii}—Cd1—N2	83.89 (5)	C3—C4—C5	119.02 (19)
O2^{iii}—Cd1—N2	96.11 (5)	C3—C4—H4	120.5
N1—Cd1—N2^{i}	105.87 (5)	C5—C4—H4	120.5
N1^{i}—Cd1—N2^{i}	74.13 (5)	N1—C5—C4	121.17 (17)
O2^{ii}—Cd1—N2^{i}	96.11 (5)	N1—C5—C6	116.99 (15)
O2^{iii}—Cd1—N2^{i}	83.89 (5)	C4—C5—C6	121.80 (17)
N2—Cd1—N2^{i}	180.0	N2—C6—C5	111.41 (14)
O1—S1—O3	114.25 (10)	N2—C6—H6A	109.3
O1—S1—O2	111.86 (9)	C5—C6—H6A	109.3
O3—S1—O2	111.57 (9)	N2—C6—H6B	109.3
O1—S1—C8	106.47 (9)	C5—C6—H6B	109.3
O3—S1—C8	107.12 (9)	H6A—C6—H6B	108.0
O2—S1—C8	104.88 (9)	N2—C7—C8	111.36 (15)
S1—O2—Cd1^{iv}	146.26 (9)	N2—C7—H7A	109.4
C5—N1—C1	119.27 (16)	C8—C7—H7A	109.4
C5—N1—Cd1	114.90 (11)	N2—C7—H7B	109.4
C1—N1—Cd1	125.37 (13)	C8—C7—H7B	109.4
C7—N2—C6	109.95 (14)	H7A—C7—H7B	108.0
C7—N2—Cd1	118.81 (11)	C7—C8—S1	111.93 (12)
C6—N2—Cd1	103.10 (10)	C7—C8—H8A	109.2
C7—N2—H2	108.2	S1—C8—H8A	109.2
C6—N2—H2	108.2	C7—C8—H8B	109.2

Cd1—N2—H2	108.2	S1—C8—H8B	109.2
N1—C1—C2	122.17 (19)	H8A—C8—H8B	107.9
O1—S1—O2—Cd1^{iv}	−124.02 (16)	Cd1—N1—C1—C2	171.82 (15)
O3—S1—O2—Cd1^{iv}	5.3 (2)	N1—C1—C2—C3	−1.1 (3)
C8—S1—O2—Cd1^{iv}	120.97 (16)	C1—C2—C3—C4	1.3 (3)
O2^{ii}—Cd1—N1—C5	−71.71 (12)	C2—C3—C4—C5	−0.3 (3)
O2^{iii}—Cd1—N1—C5	108.29 (12)	C1—N1—C5—C4	1.0 (3)
N2—Cd1—N1—C5	12.12 (12)	Cd1—N1—C5—C4	−171.65 (15)
N2^{i}—Cd1—N1—C5	−167.88 (12)	C1—N1—C5—C6	−176.72 (16)
O2^{ii}—Cd1—N1—C1	116.16 (16)	Cd1—N1—C5—C6	10.6 (2)
O2^{iii}—Cd1—N1—C1	−63.84 (16)	C3—C4—C5—N1	−0.9 (3)
N2—Cd1—N1—C1	−160.01 (16)	C3—C4—C5—C6	176.77 (19)
N2^{i}—Cd1—N1—C1	19.99 (16)	C7—N2—C6—C5	−80.67 (18)
N1—Cd1—N2—C7	90.73 (12)	Cd1—N2—C6—C5	46.99 (15)
N1^{i}—Cd1—N2—C7	−89.27 (12)	N1—C5—C6—N2	−42.0 (2)
O2^{ii}—Cd1—N2—C7	−178.19 (12)	C4—C5—C6—N2	140.29 (18)
O2^{iii}—Cd1—N2—C7	1.81 (12)	C6—N2—C7—C8	172.59 (14)
N1—Cd1—N2—C6	−31.13 (10)	Cd1—N2—C7—C8	54.25 (18)
N1^{i}—Cd1—N2—C6	148.87 (10)	N2—C7—C8—S1	177.53 (12)
O2^{ii}—Cd1—N2—C6	59.95 (10)	O1—S1—C8—C7	166.69 (13)
O2^{iii}—Cd1—N2—C6	−120.05 (10)	O3—S1—C8—C7	44.07 (16)
C5—N1—C1—C2	0.0 (3)	O2—S1—C8—C7	−74.60 (15)

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) −*x*+1, *y*−1/2, −*z*+1/2; (iii) *x*, −*y*+1/2, *z*−1/2; (iv) −*x*+1, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3^{v}	0.91	2.26	3.089 (2)	152

Symmetry codes: (v) *x*, −*y*+1/2, *z*+1/2.

Fig. 1

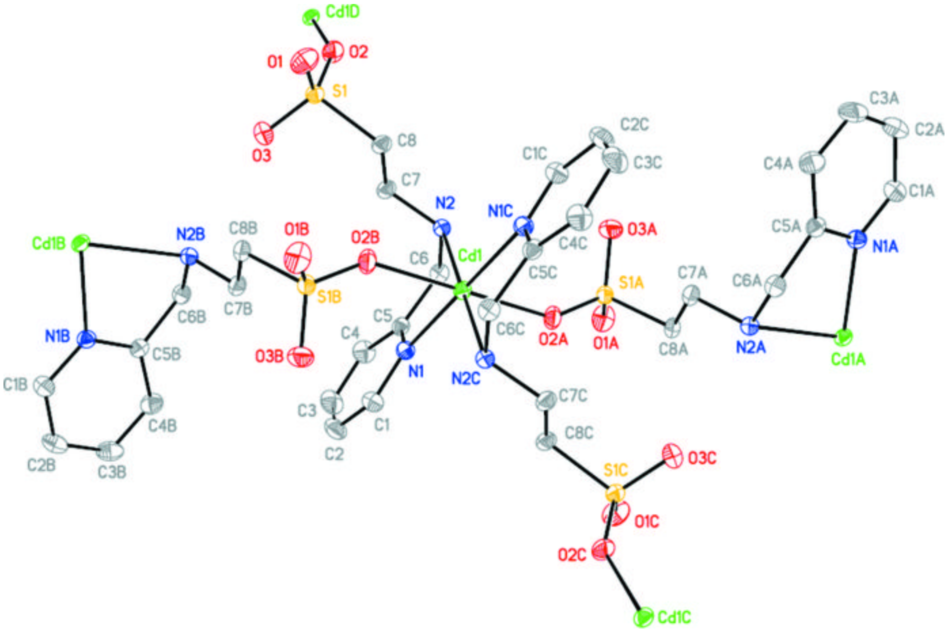
Cd1D
O1
O2
S1
O3
C8
C7
N2
C1C
C2C
C3C
C3A
C2A
C4A
C1A
Cd1B
N2B
C8B
O1B
O2B
C6
Cd1
N1C
C4C
O3A
C5A
N1A
C5C
S1A
C7A
C6A
N1B
C6B
C7B
S1B
C5
C6C
O2A
O1A
C8A
N2A
Cd1A
C5B
C4
O3B
N1
N2C
C1B
C3
C1
C7C
C4B
C2
C8C
C2B
C3B
S1C
O3C
O1C
O2C
Cd1C

Fig. 2

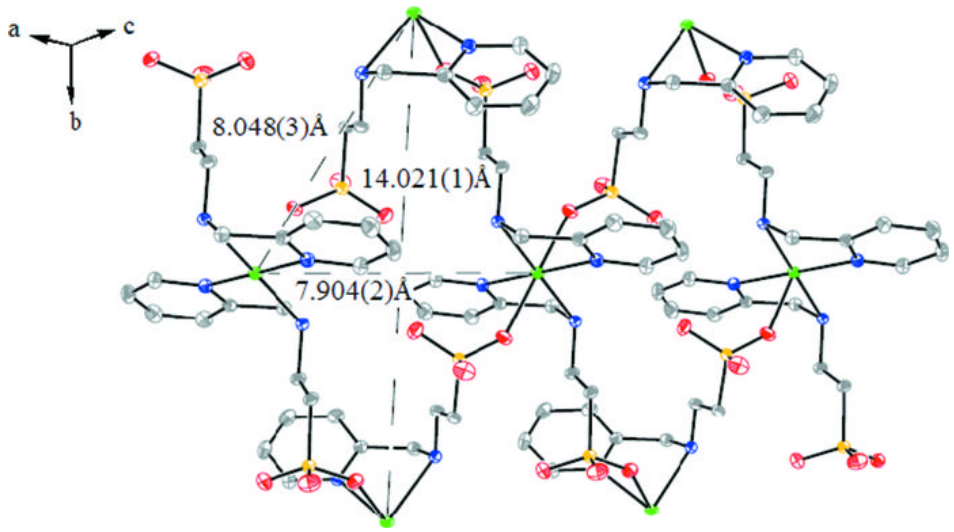

Fig. 3

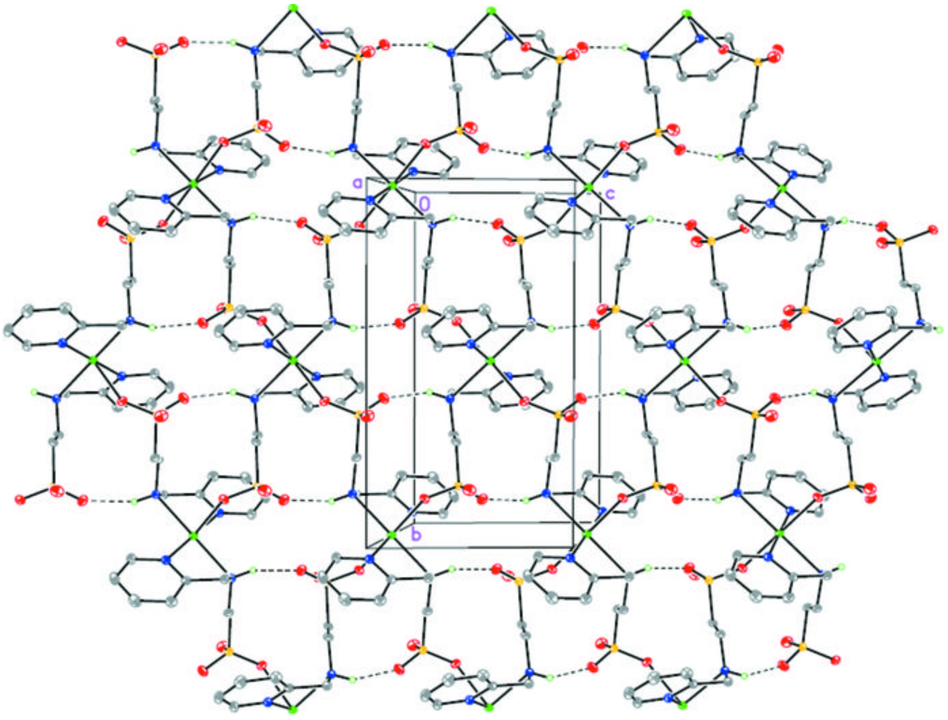

Fig. 4