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# *catena*-Poly[[diaquabis[(4-chlorophenylsulfinyl)acetato-$\kappa O$]cadmium(II)]-$\mu$-4,4′-bipyridine-$\kappa^2 N:N'$]

**Yu Su, Yan-Jun Hou, Zhi-Zhong Sun, Bai-Yan Li and Guang-Feng Hou***

College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China
Correspondence e-mail: hgf1000@163.com

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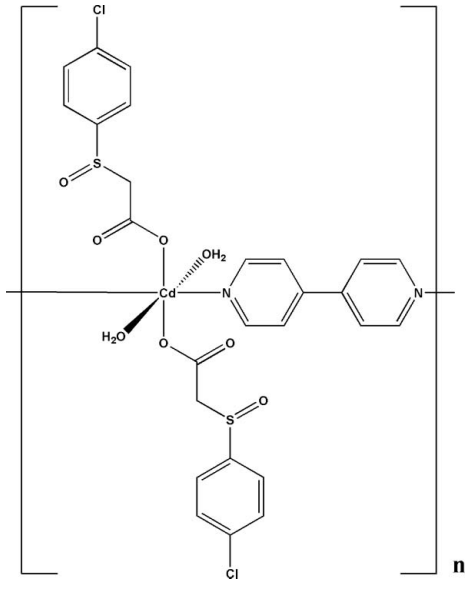
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.025; $wR$ factor = 0.062; data-to-parameter ratio = 17.9.

In the title coordination polymer, $[Cd(C_8H_6ClO_3S)_2(C_{10}H_8N_2)(H_2O)_2]_n$, the $Cd^{II}$ atom exists in an octahedral coordination environment formed by two carboxylate O atoms from two (4-chlorophenylsulfinyl)acetate ligands, two N atoms from two bipyridine ligands and two water molecules. The $Cd^{II}$ atom lies on a twofold rotation axis. Bridging by the bipyridine ligand leads to a linear chain structure, while intermolecular O—H···O hydrogen bonds link the chains into a three-dimensional network.

## Related literature

For isostructural compounds, see: Hou *et al.* (2007, 2007*a*,*b*); Su *et al.* (2007).




## Experimental

### Crystal data

$[Cd(C_8H_6ClO_3S)_2(C_{10}H_8N_2)(H_2O)_2]$
$M_r$ = 739.89
Orthorhombic, *Fdd*2
$a$ = 25.664 (5) Å
$b$ = 20.103 (7) Å
$c$ = 11.705 (2) Å
$V$ = 6039 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.09 mm$^{-1}$
$T$ = 293 (2) K
0.22 × 0.21 × 0.19 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.793, $T_{max}$ = 0.823
14361 measured reflections
3370 independent reflections
3214 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.030

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.062
$S$ = 1.06
3370 reflections
188 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.30 e Å$^{-3}$
Absolute structure: Flack (1983), 1550 Friedel pairs
Flack parameter: −0.02 (2)

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O4—H12···O1$^{i}$ | 0.85 | 1.86 | 2.710 (3) | 175 |
| O4—H12···S1$^{i}$ | 0.85 | 3.04 | 3.841 (2) | 159 |
| O4—H11···O2$^{ii}$ | 0.85 | 1.86 | 2.692 (3) | 166 |

Symmetry codes: (i) $-x+\frac{1}{4}, y-\frac{1}{4}, z-\frac{1}{4}$; (ii) $-x, -y+2, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2288).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2005 [ **doi:10.1107/S1600536807030693** ]

# *catena*-Poly[[diaquabis[(4-chlorophenylsulfinyl)acetato-*κO*]cadmium(II)]-$\mu$-4,4'-bipyridine-$\kappa^2N$:$N'$]

**Y. Su, Y.-J. Hou, Z.-Z. Sun, B.-Y. Li and G.-F. Hou**

## Comment

Recently, we reported the crystal structure of diaquabis[(4-nitrophenylsulfinylacetato)(4,4'-bipyridine)zinc(II) (Hou *et al.* 2007*a*). We also reported that of diaquabis[(4-chlorophenylsulfinylacetato)(4,4'-bipyridine)cobalt(II) (Hou *et al.* 2007*b*); diaquabis[(4-chlorophenylsulfinylacetato)(4,4'-bipyridine)zinc(II) (Hou *et al.* 2007) and diaquabis[(4-chlorophenyl-sulfinylacetato)(4,4'-bipyridine)nickel(II) (Su *et al.* 2007); this paper reports the isostructural cadmium compound.

In the title compound the cadmium bis(4-chlorophenylsulfinylacetate) moiety is bridged by 4,4'-bipyridine into a linear chain (Fig. 1). The $Cd^{II}$ atom shows an all *trans* octahedral coordination. The chains are connected into a three dimensional network *via* intermolecular O—H···O hydrogen bonds (Table 1), (Fig. 2).

## Experimental

(4-Chlorophenylsulfanyl)acetic acid was prepared by the nucleophilic reaction of chloroacetic acid and 4-chlorothiophenol under basic conditions. It was then oxidized using 30% aqueous hydrogen peroxide in acetic anhydride solution to produce 4-chlorophenylsulfinyl acetic acid. Cadmium nitrate hexahydrate (0.692 g, 2 mmol), 4,4'-bipyridine (0.312 g, 2 mmol) and 4-chlorophenylsulfinyl acetic acid (0.437 g, 2 mmol) were dissolved in water and the pH was adjusted to 6 with 0.01 *M* sodium hydroxide; colorless crystals separated from the filtered solution after several days.

## Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C) or C—H = 0.97 Å (methylene C), and with $U_{iso}$(H) = 1.2Ueq(C). Water H atoms were initially located in a difference Fourier map but they were treated as riding on their parent atoms with O—H = 0.85 Å and with $U_{iso}$(H) = 1.5Ueq(O).

The Flack parameter was refined from 1550 Friedel pairs.

## Figures

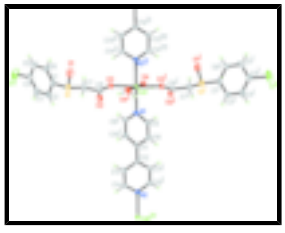

Fig. 1. Part of the polymeric structure of the title complex, with the atomlabelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii. [Symmetry codes: (I) −*x*, −*y* + 2, *z*; (II) *x*, *y*,*z* + 1; (III) −*x*, −*y* + 2, *z* + 1, (IV) *x*, *y*, *z* − 1].

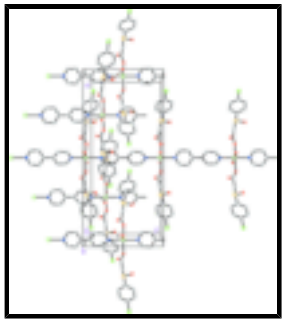

Fig. 2. A partial packing plot of (I). Dashed lines indicate the hydrogen-bonding interactions. H atoms not involved in hydrogen bonds have been omitted.

**_catena_-Poly[[diaquabis[(4-chlorophenylsulfinyl)acetato- κ*O*]cadmium(II)]-μ-4,4'-bipyridine-κ$^2$*N*:*N*']**

*Crystal data*

| | |
|---|---|
| $[Cd(C_8H_6ClO_3S)_2(C_{10}H_8N_2)(H_2O)_2]$ | $F_{000}$ = 2976 |
| $M_r$ = 739.89 | $D_x$ = 1.628 Mg m$^{-3}$ |
| Orthorhombic, *Fdd*2 | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: F 2 -2d | Cell parameters from 13606 reflections |
| *a* = 25.664 (5) Å | θ = 6.2–55.1° |
| *b* = 20.103 (7) Å | μ = 1.09 mm$^{-1}$ |
| *c* = 11.705 (2) Å | *T* = 293 (2) K |
| *V* = 6039 (3) Å$^3$ | Block, colorless |
| *Z* = 8 | 0.22 × 0.21 × 0.19 mm |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 3370 independent reflections |
| Radiation source: fine-focus sealed tube | 3214 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.030 |
| *T* = 293(2) K | $\theta_{max}$ = 27.5° |
| ω scans | $\theta_{min}$ = 3.1° |
| Absorption correction: multi-scan (ABSCOR; Higashi, 1995) | *h* = −33→33 |
| $T_{min}$ = 0.793, $T_{max}$ = 0.823 | *k* = −26→26 |
| 14361 measured reflections | *l* = −14→15 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.025 | $w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 7.9326P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.062 | $(\Delta/\sigma)_{max}$ = 0.001 |
| *S* = 1.06 | $\Delta\rho_{max}$ = 0.85 e Å$^{-3}$ |

| | |
|---|---|
| 3370 reflections | $\Delta\rho_{min} = -0.30$ e Å$^{-3}$ |
| 188 parameters | Extinction correction: none |
| 1 restraint | Absolute structure: Flack (1983), 1550 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: −0.02 (2) |
| Secondary atom site location: difference Fourier map | |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.27829 (11) | 0.97188 (15) | 1.0099 (3) | 0.0389 (7) |
| C2 | 0.29867 (13) | 0.93630 (16) | 0.9191 (3) | 0.0469 (7) |
| H1 | 0.2841 | 0.9403 | 0.8467 | 0.056* |
| C3 | 0.34059 (13) | 0.89508 (18) | 0.9366 (3) | 0.0573 (9) |
| H2 | 0.3539 | 0.8694 | 0.8773 | 0.069* |
| C4 | 0.36233 (14) | 0.89255 (17) | 1.0430 (4) | 0.0572 (9) |
| C5 | 0.34323 (17) | 0.9276 (2) | 1.1350 (4) | 0.0621 (10) |
| H3 | 0.3591 | 0.9249 | 1.2063 | 0.074* |
| C6 | 0.29992 (14) | 0.96660 (19) | 1.1179 (3) | 0.0545 (8) |
| H4 | 0.2852 | 0.9895 | 1.1789 | 0.065* |
| C7 | 0.17595 (10) | 0.96841 (14) | 0.9710 (3) | 0.0440 (6) |
| H5 | 0.1834 | 0.9395 | 0.9067 | 0.053* |
| H6 | 0.1746 | 0.9413 | 1.0395 | 0.053* |
| C8 | 0.12325 (12) | 1.00291 (16) | 0.9529 (2) | 0.0380 (8) |
| C9 | −0.03579 (12) | 1.03376 (16) | 0.7185 (3) | 0.0424 (7) |
| H7 | −0.0610 | 1.0576 | 0.7583 | 0.051* |
| C10 | −0.03732 (13) | 1.03504 (17) | 0.6005 (3) | 0.0428 (7) |
| H8 | −0.0632 | 1.0592 | 0.5634 | 0.051* |
| C11 | 0.0000 | 1.0000 | 0.5360 (7) | 0.0386 (15) |
| C12 | 0.0000 | 1.0000 | 0.4100 (6) | 0.0365 (15) |
| C13 | 0.04492 (13) | 1.0104 (2) | 0.3517 (3) | 0.0501 (9) |
| H9 | 0.0762 | 1.0168 | 0.3904 | 0.060* |
| C14 | 0.04330 (13) | 1.01123 (18) | 0.2342 (4) | 0.0497 (8) |
| H10 | 0.0738 | 1.0200 | 0.1941 | 0.060* |
| Cd1 | 0.0000 | 1.0000 | 0.97656 (3) | 0.03051 (7) |
| Cl1 | 0.41728 (5) | 0.84252 (7) | 1.06118 (18) | 0.1051 (5) |
| N1 | 0.0000 | 1.0000 | 0.7792 (5) | 0.0397 (13) |

| | | | | |
|---|---|---|---|---|
| N2 | 0.0000 | 1.0000 | 0.1761 (5) | 0.0363 (12) |
| O1 | 0.21608 (10) | 1.06206 (14) | 1.0980 (3) | 0.0711 (8) |
| O2 | 0.12289 (9) | 1.05949 (13) | 0.9125 (3) | 0.0610 (6) |
| O3 | 0.08505 (7) | 0.96899 (10) | 0.9828 (2) | 0.0439 (4) |
| O4 | −0.03001 (8) | 0.88990 (9) | 0.9748 (2) | 0.0460 (4) |
| H12 | −0.0111 | 0.8637 | 0.9356 | 0.069* |
| H11 | −0.0602 | 0.8994 | 0.9497 | 0.069* |
| S1 | 0.22630 (3) | 1.02914 (3) | 0.98480 (9) | 0.04591 (17) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0287 (12) | 0.0422 (14) | 0.0458 (19) | −0.0016 (11) | −0.0039 (11) | −0.0056 (12) |
| C2 | 0.0417 (16) | 0.0516 (17) | 0.0473 (17) | 0.0035 (13) | −0.0068 (13) | −0.0148 (14) |
| C3 | 0.0435 (18) | 0.0535 (18) | 0.075 (2) | 0.0086 (15) | 0.0005 (16) | −0.0196 (16) |
| C4 | 0.0440 (18) | 0.0443 (17) | 0.083 (3) | 0.0054 (14) | −0.0152 (17) | −0.0022 (16) |
| C5 | 0.063 (2) | 0.058 (2) | 0.065 (2) | −0.0025 (18) | −0.0300 (19) | −0.0011 (19) |
| C6 | 0.055 (2) | 0.062 (2) | 0.0466 (19) | 0.0023 (16) | −0.0026 (15) | −0.0106 (16) |
| C7 | 0.0303 (13) | 0.0449 (13) | 0.0567 (18) | −0.0001 (10) | 0.0022 (14) | −0.0052 (15) |
| C8 | 0.0348 (13) | 0.0526 (15) | 0.027 (2) | 0.0024 (12) | −0.0002 (9) | 0.0003 (13) |
| C9 | 0.0467 (16) | 0.0551 (16) | 0.0255 (15) | 0.0094 (13) | 0.0051 (14) | 0.0001 (15) |
| C10 | 0.0476 (18) | 0.0549 (18) | 0.0261 (15) | 0.0102 (14) | −0.0004 (12) | 0.0042 (13) |
| C11 | 0.038 (3) | 0.051 (3) | 0.027 (3) | −0.0046 (18) | 0.000 | 0.000 |
| C12 | 0.048 (4) | 0.050 (3) | 0.012 (3) | 0.0037 (18) | 0.000 | 0.000 |
| C13 | 0.0365 (17) | 0.089 (3) | 0.0252 (16) | −0.0037 (16) | −0.0040 (12) | −0.0114 (15) |
| C14 | 0.0384 (16) | 0.083 (2) | 0.0276 (16) | −0.0046 (14) | 0.0050 (13) | −0.0050 (19) |
| Cd1 | 0.02765 (11) | 0.04510 (12) | 0.01878 (10) | 0.00082 (12) | 0.000 | 0.000 |
| Cl1 | 0.0695 (8) | 0.0855 (8) | 0.1602 (15) | 0.0381 (7) | −0.0354 (9) | −0.0021 (9) |
| N1 | 0.041 (3) | 0.052 (3) | 0.026 (4) | −0.0011 (16) | 0.000 | 0.000 |
| N2 | 0.041 (3) | 0.051 (3) | 0.016 (3) | 0.0030 (15) | 0.000 | 0.000 |
| O1 | 0.0513 (15) | 0.0625 (15) | 0.100 (2) | 0.0063 (12) | −0.0047 (14) | −0.0428 (15) |
| O2 | 0.0376 (12) | 0.0706 (15) | 0.0746 (17) | 0.0064 (11) | 0.0094 (11) | 0.0252 (13) |
| O3 | 0.0305 (9) | 0.0614 (11) | 0.0398 (11) | 0.0023 (8) | 0.0009 (10) | 0.0052 (11) |
| O4 | 0.0456 (11) | 0.0459 (10) | 0.0464 (11) | 0.0043 (8) | −0.0044 (10) | −0.0037 (10) |
| S1 | 0.0309 (3) | 0.0403 (3) | 0.0665 (5) | −0.0002 (3) | 0.0026 (4) | −0.0005 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.384 (5) | C10—H8 | 0.9300 |
| C1—C2 | 1.384 (4) | C11—C10$^{i}$ | 1.408 (5) |
| C1—S1 | 1.787 (3) | C11—C12 | 1.475 (5) |
| C2—C3 | 1.374 (5) | C12—C13$^{i}$ | 1.356 (5) |
| C2—H1 | 0.9300 | C12—C13 | 1.356 (5) |
| C3—C4 | 1.366 (5) | C13—C14 | 1.377 (6) |
| C3—H2 | 0.9300 | C13—H9 | 0.9300 |
| C4—C5 | 1.376 (6) | C14—N2 | 1.322 (5) |
| C4—Cl1 | 1.745 (3) | C14—H10 | 0.9300 |
| C5—C6 | 1.375 (5) | Cd1—O3$^{i}$ | 2.2712 (19) |

| | | | |
|---|---|---|---|
| C5—H3 | 0.9300 | Cd1—O3 | 2.2712 (19) |
| C6—H4 | 0.9300 | Cd1—N1 | 2.310 (6) |
| C7—C8 | 1.535 (4) | Cd1—N2$^{ii}$ | 2.336 (6) |
| C7—S1 | 1.785 (3) | Cd1—O4 | 2.344 (2) |
| C7—H5 | 0.9700 | Cd1—O4$^{i}$ | 2.344 (2) |
| C7—H6 | 0.9700 | N1—C9$^{i}$ | 1.345 (5) |
| C8—O2 | 1.232 (4) | N2—C14$^{i}$ | 1.322 (5) |
| C8—O3 | 1.244 (4) | N2—Cd1$^{iii}$ | 2.336 (6) |
| C9—N1 | 1.345 (5) | O1—S1 | 1.504 (3) |
| C9—C10 | 1.382 (5) | O4—H12 | 0.8500 |
| C9—H7 | 0.9300 | O4—H11 | 0.8500 |
| C10—C11 | 1.408 (5) | | |
| C6—C1—C2 | 120.7 (3) | C13$^{i}$—C12—C11 | 120.2 (3) |
| C6—C1—S1 | 120.0 (2) | C13—C12—C11 | 120.2 (3) |
| C2—C1—S1 | 119.2 (2) | C12—C13—C14 | 118.6 (4) |
| C3—C2—C1 | 119.5 (3) | C12—C13—H9 | 120.7 |
| C3—C2—H1 | 120.2 | C14—C13—H9 | 120.7 |
| C1—C2—H1 | 120.2 | N2—C14—C13 | 122.5 (4) |
| C4—C3—C2 | 118.6 (3) | N2—C14—H10 | 118.8 |
| C4—C3—H2 | 120.7 | C13—C14—H10 | 118.8 |
| C2—C3—H2 | 120.7 | O3$^{i}$—Cd1—O3 | 176.31 (13) |
| C3—C4—C5 | 123.3 (3) | O3$^{i}$—Cd1—N1 | 91.84 (6) |
| C3—C4—Cl1 | 117.6 (3) | O3—Cd1—N1 | 91.84 (6) |
| C5—C4—Cl1 | 119.2 (3) | O3$^{i}$—Cd1—N2$^{ii}$ | 88.16 (6) |
| C6—C5—C4 | 117.8 (4) | O3—Cd1—N2$^{ii}$ | 88.16 (6) |
| C6—C5—H3 | 121.1 | N1—Cd1—N2$^{ii}$ | 180.000 (4) |
| C4—C5—H3 | 121.1 | O3$^{i}$—Cd1—O4 | 86.77 (7) |
| C5—C6—C1 | 120.1 (4) | O3—Cd1—O4 | 93.26 (7) |
| C5—C6—H4 | 120.0 | N1—Cd1—O4 | 89.50 (6) |
| C1—C6—H4 | 120.0 | N2$^{ii}$—Cd1—O4 | 90.50 (6) |
| C8—C7—S1 | 110.0 (2) | O3$^{i}$—Cd1—O4$^{i}$ | 93.26 (7) |
| C8—C7—H5 | 109.7 | O3—Cd1—O4$^{i}$ | 86.77 (7) |
| S1—C7—H5 | 109.7 | N1—Cd1—O4$^{i}$ | 89.50 (6) |
| C8—C7—H6 | 109.7 | N2$^{ii}$—Cd1—O4$^{i}$ | 90.50 (6) |
| S1—C7—H6 | 109.7 | O4—Cd1—O4$^{i}$ | 179.00 (12) |
| H5—C7—H6 | 108.2 | C9—N1—C9$^{i}$ | 116.2 (6) |
| O2—C8—O3 | 127.4 (3) | C9—N1—Cd1 | 121.9 (3) |
| O2—C8—C7 | 118.5 (3) | C9$^{i}$—N1—Cd1 | 121.9 (3) |
| O3—C8—C7 | 114.1 (3) | C14$^{i}$—N2—C14 | 118.1 (6) |
| N1—C9—C10 | 123.8 (4) | C14$^{i}$—N2—Cd1$^{iii}$ | 120.9 (3) |
| N1—C9—H7 | 118.1 | C14—N2—Cd1$^{iii}$ | 120.9 (3) |
| C10—C9—H7 | 118.1 | C8—O3—Cd1 | 126.71 (19) |
| C9—C10—C11 | 120.5 (4) | Cd1—O4—H12 | 113.7 |
| C9—C10—H8 | 119.8 | Cd1—O4—H11 | 95.2 |

| | | | |
|---|---|---|---|
| C11—C10—H8 | 119.8 | H12—O4—H11 | 118.2 |
| C10—C11—C10$^{i}$ | 115.2 (6) | O1—S1—C7 | 104.72 (17) |
| C10—C11—C12 | 122.4 (3) | O1—S1—C1 | 105.57 (16) |
| C10$^{i}$—C11—C12 | 122.4 (3) | C7—S1—C1 | 96.59 (14) |
| C13$^{i}$—C12—C13 | 119.6 (6) | | |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O4—H12···O1$^{iv}$ | 0.85 | 1.86 | 2.710 (3) | 175 |
| O4—H12···S1$^{iv}$ | 0.85 | 3.04 | 3.841 (2) | 159 |
| O4—H11···O2$^{i}$ | 0.85 | 1.86 | 2.692 (3) | 166 |

Symmetry codes: (iv) −*x*+1/4, *y*−1/4, *z*−1/4; (i) −*x*, −*y*+2, *z*.

**Fig. 1**

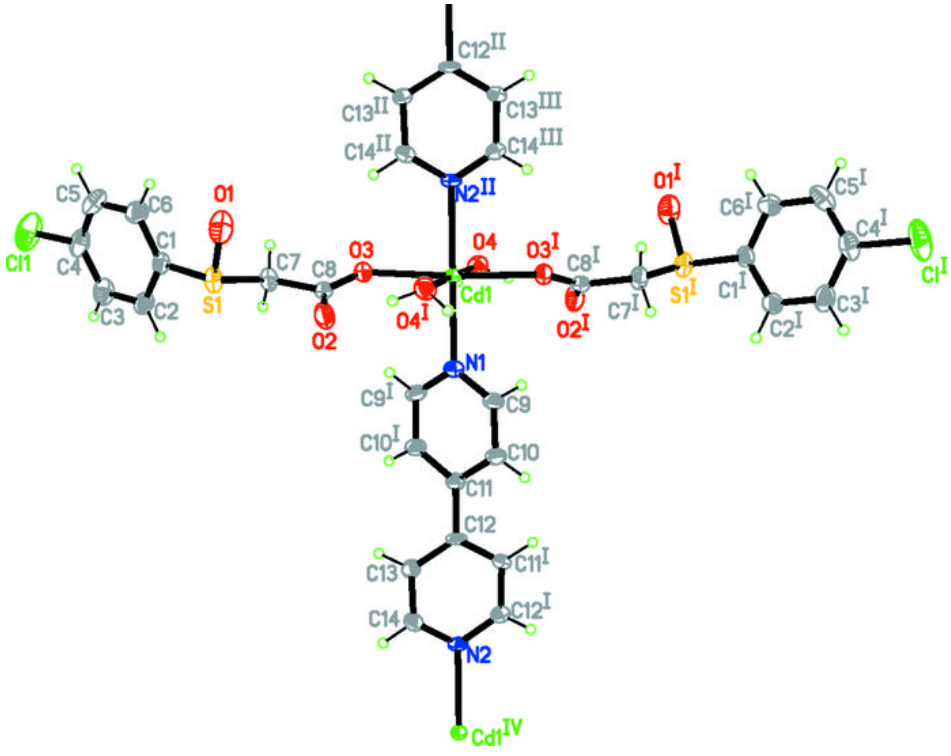
C12II
C13II
C13III
C14II
C14III
N2II
O1I
C5
C6
O1
C1
Cl1
C4
C3
C2
S1
C7
C8
O3
O4
O3I
C8I
Cd1
O4I
O2
O2I
C7I
S1I
C6I
C5I
C4I
ClI
C1I
C3I
C2I
N1
C9I
C9
C10I
C10
C11
C12
C13
C11I
C14
C12I
N2
Cd1IV

**Fig. 2**