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Hexaaquacadmium(II) bis{[1-(4-hydroxyphenyl)-1*H*-tetrazol-5-ylsulfanyl]acetate}

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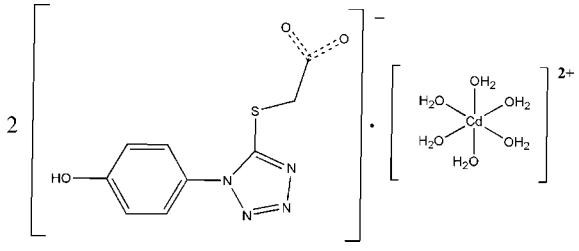
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.068; data-to-parameter ratio = 14.7.

In the title complex, $[Cd(H_2O)_6](C_9H_7N_4O_3S)_2$, the metal center is six-coordinate, forming an ideal centrosymmetric octahedral geometry. A three-dimensional supramolecular architecture is formed through hydrogen-bonding (O—H···O) and offset π–π stacking interactions (distance between pairs of adjacent benzene rings = 3.532 Å and centroid-to-centroid separation = 3.672 Å).

Related literature

For related literature, see: Chen & Suslick (1993); Desiraju *et al.* (1995); Steed & Atwood (2000); Subramanian & Zaworotko (1994); Zhang *et al.* (2007); Zhou *et al.* (1998);



Experimental

Crystal data

$[Cd(H_2O)_6](C_9H_7N_4O_3S)_2$
M_r = 722.99
Triclinic, $P\overline{1}$
a = 6.6872 (2) Å
b = 7.1478 (2) Å
c = 15.0725 (5) Å
α = 98.270 (1)°
β = 97.013 (1)°
γ = 105.353 (1)°
V = 677.76 (4) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 296 (2) K
0.49 × 0.26 × 0.03 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.650, T_{max} = 0.965
10159 measured reflections
3099 independent reflections
3009 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.068
S = 1.00
3099 reflections
211 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O3*W*	2.2635 (15)	Cd1—O2*W*	2.2857 (15)
Cd1—O1*W*	2.2727 (15)		
O3*W*^{i}—Cd1—O3*W*	180	O1*W*^{i}—Cd1—O2*W*	86.15 (6)
O3*W*—Cd1—O1*W*^{i}	89.92 (6)	O1*W*—Cd1—O2*W*	93.85 (6)
O3*W*—Cd1—O1*W*	90.08 (6)	O3*W*—Cd1—O2*W*^{i}	88.40 (7)
O1*W*^{i}—Cd1—O1*W*	180	O2*W*—Cd1—O2*W*^{i}	180
O3*W*—Cd1—O2*W*	91.60 (7)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*B*···O3^{ii}	0.82	1.77	2.586 (2)	174
O1*W*—H1*WB*···O1^{iii}	0.830 (16)	1.949 (17)	2.779 (2)	177 (3)
O2*W*—H2*WA*···O2^{iv}	0.820 (17)	1.91 (2)	2.709 (2)	164 (3)
O2*W*—H2*WB*···O2^{v}	0.829 (17)	2.002 (19)	2.815 (2)	167 (3)
O3*W*—H3*WA*···N4^{v}	0.821 (17)	2.051 (18)	2.869 (2)	174 (3)
O3*W*—H3*WB*···O2	0.815 (17)	1.974 (17)	2.788 (2)	178 (3)

Symmetry codes: (ii) $-x+1, -y+1, -z+1$; (iii) $x-1, y-1, z-1$; (iv) $x+1, y, z$; (v) $-x+1, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); 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: AT2446).

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supplementary materials

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Hexaaquacadmium(II) bis{[1-(4-hydroxyphenyl)-1*H*-tetrazol-5-ylsulfanyl]acetate}

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Comment

Beside the field of molecular chemistry based on the covalent bond, the chemistry of molecular assemblies and of intermolecular bond (Steed *et al.*, 2000) has become a new fascinating area of interest in the last two decades (Subramanian *et al.*, 1994). Efforts have been done to design and construct such kind of assemblies due to their potential multi-dimensional applications in the field of catalysis, non-linear optics, electrical conductivity, molecular recognition, and crystal engineering (Chen *et al.*,1993; Desiraju,1995). Recently, we have concentrated our attention on using H_2L (synthesized from 1-(4-hydroxyphenyl)-5-mercaptotetrazole as bridging spacer to obtain polynuclear complexes of transition-metal. Here, the synthesis and crystal structure of $[Cd(H_2O)_6](HL)_2$, (I), is presented.

The neutral compound consists of one $[Cd(H_2O)_6]^{2+}$ cation and two HL^- anions, as shown in Fig. 1, in which the complex has a crystallographic center with the Zn atom situated at the center of (0. 1/2, 0). In the cations, the Cd atom is surrounded by six aqua ligands, exhibiting an ideal octahedral geometry·On the other hand, the bond lengths within the mercaptotetrazole segment exhibit the expected pattern of four long bonds [S(1)—C(7), N(1)—N(2), N(3)—N(4) and C(7)—N(1)] and two short bonds [N(2)—N(3) and C(7)—N(4)] on the whole. As shown in Fig. 2, there exist offset-panel π-π stacking interactions. The distance between the two adjacent benzene rings is 3.532Å (centroid separation is 3.672 Å). Also intermolecular O—H···O, O—H···N hydrogen bonds are observed. Thus, all of the hydrogen bonding interactions makes the title compound extend into a three-dimensional supramolecular framework as well as the offset-panel π-π stacking interactions (Zhang *et al.*,2007).

Experimental

The synthesis of legand H_2L was prepared according to the literature (Zhou, 1998). The compound were prepared by mixing 1:2 molar ratio of cadmium chloridate and H_2L in ethanol-water(1:1,16 ml). The mixture was refluxed at 323 K for 2 h with stirring, then filtered and left to stand at the room temperature. Well shaped crystals suitable for X-ray analyses were obtained by slow evaporation of the filtrate in *ca* 40–50% yields within about a week.

Refinement

The H atoms bonded to C atoms were positioned geometrically and refined using a riding model [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C)]. The H atoms bonded to O atoms were located in a difference Fourier maps and their positions were refined isotropically, with O—H distances fixed by O—H = 0.85 (2) Å and H···H = 1.30 (2) Å, their displacement parameters were set to 1.5U_{eq}(O).

Figures

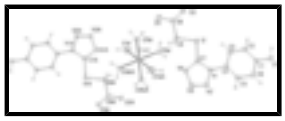

Fig. 1. View of the molecule of (I), showing the atom-numbering scheme. Displacement ellipsoids plotted at 30% probability level. [The atoms labelled with 'A' are related to the center of inversion].

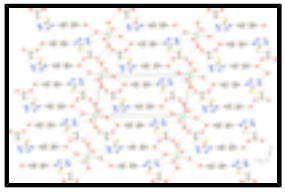

Fig. 2. Packing diagram for the title compound. The O—H···O hydrogen bonds and O—H···N interactions are depicted by dashed lines.

Hexaaquacadmium(II) bis{[1-(4-hydroxyphenyl)-1*H*-tetrazol-5-ylsulfanyl]acetate}

Crystal data

$[Cd(H_2O)_6](C_9H_7N_4O_3S)_2$	$Z = 1$
$M_r = 722.99$	$F_{000} = 366$
Triclinic, $P\overline{1}$	$D_x = 1.771$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.6872$ (2) Å	Cell parameters from 3100 reflections
$b = 7.1478$ (2) Å	$\theta = 2.8$–$26.6°$
$c = 15.0725$ (5) Å	$\mu = 1.04$ mm^{-1}
$\alpha = 98.270$ (1)°	$T = 296$ (2) K
$\beta = 97.013$ (1)°	Sheet, colourless
$\gamma = 105.353$ (1)°	0.49 × 0.26 × 0.03 mm
$V = 677.76$ (4) Å^3	

Data collection

Bruker APEXII area-detector diffractometer	3099 independent reflections
Radiation source: fine-focus sealed tube	3009 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
$T = 296(2)$ K	$\theta_{max} = 27.6°$
ω scans	$\theta_{min} = 2.8°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{min} = 0.650$, $T_{max} = 0.965$	$k = -9 \rightarrow 8$
10159 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.025$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.2797P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
3099 reflections	$\Delta\rho_{max} = 0.90$ e Å^{-3}
211 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
9 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cd1	0.5000	0.0000	0.0000	0.03204 (8)
S1	0.60568 (7)	0.61474 (8)	0.29716 (3)	0.03853 (12)
O1	1.1690 (2)	0.7681 (3)	0.72338 (9)	0.0452 (4)
H1B	1.0600	0.7148	0.7407	0.068*
O1W	0.5334 (2)	−0.0704 (3)	−0.14842 (10)	0.0492 (4)
H1WA	0.629 (4)	−0.016 (5)	−0.174 (2)	0.088 (12)*
H1WB	0.427 (3)	−0.120 (4)	−0.1879 (16)	0.055 (8)*
O2	0.1602 (2)	0.4141 (2)	0.08721 (10)	0.0419 (3)
O2W	0.7407 (2)	0.3043 (2)	0.02541 (11)	0.0455 (4)
H2WA	0.862 (3)	0.319 (5)	0.049 (2)	0.084 (11)*
H2WB	0.753 (5)	0.375 (4)	−0.0139 (17)	0.064 (9)*
O3	0.1891 (2)	0.4057 (3)	0.23510 (11)	0.0554 (5)
O3W	0.2335 (3)	0.1271 (3)	−0.04036 (11)	0.0503 (4)
H3WA	0.196 (5)	0.150 (5)	−0.0907 (12)	0.072 (10)*
H3WB	0.216 (5)	0.213 (4)	−0.0029 (15)	0.068 (9)*
N1	1.0318 (2)	0.7871 (2)	0.35349 (10)	0.0315 (3)
N2	1.2008 (2)	0.8777 (3)	0.31828 (12)	0.0393 (4)
N3	1.1337 (3)	0.8776 (3)	0.23480 (12)	0.0420 (4)
N4	0.9232 (2)	0.7909 (3)	0.21196 (11)	0.0371 (4)
C1	1.1286 (3)	0.7665 (3)	0.63276 (12)	0.0333 (4)
C2	1.2963 (3)	0.8031 (4)	0.58578 (14)	0.0421 (5)
H2	1.4325	0.8273	0.6165	0.050*

C3	1.2626 (3)	0.8040 (3)	0.49351 (14)	0.0388 (4)
H3	1.3755	0.8259	0.4621	0.047*
C4	1.0596 (3)	0.7721 (3)	0.44788 (12)	0.0300 (3)
C5	0.8922 (3)	0.7356 (3)	0.49449 (13)	0.0366 (4)
H5	0.7563	0.7149	0.4641	0.044*
C6	0.9259 (3)	0.7297 (3)	0.58611 (13)	0.0364 (4)
H6	0.8121	0.7010	0.6168	0.044*
C7	0.8611 (3)	0.7346 (3)	0.28689 (12)	0.0312 (4)
C8	0.4890 (3)	0.5720 (3)	0.17878 (12)	0.0347 (4)
H8A	0.4992	0.6971	0.1591	0.042*
H8B	0.5633	0.5002	0.1418	0.042*
C9	0.2594 (3)	0.4531 (3)	0.16719 (13)	0.0334 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02480 (10)	0.03904 (13)	0.02939 (11)	0.00194 (8)	0.00382 (7)	0.01132 (7)
S1	0.0213 (2)	0.0584 (3)	0.0299 (2)	−0.00021 (19)	0.00287 (16)	0.0122 (2)
O1	0.0292 (6)	0.0662 (10)	0.0317 (7)	−0.0008 (6)	0.0009 (5)	0.0127 (7)
O1W	0.0325 (7)	0.0733 (11)	0.0293 (7)	−0.0067 (7)	0.0063 (6)	0.0097 (7)
O2	0.0285 (6)	0.0553 (9)	0.0342 (7)	0.0014 (6)	−0.0026 (5)	0.0105 (6)
O2W	0.0287 (7)	0.0483 (9)	0.0515 (9)	−0.0053 (6)	−0.0024 (6)	0.0218 (7)
O3	0.0316 (7)	0.0843 (13)	0.0388 (8)	−0.0093 (8)	0.0050 (6)	0.0239 (8)
O3W	0.0515 (9)	0.0738 (12)	0.0351 (8)	0.0314 (9)	0.0066 (7)	0.0157 (8)
N1	0.0206 (6)	0.0382 (8)	0.0318 (7)	0.0012 (6)	0.0054 (5)	0.0070 (6)
N2	0.0250 (7)	0.0517 (10)	0.0363 (8)	0.0001 (7)	0.0083 (6)	0.0107 (7)
N3	0.0282 (8)	0.0545 (11)	0.0391 (9)	0.0008 (7)	0.0091 (6)	0.0135 (8)
N4	0.0275 (7)	0.0481 (10)	0.0334 (8)	0.0037 (7)	0.0067 (6)	0.0127 (7)
C1	0.0280 (8)	0.0343 (9)	0.0316 (9)	0.0002 (7)	0.0013 (7)	0.0063 (7)
C2	0.0218 (8)	0.0582 (13)	0.0396 (10)	0.0009 (8)	−0.0002 (7)	0.0123 (9)
C3	0.0220 (8)	0.0528 (12)	0.0381 (10)	0.0021 (8)	0.0063 (7)	0.0121 (8)
C4	0.0239 (8)	0.0318 (9)	0.0302 (8)	0.0014 (7)	0.0035 (6)	0.0056 (7)
C5	0.0210 (8)	0.0506 (11)	0.0351 (9)	0.0053 (7)	0.0025 (7)	0.0093 (8)
C6	0.0238 (8)	0.0468 (11)	0.0345 (9)	0.0031 (7)	0.0056 (7)	0.0074 (8)
C7	0.0237 (8)	0.0367 (10)	0.0313 (8)	0.0044 (7)	0.0050 (6)	0.0077 (7)
C8	0.0238 (8)	0.0463 (11)	0.0292 (8)	0.0004 (7)	0.0024 (6)	0.0114 (7)
C9	0.0242 (8)	0.0394 (10)	0.0329 (9)	0.0018 (7)	0.0029 (6)	0.0106 (7)

Geometric parameters (Å, °)

Cd1—O3W^{i}	2.2635 (15)	N1—N2	1.355 (2)
Cd1—O3W	2.2635 (15)	N1—C4	1.435 (2)
Cd1—O1W^{i}	2.2727 (15)	N2—N3	1.283 (2)
Cd1—O1W	2.2727 (15)	N3—N4	1.357 (2)
Cd1—O2W	2.2857 (15)	N4—C7	1.329 (2)
Cd1—O2W^{i}	2.2857 (15)	C1—C2	1.385 (3)
S1—C7	1.7327 (18)	C1—C6	1.388 (2)
S1—C8	1.8064 (18)	C2—C3	1.383 (3)

O1—C1	1.358 (2)	C2—H2	0.9300
O1—H1B	0.8200	C3—C4	1.389 (2)
O1W—H1WA	0.823 (17)	C3—H3	0.9300
O1W—H1WB	0.830 (16)	C4—C5	1.380 (2)
O2—C9	1.258 (2)	C5—C6	1.380 (3)
O2W—H2WA	0.820 (17)	C5—H5	0.9300
O2W—H2WB	0.829 (17)	C6—H6	0.9300
O3—C9	1.231 (2)	C8—C9	1.520 (2)
O3W—H3WA	0.821 (17)	C8—H8A	0.9700
O3W—H3WB	0.815 (17)	C8—H8B	0.9700
N1—C7	1.355 (2)		
$O3W^{i}$—Cd1—O3W	180.00 (8)	C7—N4—N3	105.59 (15)
$O3W^{i}$—Cd1—$O1W^{i}$	90.08 (6)	O1—C1—C2	118.48 (16)
O3W—Cd1—$O1W^{i}$	89.92 (6)	O1—C1—C6	122.23 (17)
$O3W^{i}$—Cd1—O1W	89.92 (6)	C2—C1—C6	119.29 (18)
O3W—Cd1—O1W	90.08 (6)	C3—C2—C1	120.47 (17)
$O1W^{i}$—Cd1—O1W	180.00 (8)	C3—C2—H2	119.8
$O3W^{i}$—Cd1—O2W	88.40 (7)	C1—C2—H2	119.8
O3W—Cd1—O2W	91.60 (7)	C2—C3—C4	119.81 (17)
$O1W^{i}$—Cd1—O2W	86.15 (6)	C2—C3—H3	120.1
O1W—Cd1—O2W	93.85 (6)	C4—C3—H3	120.1
$O3W^{i}$—Cd1—$O2W^{i}$	91.60 (7)	C5—C4—C3	119.86 (17)
O3W—Cd1—$O2W^{i}$	88.40 (7)	C5—C4—N1	121.75 (15)
$O1W^{i}$—Cd1—$O2W^{i}$	93.85 (6)	C3—C4—N1	118.33 (16)
O1W—Cd1—$O2W^{i}$	86.15 (6)	C6—C5—C4	120.16 (16)
O2W—Cd1—$O2W^{i}$	180.00 (6)	C6—C5—H5	119.9
C7—S1—C8	97.94 (9)	C4—C5—H5	119.9
C1—O1—H1B	109.5	C5—C6—C1	120.37 (17)
Cd1—O1W—H1WA	128 (2)	C5—C6—H6	119.8
Cd1—O1W—H1WB	119.9 (18)	C1—C6—H6	119.8
H1WA—O1W—H1WB	107 (2)	N4—C7—N1	108.17 (15)
Cd1—O2W—H2WA	120 (2)	N4—C7—S1	125.73 (14)
Cd1—O2W—H2WB	122 (2)	N1—C7—S1	126.10 (14)
H2WA—O2W—H2WB	104 (2)	C9—C8—S1	108.98 (12)
Cd1—O3W—H3WA	127 (2)	C9—C8—H8A	109.9
Cd1—O3W—H3WB	117 (2)	S1—C8—H8A	109.9
H3WA—O3W—H3WB	107 (2)	C9—C8—H8B	109.9
C7—N1—N2	107.85 (15)	S1—C8—H8B	109.9
C7—N1—C4	133.22 (15)	H8A—C8—H8B	108.3
N2—N1—C4	118.86 (14)	O3—C9—O2	126.70 (18)
N3—N2—N1	106.68 (15)	O3—C9—C8	118.25 (16)
N2—N3—N4	111.70 (16)	O2—C9—C8	115.05 (16)
C7—N1—N2—N3	−0.4 (2)	C4—C5—C6—C1	2.0 (3)
C4—N1—N2—N3	−177.88 (17)	O1—C1—C6—C5	177.98 (19)
N1—N2—N3—N4	0.5 (2)	C2—C1—C6—C5	−2.0 (3)
N2—N3—N4—C7	−0.4 (2)	N3—N4—C7—N1	0.1 (2)

O1—C1—C2—C3	−179.7 (2)	N3—N4—C7—S1	−179.91 (15)
C6—C1—C2—C3	0.3 (3)	N2—N1—C7—N4	0.2 (2)
C1—C2—C3—C4	1.4 (3)	C4—N1—C7—N4	177.15 (18)
C2—C3—C4—C5	−1.3 (3)	N2—N1—C7—S1	−179.80 (14)
C2—C3—C4—N1	175.88 (19)	C4—N1—C7—S1	−2.9 (3)
C7—N1—C4—C5	−15.7 (3)	C8—S1—C7—N4	7.35 (19)
N2—N1—C4—C5	160.95 (19)	C8—S1—C7—N1	−172.63 (17)
C7—N1—C4—C3	167.1 (2)	C7—S1—C8—C9	176.39 (14)
N2—N1—C4—C3	−16.2 (3)	S1—C8—C9—O3	0.1 (2)
C3—C4—C5—C6	−0.4 (3)	S1—C8—C9—O2	179.79 (15)
N1—C4—C5—C6	−177.47 (18)		

Symmetry codes: (i) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1B···O3^{ii}	0.82	1.77	2.586 (2)	174
O1W—H1WB···O1^{iii}	0.830 (16)	1.949 (17)	2.779 (2)	177 (3)
O2W—H2WA···O2^{iv}	0.820 (17)	1.91 (2)	2.709 (2)	164 (3)
O2W—H2WB···O2^{v}	0.829 (17)	2.002 (19)	2.815 (2)	167 (3)
O3W—H3WA···N4^{v}	0.821 (17)	2.051 (18)	2.869 (2)	174 (3)
O3W—H3WB···O2	0.815 (17)	1.974 (17)	2.788 (2)	178 (3)

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

Fig. 1

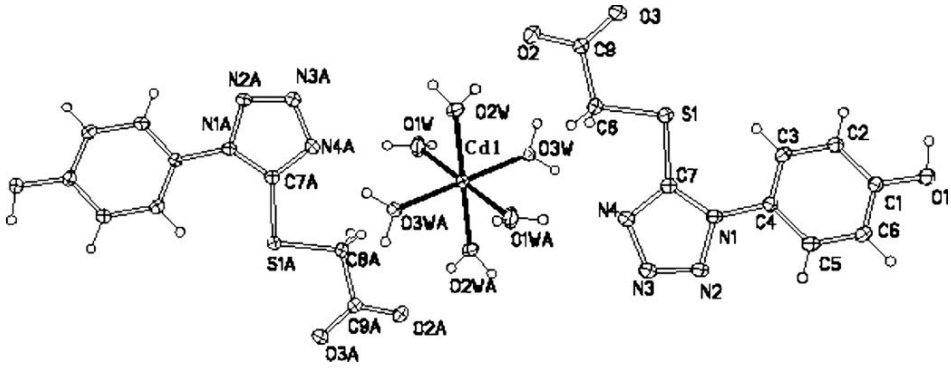
O3
O2
C8
N2A
N3A
N1A
N4A
C7A
O1W
O2W
Cd1
O3W
C6
S1
C7
C3
C2
C1
O1
N4
N1
C4
C6
C5
N3
N2
O3WA
O1WA
O2WA
S1A
C8A
C9A
O2A
O3A

Fig. 2