

## Diaquabis(dimethyl sulfoxide- $\kappa$ O)-disaccharinatocadmium

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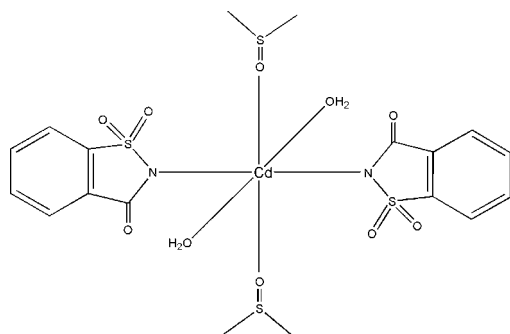
Received 19 October 2011; accepted 25 October 2011

 Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.025;  $wR$  factor = 0.061; data-to-parameter ratio = 18.4.

The title compound,  $[\text{Cd}(\text{C}_7\text{H}_4\text{NO}_3\text{S})_2(\text{C}_2\text{H}_6\text{OS})_2(\text{H}_2\text{O})_2]$ , contains a  $\text{Cd}^{2+}$  cation in an octahedral coordination environment. The metal atom is surrounded by the two different neutral ligands dimethyl sulfoxide (DMSO) and water, each coordinating through the O atom. The anionic saccharinate (sac; 1,1,3-trioxo-2,3-dihydro-1 $\lambda^6$ ,2-benzothiazol-2-ide) ligand coordinates through the N atom. Each of the three similar ligand pairs is in a *trans* configuration with respect to each other. The Cd atom lies on a crystallographic center of symmetry. The DMSO ligand coordinates through the lone pair of electrons on the O atom, as can be seen from the Cd—O—S bond angle of 123.96 (9)°.

### Related literature

For a general review article on the coordination chemistry of saccharinate ligands, see: Baran & Yilmaz (2006). For cadmium saccharinate complexes, see: Deng *et al.* (2008) and for cadmium complexes with saccharinate as a non-coordinating ligand, see: Batsanov *et al.* (2011). For a cadmium complex that contains both saccharinate and DMSO, see: Yilmaz *et al.* (2003). For the preparation of cadmium precursor complexes, see: Haider *et al.* (1984).



### Experimental

#### Crystal data

$[\text{Cd}(\text{C}_7\text{H}_4\text{NO}_3\text{S})_2(\text{C}_2\text{H}_6\text{OS})_2(\text{H}_2\text{O})_2]$   
 $M_r = 669.03$   
 Monoclinic,  $P2_1/c$   
 $a = 10.2613$  (5) Å  
 $b = 15.4294$  (8) Å  
 $c = 7.9951$  (4) Å

$\beta = 98.889$  (1)°  
 $V = 1250.63$  (11) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.26$  mm<sup>-1</sup>  
 $T = 173$  K  
 $0.14 \times 0.11 \times 0.08$  mm

#### Data collection

Bruker Kappa DUO APEXII diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1997)  
 $T_{\min} = 0.843$ ,  $T_{\max} = 0.906$

12452 measured reflections  
 3121 independent reflections  
 2624 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.038$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.061$   
 $S = 1.03$   
 3121 reflections  
 170 parameters  
 2 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.42$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.41$  e Å<sup>-3</sup>

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2006); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: SHELXL97.

WeVZ gratefully acknowledges financial support from the University of KwaZulu-Natal. FSWP thanks the National Research Foundation (NRF) for an Innovative Grant.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2035).

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## supporting information

*Acta Cryst.* (2011). E67, m1635 [doi:10.1107/S1600536811044497]

## Diaquabis(dimethyl sulfoxide- $\kappa$ O)disaccharinatocadmium

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### S1. Comment

Saccharin (*o*-sulfobenzimide; 1,2-benzothiazole-3(2*H*)-one 1,1-dioxide; Hsac) is a widely used artificial sweetening agent. The imino hydrogen is acidic and can be readily deprotonated. The coordination chemistry of this anion is versatile due to the different coordination sites to metallic centers it can accommodate, *i.e.*, one N, one O (carbonylic) and two O (sulfonic) atoms. These donor atoms of the anion can thus readily generate either N- or O-monodentate or bidentate (N, O) coordination. Saccharin is normally used as the sodium or calcium salt which dramatically improves water solubility. Most metal complexes contain the deprotonated form of saccharin, and this saccharinate anion (sac) is commercially available as the sodium salt, used in the present study. The reaction of sodium saccharinate with a variety of divalent transition metal ions results in coordination complexes with general formula  $[M(\text{sac})_2(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$  ( $M = \text{V}, \text{Cr}, \text{Mn}, \text{Fe}, \text{Co}, \text{Ni}, \text{Cu}, \text{Zn}, \text{Cd}$ ), which all show a clear preference to bind through the deprotonated anionic N-atom (Baran and Yilmaz, 2006). These octahedral complexes contain two N-bonded sac ligands in *trans* positions, and complexes of the type  $[M(\text{sac})_2(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$  are thus commonly used as precursors in the synthesis of mixed-ligand saccharinate complexes. The aqua ligands in these metal complexes are labile and readily displaced by direct reaction of neutral ligands. The addition of the ligands to the solutions of the complexes usually results in the substitution of all four aqua ligands, thereby forming stable new mixed-ligand complexes. In cases where the incoming neutral ligand is relatively bulky, as in the present study, it causes steric hindrance and only two of the four aqua ligands become displaced in order for the Cd center to remain octahedral. Although there are a number of Cd(II) saccharinate complexes previously reported (Batsanov *et al.*, 2011, and refs. therein), we are aware of only one other report that contains both saccharinate and dmsu as ligands in a structurally characterized Cd(II) complex (Yilmaz *et al.*, 2003).

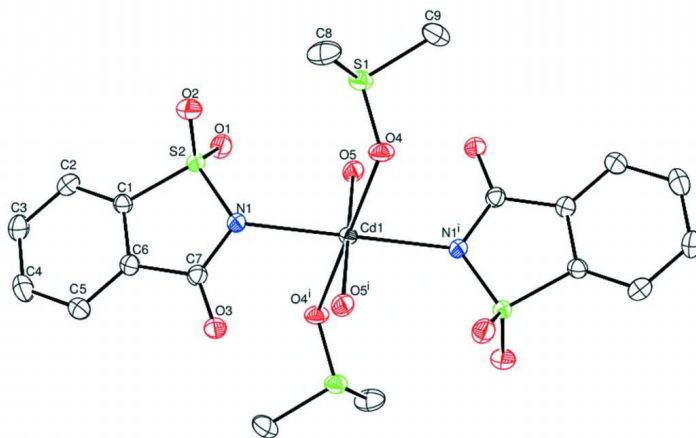
### S2. Experimental

$[\text{Cd}(\text{sac})_2(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$  was prepared as per literature method (Haider *et al.*, 1984). Colorless crystals of  $[\text{Cd}(\text{sac})_2(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$  (1.13 g; 2.10 mmol) was placed in a 100 ml beaker and dissolved in excess amount of dimethyl sulfoxide (dmsu) (20 ml). The reaction mixture was gently heated on a heating mantle with stirring to reduce the volume of dmsu to ~7 ml. The beaker was removed from the heat source and allowed to stand for 6 days during which time large colorless blocky crystals of the title compound were obtained. Yield (1.30 g, 92%); Mp 114°C;  $^{13}\text{C}$  NMR ( $\text{CD}_3\text{OD}$ , 101 MHz) d(p.p.m.): 40.39 ( $\text{CH}_3$ -dmsu), 121.20 ( $\text{C}_6$ -ring), 124.91 ( $\text{C}_6$ -ring), 133.42 ( $\text{C}_6$ -ring), 134.21 ( $\text{C}_6$ -ring), 134.24 ( $\text{C}_6$ -ring), 144.90 ( $\text{C}_6$ -ring) 171.90 (C=O); IR (ATR) 3481, 3016 n(OH), 1646, 1609 n(C=O), 1583, 1460 n(C=C), 1271, 1256 n(O=S=O); 1054, 1036 n(S=O).

### S3. Refinement

All non-H atoms were refined anisotropically. All hydrogen atoms could be found in the difference electron density maps. All, except H5A and H5B on O5, were placed in idealized positions refining in riding models with  $U_{\text{iso}}$  set at 1.2 or 1.5

times those of their parent atoms. The water hydrogen atoms H5A and H5B were located in the difference electron density maps and refined with independent isotropic temperature factors and simple bond length constraints of  $d(\text{O—H}) = 0.980(2) \text{ \AA}$ . The structure was refined to  $R$  factor of 0.0253.



**Figure 1**

The ORTEP molecular structure of the title complex, shown with 50% probability ellipsoids. [Symmetry codes: (i)  $1-x, 2-y, -z$ ]

**Diaquabis(dimethyl sulfoxide)bis(1,1,3,3-trioxo-2,3-dihydro-1 $\lambda$ <sup>6</sup>,2-benzothiazol-2-ido)cadmium**

*Crystal data*

$[\text{Cd}(\text{C}_7\text{H}_4\text{NO}_3\text{S})_2(\text{C}_2\text{H}_6\text{OS})_2(\text{H}_2\text{O})_2]$

$M_r = 669.03$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P 2_1/c$

$a = 10.2613(5) \text{ \AA}$

$b = 15.4294(8) \text{ \AA}$

$c = 7.9951(4) \text{ \AA}$

$\beta = 98.889(1)^\circ$

$V = 1250.63(11) \text{ \AA}^3$

$Z = 2$

$F(000) = 676$

$D_x = 1.777 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 12452 reflections

$\theta = 2.0\text{--}28.4^\circ$

$\mu = 1.26 \text{ mm}^{-1}$

$T = 173 \text{ K}$

Plate, colourless

$0.14 \times 0.11 \times 0.08 \text{ mm}$

*Data collection*

Bruker Kappa DUO APEXII  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$0.5^\circ \varphi$  scans and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1997)

$T_{\text{min}} = 0.843, T_{\text{max}} = 0.906$

12452 measured reflections

3121 independent reflections

2624 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\text{max}} = 28.4^\circ, \theta_{\text{min}} = 2.0^\circ$

$h = -13 \rightarrow 13$

$k = -20 \rightarrow 19$

$l = -10 \rightarrow 10$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.061$   
 $S = 1.03$   
 3121 reflections  
 170 parameters  
 2 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  
 $w = 1/[\sigma^2(F_o^2) + (0.026P)^2 + 0.4033P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.41 \text{ e } \text{\AA}^{-3}$

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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.5000	1.0000	0.0000	0.01487 (7)
S1	0.52294 (5)	0.80523 (4)	0.19576 (7)	0.02107 (12)
S2	0.26624 (5)	0.99004 (4)	0.27847 (6)	0.01863 (12)
O1	0.37534 (15)	1.02578 (12)	0.39322 (19)	0.0269 (4)
O2	0.23352 (16)	0.90145 (11)	0.3102 (2)	0.0286 (4)
O3	0.17818 (14)	1.06754 (10)	-0.15887 (18)	0.0236 (3)
O4	0.52173 (15)	0.85326 (10)	0.02902 (18)	0.0226 (3)
O5	0.62293 (15)	1.02147 (11)	0.25981 (19)	0.0219 (3)
H5A	0.7063 (14)	0.9905 (16)	0.261 (4)	0.053 (10)*
H5B	0.599 (3)	1.0050 (18)	0.3695 (18)	0.056 (11)*
N1	0.28899 (17)	1.00406 (12)	0.0832 (2)	0.0187 (4)
C1	0.12665 (19)	1.05728 (14)	0.2691 (3)	0.0173 (4)
C2	0.0586 (2)	1.08352 (15)	0.3962 (3)	0.0226 (5)
H2	0.0842	1.0655	0.5101	0.027*
C3	-0.0494 (2)	1.13759 (16)	0.3494 (3)	0.0285 (5)
H3	-0.0998	1.1564	0.4329	0.034*
C4	-0.0848 (2)	1.16459 (17)	0.1830 (3)	0.0315 (6)
H4	-0.1590	1.2016	0.1548	0.038*
C5	-0.0139 (2)	1.13854 (15)	0.0564 (3)	0.0240 (5)
H5	-0.0382	1.1572	-0.0574	0.029*
C6	0.09327 (19)	1.08447 (14)	0.1024 (3)	0.0173 (4)
C7	0.1890 (2)	1.05113 (14)	-0.0059 (3)	0.0181 (4)
C8	0.3957 (2)	0.72722 (17)	0.1524 (3)	0.0338 (6)
H8A	0.3100	0.7565	0.1340	0.051*

H8B	0.3996	0.6874	0.2485	0.051*
H8C	0.4071	0.6945	0.0505	0.051*
C9	0.6623 (2)	0.73625 (17)	0.2127 (4)	0.0379 (6)
H9A	0.6571	0.7007	0.1103	0.057*
H9B	0.6642	0.6985	0.3116	0.057*
H9C	0.7428	0.7714	0.2254	0.057*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cd1	0.01608 (10)	0.01350 (11)	0.01516 (10)	0.00098 (8)	0.00279 (7)	0.00131 (8)
S1	0.0264 (3)	0.0166 (3)	0.0201 (2)	0.0016 (2)	0.0034 (2)	0.0023 (2)
S2	0.0167 (2)	0.0241 (3)	0.0156 (2)	0.0032 (2)	0.00400 (19)	0.0044 (2)
O1	0.0193 (8)	0.0431 (10)	0.0180 (8)	0.0014 (7)	0.0016 (6)	0.0029 (7)
O2	0.0331 (9)	0.0243 (9)	0.0296 (9)	0.0055 (7)	0.0089 (7)	0.0086 (7)
O3	0.0227 (8)	0.0323 (9)	0.0156 (7)	0.0056 (7)	0.0027 (6)	0.0038 (7)
O4	0.0322 (9)	0.0142 (8)	0.0219 (8)	0.0017 (6)	0.0060 (7)	0.0041 (6)
O5	0.0233 (8)	0.0270 (9)	0.0156 (7)	0.0019 (6)	0.0039 (6)	-0.0007 (6)
N1	0.0180 (8)	0.0238 (10)	0.0149 (8)	0.0040 (7)	0.0045 (7)	0.0028 (8)
C1	0.0144 (9)	0.0180 (10)	0.0191 (10)	-0.0006 (8)	0.0013 (8)	0.0018 (8)
C2	0.0245 (11)	0.0245 (12)	0.0194 (10)	-0.0031 (9)	0.0055 (9)	0.0010 (9)
C3	0.0290 (12)	0.0309 (13)	0.0286 (12)	0.0065 (10)	0.0136 (10)	-0.0020 (11)
C4	0.0244 (12)	0.0355 (14)	0.0356 (13)	0.0106 (11)	0.0076 (10)	0.0008 (12)
C5	0.0220 (11)	0.0272 (13)	0.0225 (10)	0.0047 (9)	0.0026 (9)	0.0031 (10)
C6	0.0155 (9)	0.0181 (10)	0.0179 (10)	-0.0020 (8)	0.0017 (8)	-0.0013 (8)
C7	0.0165 (9)	0.0202 (11)	0.0176 (10)	-0.0009 (8)	0.0029 (8)	0.0007 (9)
C8	0.0393 (14)	0.0272 (13)	0.0339 (13)	-0.0102 (11)	0.0024 (11)	0.0086 (11)
C9	0.0325 (13)	0.0331 (15)	0.0490 (16)	0.0124 (11)	0.0089 (12)	0.0184 (13)

*Geometric parameters (Å, °)*

Cd1—O5 <sup>i</sup>	2.2817 (15)	C1—C2	1.379 (3)
Cd1—O5	2.2817 (15)	C1—C6	1.388 (3)
Cd1—O4	2.2833 (15)	C2—C3	1.391 (3)
Cd1—O4 <sup>i</sup>	2.2833 (15)	C2—H2	0.9500
Cd1—N1 <sup>i</sup>	2.3620 (17)	C3—C4	1.388 (3)
Cd1—N1	2.3620 (17)	C3—H3	0.9500
S1—O4	1.5236 (15)	C4—C5	1.394 (3)
S1—C8	1.770 (2)	C4—H4	0.9500
S1—C9	1.771 (2)	C5—C6	1.384 (3)
S2—O2	1.4393 (17)	C5—H5	0.9500
S2—O1	1.4429 (17)	C6—C7	1.498 (3)
S2—N1	1.6286 (17)	C8—H8A	0.9800
S2—C1	1.761 (2)	C8—H8B	0.9800
O3—C7	1.237 (2)	C8—H8C	0.9800
O5—H5A	0.979 (2)	C9—H9A	0.9800
O5—H5B	0.979 (2)	C9—H9B	0.9800
N1—C7	1.364 (3)	C9—H9C	0.9800

O5 <sup>i</sup> —Cd1—O5	180.0	C2—C1—S2	129.98 (17)
O5 <sup>i</sup> —Cd1—O4	88.86 (6)	C6—C1—S2	107.30 (15)
O5—Cd1—O4	91.14 (6)	C1—C2—C3	116.8 (2)
O5 <sup>i</sup> —Cd1—O4 <sup>i</sup>	91.14 (6)	C1—C2—H2	121.6
O5—Cd1—O4 <sup>i</sup>	88.86 (6)	C3—C2—H2	121.6
O4—Cd1—O4 <sup>i</sup>	180.0	C4—C3—C2	121.1 (2)
O5 <sup>i</sup> —Cd1—N1 <sup>i</sup>	98.15 (6)	C4—C3—H3	119.4
O5—Cd1—N1 <sup>i</sup>	81.85 (6)	C2—C3—H3	119.4
O4—Cd1—N1 <sup>i</sup>	85.58 (6)	C3—C4—C5	121.4 (2)
O4 <sup>i</sup> —Cd1—N1 <sup>i</sup>	94.42 (6)	C3—C4—H4	119.3
O5 <sup>i</sup> —Cd1—N1	81.85 (6)	C5—C4—H4	119.3
O5—Cd1—N1	98.15 (6)	C6—C5—C4	117.6 (2)
O4—Cd1—N1	94.42 (6)	C6—C5—H5	121.2
O4 <sup>i</sup> —Cd1—N1	85.58 (6)	C4—C5—H5	121.2
N1 <sup>i</sup> —Cd1—N1	180.00 (9)	C5—C6—C1	120.35 (19)
O4—S1—C8	104.67 (10)	C5—C6—C7	128.20 (19)
O4—S1—C9	104.85 (11)	C1—C6—C7	111.39 (18)
C8—S1—C9	99.72 (13)	O3—C7—N1	124.79 (19)
O2—S2—O1	115.48 (10)	O3—C7—C6	122.33 (19)
O2—S2—N1	111.53 (10)	N1—C7—C6	112.85 (17)
O1—S2—N1	110.29 (9)	S1—C8—H8A	109.5
O2—S2—C1	110.89 (9)	S1—C8—H8B	109.5
O1—S2—C1	110.36 (10)	H8A—C8—H8B	109.5
N1—S2—C1	96.72 (9)	S1—C8—H8C	109.5
S1—O4—Cd1	123.96 (9)	H8A—C8—H8C	109.5
Cd1—O5—H5A	107.3 (19)	H8B—C8—H8C	109.5
Cd1—O5—H5B	126.8 (19)	S1—C9—H9A	109.5
H5A—O5—H5B	102 (3)	S1—C9—H9B	109.5
C7—N1—S2	111.33 (14)	H9A—C9—H9B	109.5
C7—N1—Cd1	121.01 (13)	S1—C9—H9C	109.5
S2—N1—Cd1	122.67 (9)	H9A—C9—H9C	109.5
C2—C1—C6	122.70 (19)	H9B—C9—H9C	109.5
C8—S1—O4—Cd1	124.57 (12)	O1—S2—C1—C2	-58.7 (2)
C9—S1—O4—Cd1	-130.95 (13)	N1—S2—C1—C2	-173.3 (2)
O5 <sup>i</sup> —Cd1—O4—S1	-143.39 (10)	O2—S2—C1—C6	-111.05 (16)
O5—Cd1—O4—S1	36.61 (10)	O1—S2—C1—C6	119.69 (15)
O4 <sup>i</sup> —Cd1—O4—S1	140 (100)	N1—S2—C1—C6	5.10 (16)
N1 <sup>i</sup> —Cd1—O4—S1	118.34 (11)	C6—C1—C2—C3	1.7 (3)
N1—Cd1—O4—S1	-61.66 (11)	S2—C1—C2—C3	179.95 (18)
O2—S2—N1—C7	109.33 (16)	C1—C2—C3—C4	-1.0 (4)
O1—S2—N1—C7	-120.95 (16)	C2—C3—C4—C5	0.1 (4)
C1—S2—N1—C7	-6.30 (17)	C3—C4—C5—C6	0.1 (4)
O2—S2—N1—Cd1	-95.51 (12)	C4—C5—C6—C1	0.5 (3)
O1—S2—N1—Cd1	34.20 (14)	C4—C5—C6—C7	-176.6 (2)
C1—S2—N1—Cd1	148.86 (11)	C2—C1—C6—C5	-1.5 (3)
O5 <sup>i</sup> —Cd1—N1—C7	-45.91 (16)	S2—C1—C6—C5	179.89 (17)

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O5—Cd1—N1—C7	134.09 (16)	C2—C1—C6—C7	176.04 (19)
O4—Cd1—N1—C7	-134.12 (16)	S2—C1—C6—C7	-2.5 (2)
O4 <sup>i</sup> —Cd1—N1—C7	45.88 (16)	S2—N1—C7—O3	-176.23 (18)
N1 <sup>i</sup> —Cd1—N1—C7	142 (3)	Cd1—N1—C7—O3	28.1 (3)
O5 <sup>i</sup> —Cd1—N1—S2	161.27 (12)	S2—N1—C7—C6	5.7 (2)
O5—Cd1—N1—S2	-18.73 (12)	Cd1—N1—C7—C6	-149.94 (14)
O4—Cd1—N1—S2	73.06 (11)	C5—C6—C7—O3	-2.6 (4)
O4 <sup>i</sup> —Cd1—N1—S2	-106.94 (11)	C1—C6—C7—O3	-180.0 (2)
N1 <sup>i</sup> —Cd1—N1—S2	-11 (2)	C5—C6—C7—N1	175.5 (2)
O2—S2—C1—C2	70.5 (2)	C1—C6—C7—N1	-1.8 (3)

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