

catena-Poly[bis(sulfamethoxazolium) [[trichloridocadmate(II)]- μ -chlorido] monohydrate]

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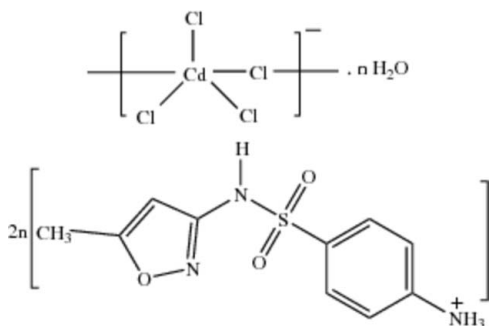
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.041; wR factor = 0.111; data-to-parameter ratio = 14.0.

In the title compound, $\{(\text{C}_{10}\text{H}_{12}\text{N}_3\text{O}_3\text{S})_2[\text{CdCl}_4]\cdot\text{H}_2\text{O}\}_n$, the Cd^{II} atom is five-coordinate with a distorted trigonal-bipyramidal geometry formed by chloride ions. The Cd atom and two of the Cl atoms lie on a mirror plane. The cation is protonated on the amino group N atom; it is not coordinated to cadmium, but is hydrogen bonded to the chlorido ligands. Each water molecule bridges two chlorido ligands, generating ring motifs along the $-\text{Cd}-\text{Cl}-\text{Cd}-$ chains. The isoxazole unit and the amide groups are linked through a pair of $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds. The crystal structure is stabilized by $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{Cl}$, $\text{C}-\text{H}\cdots\text{N}$, $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For related literature, see: Abramenco & Sergienko (2002); Bettinetti *et al.* (1982); Dai *et al.* (2002); Fawcett *et al.* (1978); Haridas *et al.* (1984); Kagi & Vallee (1960); Kálmán *et al.* (1981); Kendi *et al.* (2000); Schaffers & Keszler (1993); Singh *et al.* (1984); Subashini *et al.* (2007); Subha Nandhini *et al.* (2002); Takasuka & Nakai (2001); Tao *et al.* (2003); Yukawa *et al.* (1982).



Experimental

Crystal data

$(\text{C}_{10}\text{H}_{12}\text{N}_3\text{O}_3\text{S})_2[\text{CdCl}_4]\cdot\text{H}_2\text{O}$
 $M_r = 780.82$
 Orthorhombic, $Pnma$
 $a = 15.088$ (2) Å
 $b = 35.028$ (3) Å
 $c = 5.562$ (3) Å

$V = 2939.5$ (17) Å³
 $Z = 4$
 Cu $K\alpha$ radiation
 $\mu = 11.07$ mm⁻¹
 $T = 293$ K
 $0.19 \times 0.16 \times 0.14$ mm

Data collection

Siemens AED single-crystal diffractometer
 Absorption correction: ψ scan (North *et al.*, 1968)

$T_{\text{min}} = 0.227$, $T_{\text{max}} = 0.306$ (expected range = 0.157–0.212)
 2834 measured reflections
 2834 independent reflections
 2470 reflections with $I > 2\sigma(I)$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.111$
 $S = 1.05$
 2834 reflections
 203 parameters
 4 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 1.04$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.64$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cd1—Cl2	2.4828 (17)	Cd1—Cl2 ⁱⁱ	2.4828 (17)
Cd1—Cl3	2.469 (2)	Cd1—Cl1	2.6688 (19)
Cd1—Cl1 ⁱ	2.902 (2)		
Cl1—Cd1—Cl2 ⁱⁱ	92.51 (3)	Cl1—Cd1—Cl1 ⁱ	173.60 (5)
Cl2—Cd1—Cl3	113.69 (3)	Cl1 ⁱ —Cd1—Cl2 ⁱⁱ	84.90 (3)
Cl1 ⁱ —Cd1—Cl2	84.90 (3)	Cl1 ⁱ —Cd1—Cl3	91.27 (5)
Cl2—Cd1—Cl2 ⁱⁱ	131.63 (4)	Cl2 ⁱⁱ —Cd1—Cl3	113.69 (3)
Cl1—Cd1—Cl2	92.51 (3)	Cd1—Cl1—Cd1 ⁱⁱⁱ	173.60 (7)
Cl1—Cd1—Cl3	95.12 (5)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1W—H1W ^{..} Cl3 ⁱ	0.96	2.11	3.035 (5)	161
O1W—H2W ^{..} Cl3	0.95	2.11	3.036 (5)	164
N4—H4A ^{..} Cl2 ^{iv}	0.94 (5)	2.26 (5)	3.184 (4)	171 (4)
N4—H4B ^{..} O1W ^v	0.91 (5)	1.86 (5)	2.758 (4)	169 (4)
N4—H4B ^{..} O1W ⁱⁱⁱ	0.91 (5)	1.86 (5)	2.758 (4)	169 (4)
N4—H4C ^{..} Cl2 ^{vi}	0.85 (4)	2.49 (4)	3.196 (4)	141 (4)
N4—H4C ^{..} O1 ^{vi}	0.85 (4)	2.33 (5)	2.871 (4)	122 (4)
N7—H7 ^{..} N8 ^{vii}	0.86	2.58	3.188 (5)	129
C2—H2 ^{..} O2	0.93	2.55	2.911 (4)	103
C9—H9 ^{..} O2	0.93	2.50	2.991 (4)	113
C9—H9 ^{..} N8 ⁱ	0.93	2.58	3.354 (5)	141

Symmetry codes: (i) $x, y, z + 1$; (iii) $x, -y + \frac{1}{2}, z - 1$; (iv) $x - \frac{1}{2}, y, -z + \frac{3}{2}$; (v) $x, y, z - 1$; (vi) $x - \frac{1}{2}, y, -z + \frac{3}{2}$; (vii) $-x + 1, -y, -z + 1$.

Data collection: local program (Belletti *et al.*, 1993); cell refinement: local program; data reduction: local program; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2052).

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supporting information

Acta Cryst. (2008). E64, m250–m251 [https://doi.org/10.1107/S1600536807067190]

catena-Poly[bis(sulfamethoxazolium) [[trichloridocadmiate(II)]- μ -chlorido] monohydrate]**Annamalai Subashini, Packianathan Thomas Muthiah, Gabriele Bocelli and Andrea Cantoni****S1. Comment**

Polynuclear d^{10} -metal complexes have been found to exhibit intriguing structural and photoluminescent properties (Dai *et al.*, 2002; Tao *et al.*, 2003). Chloride-bridged cadmium(II) polymeric complexes are of considerable interest, because they may act as photoactive materials. Cadmium is found to occur naturally in at least one protein, metallothionein (Kagi & Vallee, 1960). Sulfonamides constitute an important class of antimicrobial agents. The drug, 4-[5-methylisoxazol-3-yl]aminosulfonyl aniline [Sulfamethoxazole (SMZ)] prevents the formation of dihydrofolic acid, a compound that bacteria must be able to make in order to survive. The two polymorphs of SMZ (Bettinetti *et al.*, 1982) have already been reported in literature. Recently, the crystal structure of sulfamethoxazole hydrochloride (Subashini *et al.*, 2007) has been reported from our laboratory. X-ray analysis reveals that (I) possesses a polynuclear structure with the Cd atom and two of the Cl atoms on a special positions(*m*). The Cd atom has trigonal bipyramidal coordination geometry formed by five chloride anions. The Cd1—Cl1, Cd1—Cl2, Cd1—Cl3, and Cd—Clⁱ bond lengths are 2.669 (2), 2.4828 (17), 2.469 (2) and 2.902 (2) Å respectively. The mean Cd—Cl distance, 2.630 (2) Å, is in agreement with the corresponding distances reported in the structures of complexes of CdCl₂ with 4-hydroxy-*L*-proline [2.620 (2) Å] (Yukawa *et al.*, 1982), β -alanine [2.619 (5) Å] (Subha Nandhini *et al.*, 2002) and *L*-alanine [2.61 (1) Å] (Schaffers & Keszler, 1993). The Cd—Cl distances reported for tetrameric cadmium(II) complex (Fawcett *et al.*, 1978), *viz.* 2.946 (6) and 2.946 (5) Å, are longer compared to those in the present structure.

The atoms around the sulfonamide S atom in (I) are arranged in a slightly distorted tetrahedral configuration. The largest deviation is in the angle O1—S1—O2 [121.22 (17)°], but it confirms to the non-tetrahedral nature commonly observed in sulfonamides (Haridas *et al.*, 1984; Kendi *et al.*, 2000; Takasuka & Nakai, 2001). The S1—C1 distance of 1.760 (3) Å (I) is a normal single-bond value and matches well with those observed in other sulfonamides (Singh *et al.*, 1984; Abramenko & Sergienko, 2002). In the present structure the dihedral angle between the isoxazole and amino phenyl plane is found to be 88.31 (18)°, whereas in neutral SMZ structures the dihedral angles are 73.1 (5)° for Form 1 and 79.6 (6)° for Form 2 (Bettinetti *et al.*, 1982) respectively. The two torsion angles τ_1 (C—C—S—N) and τ_2 (C—S—N—C) defining the conformation of the sulfonamide group are reported to lie in the range 70–120° and 60–90°, respectively (Kálmán *et al.*, 1981). The torsion angles τ_1 is -81.9 (3)° (C6—C1—S1—N7) and τ_2 is -73.6 (3)° (C1—S1—N7—C8). In neutral forms, the torsion angles τ_1 are -76.5 (9)° (Form 1) and -78.5 (5)° (Form 2). The torsion angles τ_2 are -56.1 (4)° in form 1 and -61.5 (8)° in form 2. In sulfamethoxazole hydrochloride the torsion angles are (τ_1) 73.2 (3)° and (τ_2) -71.2 (3)° (Subashini *et al.*, 2007). The cation is protonated on the amine nitrogen (N4) atom. The drug is not coordinated to cadmium and the amino group (N4) of the drug is hydrogen bonded to the chloride ions. 4-ammonio group acts as a bridge between the sulfonamide oxygen atom and water molecules. Four smz cations and two water molecules are connected through N—H \cdots O hydrogen bonds forming a 24 membered ring with graph-set $R^4_6(24)$ (Fig. 2). The

isoxazole moiety and the amide groups are paired through a pair of N—H···N hydrogen bonds. A C—H···N hydrogen bond is observed between isoxazole carbon (C9) and nitrogen (N8). The water O1W atom does not participate in coordination with cadmium. Each water molecule bridges two chloride ions generating ring motifs along the —Cd—Cl—Cd— chains as shown in Fig 3.

S2. Experimental

Hot ethanol solution of sulfamethoxazole (Qualigens, 63 mg) and an aqueous solution of cadmium chloride ($\text{CdCl}_2 \cdot 2\text{H}_2\text{O}$, 98%) (SISCO CHEM, 54 mg) were mixed in a 1:1 stoichiometric ratio. On slow evaporation light brown prismatic crystals of the title complex were formed.

S3. Refinement

The hydrogen atoms of the aromatic groups were positioned geometrically and refined using a riding model, with $\text{C—H} = 0.93\text{--}0.96\text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl hydrogen atoms and $1.2U_{\text{eq}}(\text{C})$ for all other hydrogen atoms. The hydrogen atoms of the water molecule and ammonio group (N4) were located in a difference Fourier maps and were refined, subject to bond length restraints of 0.96 \AA (O—H), 1.5 \AA (H..H) and 0.86 \AA for ammonio N—H(H4C). The highest peak in the final difference map was found at a distance of 1.04 \AA from Cd1 and the deepest hole was -0.64 \AA from Cl1.

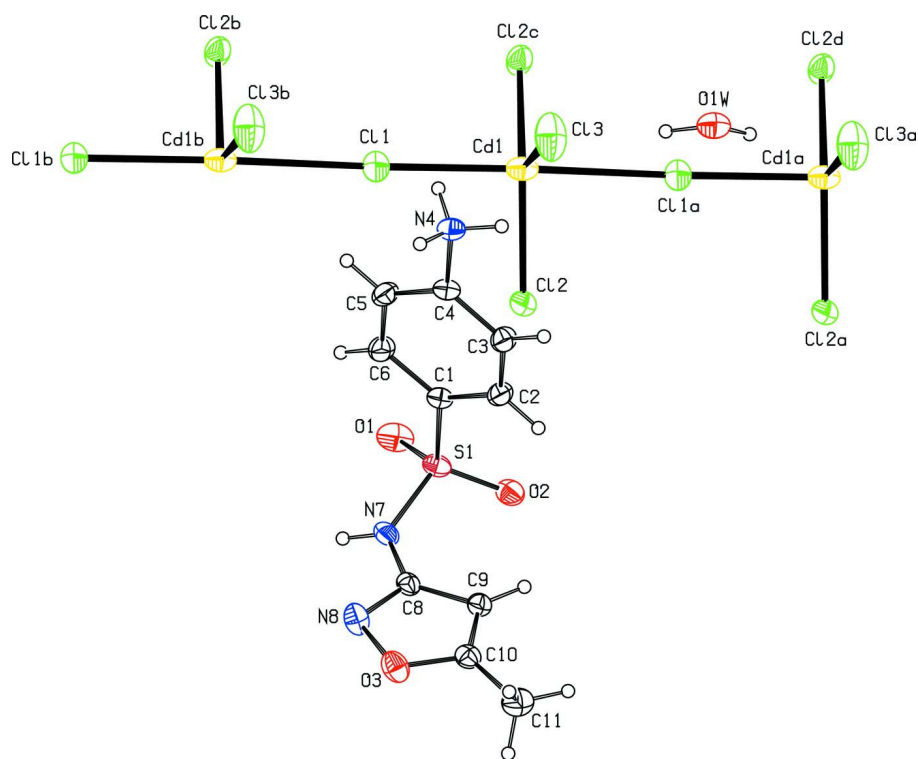


Figure 1

An ORTEP view of the asymmetric unit of (I) showing 30% probability displacement ellipsoids. Symmetry codes: (i) $x, y, z + 1$; (ii) $x, -y + 1/2, z$.

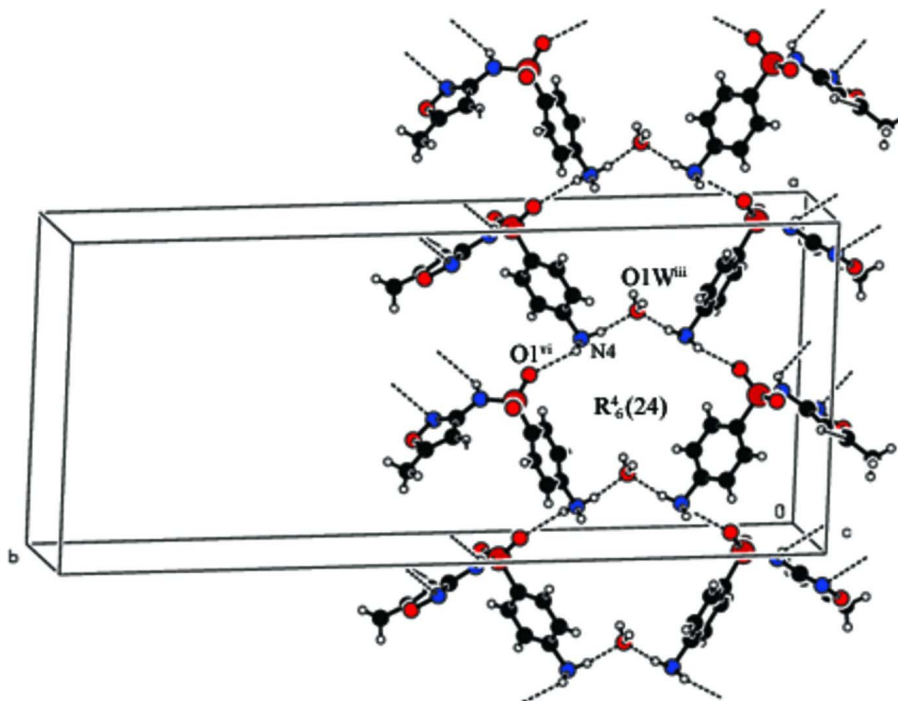


Figure 2

Packing view of compound (I). Symmetry codes: (iii) $x, -y + 1/2, z - 1$; (vi) $x - 1/2, y, -z + 3/2$.

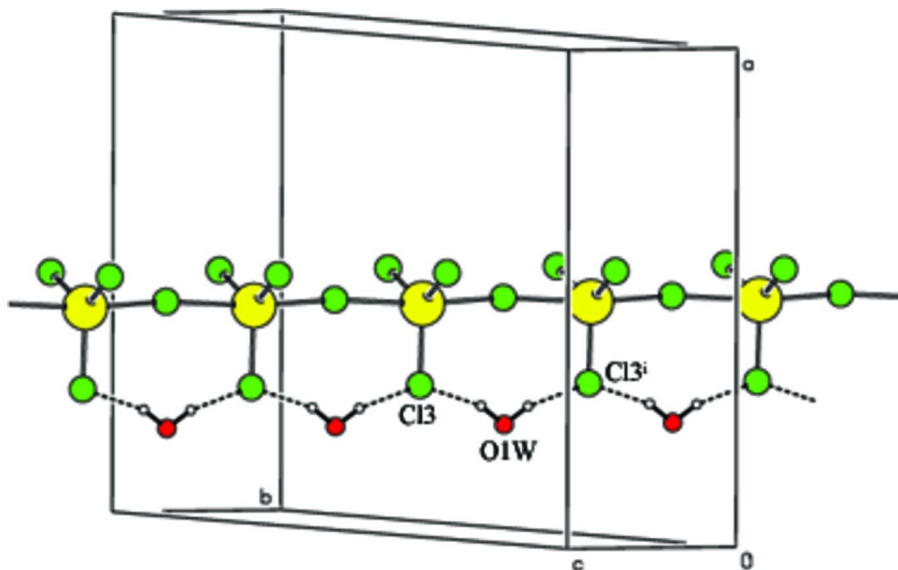


Figure 3

Water molecules bridging chloride ions generating ring motifs along $-\text{Cd}-\text{Cl}-\text{Cd}$ chains. Symmetry codes: (i) $x, y, z + 1$.

catena-Poly[bis(sulfamethoxazolium) [[trichloridocadmium(II)]- μ -chlorido] monohydrate]

Crystal data

$(\text{C}_{10}\text{H}_{12}\text{N}_3\text{O}_3\text{S})_2[\text{CdCl}_4] \cdot \text{H}_2\text{O}$

$M_r = 780.82$

Orthorhombic, *Pnma*

Hall symbol: -P 2ac 2n

$a = 15.088 (2) \text{ \AA}$

$b = 35.028 (3) \text{ \AA}$

$c = 5.562 (3) \text{ \AA}$
 $V = 2939.5 (17) \text{ \AA}^3$
 $Z = 4$
 $F(000) = 1568$
 $D_x = 1.764 \text{ Mg m}^{-3}$
 Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$

Cell parameters from 45 reflections

$\theta = 5.1\text{--}70.1^\circ$
 $\mu = 11.07 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
 Prism-like, light-brown
 $0.19 \times 0.16 \times 0.14 \text{ mm}$

Data collection

Siemens AED single-crystal
 diffractometer
 Radiation source: fine- focus sealed tube
 Graphite monochromator
 ω - 2θ scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.227$, $T_{\max} = 0.306$

2834 measured reflections
 2834 independent reflections
 2470 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.000$
 $\theta_{\max} = 70.1^\circ$, $\theta_{\min} = 5.1^\circ$
 $h = -2 \rightarrow 18$
 $k = -2 \rightarrow 42$
 $l = -6 \rightarrow 6$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.111$
 $S = 1.05$
 2834 reflections
 203 parameters
 4 restraints
 Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map

Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0706P)^2 + 2.0804P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.04 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.64 \text{ e \AA}^{-3}$
 Extinction correction: *SHELXL*,
 $FC^* = KFC[1 + 0.001XFC^2\Lambda^3/\text{SIN}(2\Theta)]^{-1/4}$
 Extinction coefficient: 0.00108 (10)

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All e.s.d.'s are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.47494 (5)	0.09076 (2)	0.89098 (17)	0.0348 (3)
O1	0.54498 (17)	0.11258 (8)	0.7896 (6)	0.0526 (9)
O2	0.47844 (16)	0.07794 (8)	1.1338 (5)	0.0433 (8)
O3	0.34703 (17)	-0.03052 (8)	0.6783 (5)	0.0465 (8)
N4	0.1435 (2)	0.18175 (9)	0.7834 (6)	0.0367 (9)
N7	0.46903 (19)	0.05310 (9)	0.7171 (5)	0.0383 (9)
N8	0.39733 (19)	-0.00044 (9)	0.5779 (6)	0.0450 (10)
C1	0.3753 (2)	0.11622 (9)	0.8542 (6)	0.0311 (8)
C2	0.3077 (2)	0.11213 (9)	1.0198 (6)	0.0376 (9)

C3	0.2303 (2)	0.13307 (10)	0.9951 (6)	0.0380 (10)
C4	0.2224 (2)	0.15783 (9)	0.8048 (6)	0.0322 (9)
C5	0.2887 (2)	0.16153 (10)	0.6346 (7)	0.0400 (10)
C6	0.3658 (2)	0.14054 (10)	0.6588 (6)	0.0403 (10)
C8	0.4174 (2)	0.02120 (9)	0.7613 (6)	0.0315 (8)
C9	0.3822 (2)	0.00750 (9)	0.9784 (6)	0.0348 (9)
C10	0.3395 (2)	-0.02479 (9)	0.9160 (6)	0.0345 (9)
C11	0.2894 (3)	-0.05362 (11)	1.0534 (8)	0.0500 (11)
Cd1	0.47373 (2)	0.25000	1.18772 (7)	0.0430 (1)
Cl1	0.48401 (11)	0.25000	0.7087 (2)	0.0541 (5)
Cl2	0.54023 (7)	0.18534 (3)	1.21780 (16)	0.0511 (3)
Cl3	0.31017 (11)	0.25000	1.2016 (3)	0.0795 (7)
O1W	0.2295 (3)	0.25000	1.7017 (8)	0.0513 (14)
H2	0.31420	0.09530	1.14790	0.0450*
H3	0.18440	0.13040	1.10560	0.0460*
H4A	0.119 (3)	0.1815 (15)	0.938 (10)	0.073 (15)*
H4B	0.165 (3)	0.2055 (13)	0.753 (7)	0.046 (11)*
H4C	0.118 (3)	0.1707 (14)	0.666 (7)	0.076 (17)*
H5	0.28150	0.17800	0.50500	0.0480*
H6	0.41080	0.14270	0.54540	0.0480*
H7	0.50050	0.05320	0.58820	0.0460*
H9	0.38720	0.01830	1.13060	0.0420*
H11A	0.22950	-0.05460	0.99580	0.0750*
H11B	0.28950	-0.04690	1.22070	0.0750*
H11C	0.31670	-0.07820	1.03310	0.0750*
H1W	0.26750	0.25000	1.83940	0.13 (4)*
H2W	0.26530	0.25000	1.56040	0.08 (2)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0272 (4)	0.0305 (4)	0.0468 (5)	0.0038 (3)	-0.0006 (3)	-0.0050 (3)
O1	0.0300 (12)	0.0449 (15)	0.083 (2)	-0.0033 (11)	0.0069 (12)	-0.0036 (14)
O2	0.0447 (13)	0.0426 (14)	0.0427 (13)	0.0104 (11)	-0.0108 (11)	-0.0063 (11)
O3	0.0442 (14)	0.0511 (15)	0.0441 (14)	-0.0099 (12)	0.0004 (11)	-0.0139 (11)
N4	0.0343 (15)	0.0302 (15)	0.0456 (18)	0.0058 (12)	-0.0034 (13)	-0.0003 (13)
N7	0.0427 (16)	0.0326 (15)	0.0395 (15)	0.0050 (11)	0.0113 (12)	-0.0059 (12)
N8	0.0426 (15)	0.0549 (19)	0.0374 (16)	-0.0080 (14)	0.0044 (13)	-0.0087 (14)
C1	0.0283 (14)	0.0255 (14)	0.0394 (16)	0.0020 (12)	0.0004 (12)	-0.0023 (12)
C2	0.0384 (16)	0.0345 (16)	0.0400 (17)	0.0067 (14)	0.0072 (14)	0.0087 (14)
C3	0.0338 (16)	0.0388 (17)	0.0415 (17)	0.0041 (13)	0.0080 (14)	0.0067 (14)
C4	0.0295 (15)	0.0242 (15)	0.0428 (17)	0.0005 (11)	-0.0017 (13)	-0.0026 (12)
C5	0.0436 (18)	0.0335 (16)	0.0429 (17)	0.0035 (14)	0.0070 (15)	0.0110 (15)
C6	0.0387 (17)	0.0375 (18)	0.0447 (19)	0.0020 (14)	0.0112 (15)	0.0072 (15)
C8	0.0287 (14)	0.0343 (15)	0.0314 (15)	0.0091 (12)	-0.0009 (12)	-0.0036 (13)
C9	0.0388 (16)	0.0329 (16)	0.0328 (16)	0.0068 (13)	-0.0004 (13)	-0.0014 (13)
C10	0.0292 (14)	0.0356 (16)	0.0388 (17)	0.0064 (12)	-0.0008 (13)	-0.0018 (14)
C11	0.0441 (19)	0.045 (2)	0.061 (2)	-0.0010 (16)	0.0025 (18)	0.0030 (18)

Cd1	0.0368 (2)	0.0306 (2)	0.0615 (3)	0.0000	0.0019 (2)	0.0000
Cl1	0.0672 (9)	0.0529 (8)	0.0422 (7)	0.0000	0.0054 (6)	0.0000
Cl2	0.0724 (6)	0.0427 (5)	0.0383 (5)	0.0192 (4)	0.0009 (4)	-0.0018 (4)
Cl3	0.0402 (7)	0.1403 (19)	0.0581 (9)	0.0000	0.0057 (6)	0.0000
O1W	0.052 (2)	0.037 (2)	0.065 (3)	0.0000	0.000 (2)	0.0000

Geometric parameters (Å, °)

Cd1—Cl2	2.4828 (17)	N7—H7	0.8599
Cd1—Cl3	2.469 (2)	C1—C6	1.388 (5)
Cd1—Cl1 ⁱ	2.902 (2)	C1—C2	1.382 (5)
Cd1—Cl2 ⁱⁱ	2.4828 (17)	C2—C3	1.386 (4)
Cd1—Cl1	2.6688 (19)	C3—C4	1.374 (5)
S1—C1	1.760 (3)	C4—C5	1.383 (5)
S1—O1	1.421 (3)	C5—C6	1.383 (5)
S1—O2	1.424 (3)	C8—C9	1.404 (5)
S1—N7	1.638 (3)	C9—C10	1.347 (4)
O3—N8	1.413 (4)	C10—C11	1.475 (5)
O3—C10	1.342 (4)	C2—H2	0.9299
O1W—H1W	0.9567	C3—H3	0.9306
O1W—H2W	0.9536	C5—H5	0.9296
N4—C4	1.461 (4)	C6—H6	0.9298
N7—C8	1.384 (4)	C9—H9	0.9303
N8—C8	1.306 (5)	C11—H11A	0.9595
N4—H4A	0.94 (5)	C11—H11B	0.9598
N4—H4B	0.91 (5)	C11—H11C	0.9611
N4—H4C	0.85 (4)		
Cd1...H1W ⁱⁱⁱ	3.6654	N8...H7 ^{xi}	2.5778
Cd1...H2W	3.7665	C3...O1 ^{xii}	3.293 (5)
Cd1...H4A ^{iv}	3.86 (5)	C4...O1 ^{xii}	3.155 (4)
Cd1...H4A ^v	3.86 (5)	C4...O1W ^{vi}	3.281 (4)
Cd1...H1W ^{vi}	3.6654	C4...O1W ⁱⁱⁱ	3.281 (4)
Cd1...H2W ⁱⁱ	3.7665	C5...O1W ^{vi}	3.247 (4)
Cl1...Cd1 ⁱⁱⁱ	2.902 (2)	C5...O1W ⁱⁱⁱ	3.247 (4)
Cl1...N4 ^{vii}	3.392 (4)	C8...C11 ^{xv}	3.516 (6)
Cl1...N4 ^{viii}	3.392 (4)	C8...N8 ^{xi}	3.450 (5)
Cl1...Cl2 ⁱⁱⁱ	3.648 (2)	C8...C9 ^x	3.500 (5)
Cl2...N4 ^{vii}	3.196 (4)	C9...O2	2.991 (4)
Cl2...N4 ^v	3.184 (4)	C9...N8 ⁱ	3.354 (5)
Cl3...O1W ⁱⁱⁱ	3.035 (5)	C9...C8 ^x	3.500 (5)
Cl3...O1W ^{vi}	3.035 (5)	C10...O2 ^x	3.330 (4)
Cl3...O1W ⁱⁱ	3.036 (5)	C11...C8 ^{xvi}	3.516 (6)
Cl3...O1W	3.036 (5)	C11...N8 ^{xvi}	3.397 (6)
Cl2...H3 ^v	3.0659	C11...O1 ^x	3.357 (5)
Cl2...H4C ^{vii}	2.49 (4)	C8...H11A ^{xv}	2.9089
Cl2...H4A ^v	2.26 (5)	H1W...H4B ⁱ	2.2477
Cl2...H6 ⁱ	3.0601	H1W...Cd1 ⁱ	3.6654

Cl3...H1W ⁱⁱⁱ	2.1149	H1W...H4B ^{ix}	2.2477
Cl3...H2W	2.1074	H1W...Cl3 ⁱ	2.1149
Cl3...H5 ⁱ	3.0652	H1W...Cl3 ⁱ	2.1149
Cl3...H5 ^{ix}	3.0652	H1W...Cd1 ⁱ	3.6654
Cl3...H2W ⁱⁱ	2.1074	H2...O2	2.5528
Cl3...H1W ^{vi}	2.1149	H2...H11A ^{xvi}	2.4923
S1...H9	3.1577	H2W...Cd1	3.7665
O1...C11 ^x	3.357 (5)	H2W...Cl3	2.1074
O1...C3 ^{vii}	3.293 (5)	H2W...H4B ^{ix}	2.4223
O1...N4 ^{vii}	2.871 (4)	H2W...H5 ^{ix}	2.5525
O1...C4 ^{vii}	3.155 (4)	H2W...Cl3	2.1074
O1W...N4 ⁱ	2.758 (4)	H2W...H4B ⁱ	2.4223
O1W...C4 ⁱ	3.281 (4)	H2W...H5 ⁱ	2.5525
O1W...Cl3 ⁱ	3.035 (5)	H2W...Cd1	3.7665
O1W...Cl3	3.036 (5)	H3...H4A	2.2464
O1W...C5 ^{ix}	3.247 (4)	H3...Cl2 ^{xiv}	3.0659
O1W...C5 ⁱ	3.247 (4)	H4A...H3	2.2464
O1W...Cl3 ⁱ	3.035 (5)	H4A...Cd1 ^{xiv}	3.86 (5)
O1W...N4 ^{ix}	2.758 (4)	H4A...Cl2 ^{xiv}	2.26 (5)
O1W...Cl3	3.036 (5)	H4A...Cd1 ^{xvii}	3.86 (5)
O1W...C4 ^{ix}	3.281 (4)	H4B...H5	2.4332
O2...C9	2.991 (4)	H4B...O1W ^{vi}	1.86 (5)
O2...C10 ^x	3.330 (4)	H4B...O1W ⁱⁱⁱ	1.86 (5)
O1...H4C ^{vii}	2.33 (5)	H4B...H1W ⁱⁱⁱ	2.2477
O1...H11C ^x	2.6035	H4B...H2W ⁱⁱⁱ	2.4223
O1...H6	2.6564	H4B...H1W ^{vi}	2.2477
O1W...H5 ^{ix}	2.8589	H4B...H2W ^{vi}	2.4223
O1W...H5 ⁱ	2.8589	H4C...Cl2 ^{xii}	2.49 (4)
O1W...H4B ^{ix}	1.86 (5)	H4C...O1 ^{xii}	2.33 (5)
O1W...H4B ⁱ	1.86 (5)	H5...H2W ⁱⁱⁱ	2.5525
O2...H7 ⁱ	2.6925	H5...Cl3 ⁱⁱⁱ	3.0652
O2...H2	2.5528	H5...O1W ⁱⁱⁱ	2.8589
O2...H9	2.5019	H5...Cl3 ^{vi}	3.0652
O3...H11B ⁱⁱⁱ	2.7496	H5...O1W ^{vi}	2.8589
O3...H7 ^{xi}	2.8496	H5...H4B	2.4332
N4...Cl1 ^{xii}	3.392 (4)	H5...H2W ^{vi}	2.5525
N4...Cl2 ^{xii}	3.196 (4)	H6...O1	2.6564
N4...Cl1 ^{xiii}	3.392 (4)	H6...Cl2 ⁱⁱⁱ	3.0601
N4...O1 ^{xii}	2.871 (4)	H7...O3 ^{xi}	2.8496
N4...O1W ^{vi}	2.758 (4)	H7...N8 ^{xi}	2.5778
N4...Cl2 ^{xiv}	3.184 (4)	H7...O2 ⁱⁱⁱ	2.6925
N4...O1W ⁱⁱⁱ	2.758 (4)	H9...O2	2.5019
N7...N8 ^{xi}	3.188 (5)	H9...N8 ⁱ	2.5776
N8...C8 ^{xi}	3.450 (5)	H9...S1	3.1577
N8...C9 ⁱⁱⁱ	3.354 (5)	H11A...N8 ^{xvi}	2.7545
N8...N7 ^{xi}	3.188 (5)	H11A...C8 ^{xvi}	2.9089
N8...C11 ^{xv}	3.397 (6)	H11A...H2 ^{xv}	2.4923
N8...N8 ^{xi}	3.217 (4)	H11B...O3 ⁱ	2.7496

N8...H11A ^{xv}	2.7545	H11C...O1 ^x	2.6035
N8...H9 ⁱⁱⁱ	2.5776		
C11—Cd1—C12 ⁱⁱ	92.51 (3)	S1—C1—C2	120.0 (2)
C12—Cd1—C13	113.69 (3)	C1—C2—C3	120.1 (3)
C11 ⁱ —Cd1—C12	84.90 (3)	C2—C3—C4	118.9 (3)
C12—Cd1—C12 ⁱⁱ	131.63 (4)	N4—C4—C3	119.7 (3)
C11—Cd1—C12	92.51 (3)	C3—C4—C5	121.6 (3)
C11—Cd1—C13	95.12 (5)	N4—C4—C5	118.7 (3)
C11—Cd1—C11 ⁱ	173.60 (5)	C4—C5—C6	119.5 (3)
C11 ⁱ —Cd1—C12 ⁱⁱ	84.90 (3)	C1—C6—C5	119.3 (3)
C11 ⁱ —Cd1—C13	91.27 (5)	N7—C8—C9	129.9 (3)
C12 ⁱⁱ —Cd1—C13	113.69 (3)	N8—C8—C9	112.7 (3)
Cd1—C11—Cd1 ^{vi}	173.60 (7)	N7—C8—N8	117.4 (3)
O1—S1—N7	103.85 (17)	C8—C9—C10	104.3 (3)
O1—S1—C1	108.46 (16)	C9—C10—C11	133.4 (3)
O2—S1—N7	107.94 (16)	O3—C10—C11	116.8 (3)
O1—S1—O2	121.22 (17)	O3—C10—C9	109.8 (3)
O2—S1—C1	107.56 (16)	C1—C2—H2	119.91
N7—S1—C1	107.03 (15)	C3—C2—H2	120.02
N8—O3—C10	108.9 (3)	C2—C3—H3	120.56
H1W—O1W—H2W	108.68	C4—C3—H3	120.52
S1—N7—C8	125.2 (2)	C6—C5—H5	120.25
O3—N8—C8	104.4 (3)	C4—C5—H5	120.28
H4A—N4—H4C	121 (4)	C1—C6—H6	120.37
C4—N4—H4A	104 (3)	C5—C6—H6	120.33
H4B—N4—H4C	116 (4)	C8—C9—H9	127.81
H4A—N4—H4B	109 (4)	C10—C9—H9	127.93
C4—N4—H4B	104 (3)	H11B—C11—H11C	109.45
C4—N4—H4C	100 (3)	H11A—C11—H11B	109.51
C8—N7—H7	117.52	H11A—C11—H11C	109.42
S1—N7—H7	117.31	C10—C11—H11A	109.53
S1—C1—C6	119.3 (2)	C10—C11—H11B	109.49
C2—C1—C6	120.6 (3)	C10—C11—H11C	109.44
O1—S1—N7—C8	171.7 (3)	O3—N8—C8—C9	-0.8 (4)
O2—S1—N7—C8	41.8 (3)	S1—C1—C6—C5	-177.8 (3)
C1—S1—N7—C8	-73.7 (3)	S1—C1—C2—C3	178.0 (3)
O1—S1—C1—C2	-150.0 (3)	C6—C1—C2—C3	-1.5 (5)
O1—S1—C1—C6	29.6 (3)	C2—C1—C6—C5	1.7 (5)
O2—S1—C1—C2	-17.2 (3)	C1—C2—C3—C4	-0.2 (5)
O2—S1—C1—C6	162.3 (3)	C2—C3—C4—N4	-176.5 (3)
N7—S1—C1—C2	98.6 (3)	C2—C3—C4—C5	1.8 (5)
N7—S1—C1—C6	-81.9 (3)	C3—C4—C5—C6	-1.6 (5)
N8—O3—C10—C11	-179.5 (3)	N4—C4—C5—C6	176.7 (3)
C10—O3—N8—C8	0.5 (3)	C4—C5—C6—C1	-0.2 (5)
N8—O3—C10—C9	0.0 (4)	N8—C8—C9—C10	0.8 (4)
S1—N7—C8—N8	158.6 (3)	N7—C8—C9—C10	-178.6 (3)

S1—N7—C8—C9	-22.0 (5)	C8—C9—C10—O3	-0.5 (4)
O3—N8—C8—N7	178.7 (3)	C8—C9—C10—C11	178.9 (4)

Symmetry codes: (i) $x, y, z+1$; (ii) $x, -y+1/2, z$; (iii) $x, y, z-1$; (iv) $x+1/2, -y+1/2, -z+5/2$; (v) $x+1/2, y, -z+5/2$; (vi) $x, -y+1/2, z-1$; (vii) $x+1/2, y, -z+3/2$; (viii) $x+1/2, -y+1/2, -z+3/2$; (ix) $x, -y+1/2, z+1$; (x) $-x+1, -y, -z+2$; (xi) $-x+1, -y, -z+1$; (xii) $x-1/2, y, -z+3/2$; (xiii) $x-1/2, -y+1/2, -z+3/2$; (xiv) $x-1/2, y, -z+5/2$; (xv) $-x+1/2, -y, z-1/2$; (xvi) $-x+1/2, -y, z+1/2$; (xvii) $x-1/2, -y+1/2, -z+5/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1 W —H1 W ···Cl3 ⁱ	0.96	2.11	3.035 (5)	161
O1 W —H2 W ···Cl3	0.95	2.11	3.036 (5)	164
N4—H4A···Cl2 ^{xiv}	0.94 (5)	2.26 (5)	3.184 (4)	171 (4)
N4—H4B···O1 W ⁱⁱⁱ	0.91 (5)	1.86 (5)	2.758 (4)	169 (4)
N4—H4B···O1 W ^{vi}	0.91 (5)	1.86 (5)	2.758 (4)	169 (4)
N4—H4C···Cl2 ^{xii}	0.85 (4)	2.49 (4)	3.196 (4)	141 (4)
N4—H4C···O1 ^{xii}	0.85 (4)	2.33 (5)	2.871 (4)	122 (4)
N7—H7···N8 ^{xi}	0.86	2.58	3.188 (5)	129
C2—H2···O2	0.93	2.55	2.911 (4)	103
C9—H9···O2	0.93	2.50	2.991 (4)	113
C9—H9···N8 ⁱ	0.93	2.58	3.354 (5)	141

Symmetry codes: (i) $x, y, z+1$; (iii) $x, y, z-1$; (vi) $x, -y+1/2, z-1$; (xi) $-x+1, -y, -z+1$; (xii) $x-1/2, y, -z+3/2$; (xiv) $x-1/2, y, -z+5/2$.