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Di-μ_2-aqua-bis[aqua(2,2′-diamino-4,4′-bi-1,3-thiazole-κ^2N,N')(4-nitrobenzoato-κO)cadmium(II)] bis(4-nitrobenzoate)

Guang-Hua Chen, Yuan-Yuan Lin, Yan-Ping Yu and Bing-Xin Liu*

Department of Chemistry, Shanghai University, People's Republic of China
Correspondence e-mail: r5744011@yahoo.com.cn

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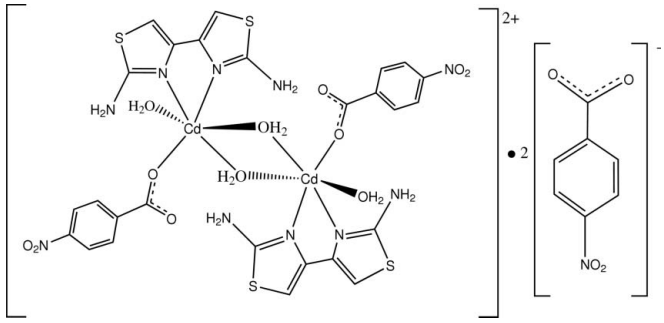
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.032; wR factor = 0.072; data-to-parameter ratio = 12.2.

The title compound, $[Cd_2(C_7H_4NO_4)_2(C_6H_{10}N_4O_2S_2)_2]$-$(C_7H_4NO_4)_2$, consists of dimeric Cd^{II} complex cations and uncoordinated 4-nitrobenzoate anions. Within the complex cation, each Cd^{II} cation assumes a distorted octahedral coordination geometry, formed by a diaminobithiazole (DABT) ligand, a 4-nitrobenzoate anion and two coordinated water molecules. Two coordinated water molecules bridge two Cd^{II} cations to form the dimeric complex cation across an inversion centre. The two thiazole rings of the chelating DABT ligand are twisted with respect to each other, forming a dihedral angle of 3.91 (18)°. The centroid-to-centroid separation of 3.7601 (19) Å indicates the existence of π–π stacking between nearly parallel thiazole rings in the crystal structure. O—H···O and N—H···O hydrogen bonding between complex cations and uncoordinated 4-nitrobenzoate anions, and between complex cations, helps to stabilize the crystal structure.

Related literature

For general background, see: Sun *et al.* (1997); Waring (1981); Fisher *et al.* (1985); Liu & Xu (2004). For related structures, see: Luo *et al.* (2004); Liu *et al.* (2004, 2006); Liu & Xu (2005).



Experimental

Crystal data

$[Cd_2(C_7H_4NO_4)_2(C_6H_{10}N_4O_2S_2)_2]$-$(C_7H_4NO_4)_2$
M_r = 1357.85
Triclinic, $P\overline{1}$
a = 7.6045 (10) Å
b = 10.7869 (14) Å
c = 16.118 (2) Å
α = 97.741 (1)°
β = 102.600 (1)°
γ = 100.817 (1)°
V = 1245.9 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 295 (2) K
0.30 × 0.26 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.710, T_{max} = 0.825
6467 measured reflections
4310 independent reflections
3751 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.072
S = 1.05
4310 reflections
352 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd—O1	2.294 (2)	Cd—O21	2.313 (2)
Cd—O1^{i}	2.393 (2)	Cd—N11	2.266 (3)
Cd—O2	2.250 (2)	Cd—N13	2.344 (2)
Cd—O1—Cd^{i}	105.70 (8)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O22	0.83	1.90	2.662 (3)	151
O1—H1B···O31^{ii}	0.88	1.66	2.522 (3)	164
O2—H2A···O32	0.84	1.83	2.650 (4)	164
O2—H2B···O22^{ii}	0.83	1.95	2.766 (3)	165
N12—H12A···O33^{iii}	0.86	2.45	3.164 (4)	141
N12—H12A···O34^{iii}	0.86	2.35	3.192 (5)	165
N12—H12B···O21	0.89	2.07	2.901 (4)	156
N14—H14A···O24^{iv}	0.86	2.54	3.292 (4)	147
N14—H14B···O31^{ii}	0.87	2.19	3.014 (4)	158

Symmetry codes: (ii) $-x+2, -y+1, -z+1$; (iii) $-x+1, -y, -z$; (iv) $x, y, z+1$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC and Rigaku, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The project was supported by the Educational Development Foundation of Shanghai Educational Committee, China (grant No. AB0448).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2275).

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supplementary materials

Acta Cryst. (2007). E**63**, m1915-m1916 [**doi:10.1107/S1600536807028462**]

Di-μ_2-aqua-bis[aqua(2,2'-diamino-4,4'-bi-1,3-thiazole-κ^2N,N')(4-nitrobenzoato-κO)cadmium(II)] bis(4-nitrobenzoate)

G.-H. Chen, Y.-Y. Lin, Y.-P. Yu and B.-X. Liu

Comment

Transition metal complexes of 2,2'-diamino-4,4'-bi-1,3-thiazole (DABT) have shown potential application in the field of soft magnetic material (Sun *et al.*, 1997) and biological activities, such as the effective inhibitors of DNA synthesis of the tumor cells (Waring, 1981; Fisher *et al.*, 1985). As part of serial structural investigation of metal complexes with DABT (Liu & Xu, 2004), the title Cd^{II} complex was recently prepared and its X-ray structure is presented here.

The molecular structure of the title compound is shown in Fig. 1. The crystal of the title compound consists of the dimeric Cd^{II} complex cations and uncoordinated 4-nitrobenzoate anions. Within the complex cation, each Cd^{II} cation assumes a distorted octahedral coordination geometry (Table 1), formed by DABT, 4-nitrobenzoate anion and two coordinated water molecules. Two coordinated water molecules bridges two Cd^{II} cations to form the dimeric complex cation across on an inversion center.

Whithin the complex, the DABT molecule shows approximately coplanar configuration with the dihedral angle 3.91 (18)° between two thiazole rings, which comparable to 2.6 (1)° found in $[Mn(C_6H_6N_4S_2)(C_8H_4O_4)(H_2O)_2]\cdot 2H_2O$ (Liu *et al.*, 2006) and 4.57 (7)° in [Mn(DABT)(oxydiacetate)] (Luo *et al.*, 2004), but different from 17.23 (7)° found in $[Cr(C_4H_5NO_4)(C_6H_6N_4S_2)(H_2O)]Cl\cdot H_2O$, (Liu *et al.*, 2004) and 20.02 (8)° found in [Ni(DABT)(iminodiacetate)] (Liu & Xu, 2005).

One oxygen atom O21 of carboxyl group of the 4-nitrobenzoate anion chelates to Cd^{II} atom, and hydrogen bonded to the amino group of DABT within the complex, another uncoordinated oxygen atom(O22) is hydrogen bonded to the coordinated water within the complex (Table 2), which helps to stabilize the crystal structure.

The separations of 3.7601 (19) Å between nearly parallel thiazole rings ($1-x,-y,1-z$) suggests the existence of π-π stacking (Fig. 2).

Experimental

An ethanol solution (20 ml) containing DABT (0.20 g, 1 mmol) and $CdCl_2\cdot 2.5(H_2O)$ (0.22 g, 1 mmol) was mixed with an aqueous solution (10 ml) of 4-nitrobenzoic acid (0.34 g, 2 mmol) and NaOH (0.08 g, 2 mmol). The mixture was refluxed for 6 h. After cooling to room temperature the solution was filtered. Single crystals of the title compound were obtained from the filtrate after 7 d.

Refinement

H atoms on carbon atoms were placed in calculated positions with C—H distances = 0.93 Å (aromatic), and were included in the final cycles of refinement in riding mode with U_{iso}(H) = 1.2U_{eq}(C). H atoms of amino groups and water molecules were located in a difference Fourier map and included in the structure factor calculations with fixed positional and U_{iso}(H) = 0.05 Å^2.

Figures

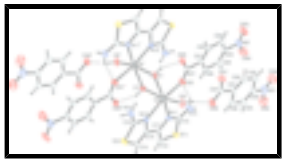

Fig. 1. The molecular structure of the title compound with 30% probability displacement ellipsoids (arbitrary spheres for H atoms), dashed lines showing the hydrogen bonding.

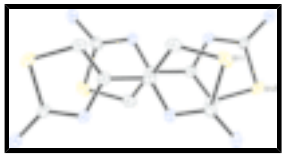

Fig. 2. The unit cell packing diagram showing π-π stacking between the S11-thiazole and S12^{i}-thiazole rings [symmetry code: (i) 1 − *x*,-*y*,1 − *z*]. H atoms have been omitted for clarity.

Di-μ$_2$-aqua-bis[aqua(2,2'-diamino-4,4'-bi-1,3-thiazole-κ^2*N*,*N*')(4- nitrobenzoato-κ*O*)cadmium(II)] bis(4-nitrobenzoate)

Crystal data

$[Cd_2(C_7H_4NO_4)_2(C_6H_{10}N_4O_2S_2)_2](C_7H_4NO_4)_2$	Z = 1
M_r = 1357.85	F_{000} = 680
Triclinic, $P\overline{1}$	D_x = 1.810 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.6045 (10) Å	Cell parameters from 4280 reflections
b = 10.7869 (14) Å	θ = 2.0–25.0º
c = 16.118 (2) Å	μ = 1.11 mm^{-1}
α = 97.741 (1)º	T = 295 (2) K
β = 102.600 (1)º	Prism, red
γ = 100.817 (1)º	0.30 × 0.26 × 0.17 mm
V = 1245.9 (3) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	4310 independent reflections
Radiation source: fine-focus sealed tube	3751 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 25.0º
T = 295(2) K	θ_{min} = 1.9º

ω scans

Absorption correction: multi-scan (ABSCOR; Higashi, 1995)

T_{min} = 0.710, T_{max} = 0.825

6467 measured reflections

$h = -8 \rightarrow 9$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.072$

$S = 1.05$

4310 reflections

352 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.027P)^2 + 0.7682P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.32$ e Å^{-3}

$\Delta\rho_{min} = -0.40$ e Å^{-3}

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_{iso}*/U_{eq}
Cd	0.57818 (3)	0.34675 (2)	0.481336 (15)	0.03068 (9)
O1	0.6890 (3)	0.56396 (19)	0.52648 (14)	0.0318 (5)
H1A	0.7300	0.5938	0.4877	0.050*
H1B	0.7772	0.5890	0.5750	0.050*
O2	0.8663 (3)	0.3128 (2)	0.50161 (16)	0.0460 (6)
H2A	0.9032	0.2898	0.4578	0.050*
H2B	0.9550	0.3491	0.5432	0.050*
O21	0.5914 (3)	0.3862 (2)	0.34503 (14)	0.0425 (6)
O22	0.7996 (3)	0.5726 (2)	0.38119 (14)	0.0419 (6)
O23	0.8204 (5)	0.5367 (3)	−0.0475 (2)	0.0797 (10)
O24	0.6407 (6)	0.3528 (4)	−0.0772 (2)	0.0953 (12)
O31	1.1054 (3)	0.3710 (2)	0.32199 (15)	0.0488 (7)
O32	0.9237 (4)	0.2072 (2)	0.35451 (16)	0.0506 (7)

O33	0.6588 (5)	−0.0802 (4)	−0.0749 (2)	0.0964 (13)
O34	0.8323 (6)	0.0790 (4)	−0.1054 (2)	0.0932 (12)
N11	0.3961 (4)	0.1488 (2)	0.42375 (17)	0.0316 (6)
N12	0.3833 (5)	0.1243 (3)	0.27703 (19)	0.0543 (9)
H12A	0.3311	0.0815	0.2257	0.050*
H12B	0.4630	0.1992	0.2858	0.050*
N13	0.5098 (3)	0.2598 (2)	0.59931 (16)	0.0301 (6)
N14	0.6762 (4)	0.4014 (3)	0.72924 (18)	0.0460 (8)
H14A	0.6824	0.4245	0.7832	0.050*
H14B	0.7225	0.4557	0.7000	0.050*
N21	0.7267 (5)	0.4480 (4)	−0.0264 (2)	0.0540 (9)
N31	0.7664 (6)	0.0236 (4)	−0.0541 (2)	0.0660 (11)
S11	0.16984 (14)	−0.05631 (9)	0.33490 (6)	0.0464 (2)
S12	0.44067 (14)	0.18707 (9)	0.73631 (6)	0.0455 (2)
C11	0.3181 (4)	0.0854 (3)	0.4812 (2)	0.0321 (8)
C12	0.1944 (5)	−0.0249 (3)	0.4448 (2)	0.0436 (9)
H12	0.1305	−0.0774	0.4749	0.052*
C13	0.3308 (5)	0.0853 (3)	0.3445 (2)	0.0358 (8)
C14	0.3819 (4)	0.1423 (3)	0.5736 (2)	0.0320 (8)
C15	0.3295 (5)	0.0901 (3)	0.6382 (2)	0.0424 (9)
H15	0.2450	0.0125	0.6308	0.051*
C16	0.5543 (5)	0.2946 (3)	0.6835 (2)	0.0314 (7)
C21	0.7022 (4)	0.4717 (3)	0.2335 (2)	0.0315 (7)
C22	0.8271 (5)	0.5632 (3)	0.2099 (2)	0.0427 (9)
H22	0.9064	0.6296	0.2520	0.051*
C23	0.8349 (5)	0.5569 (4)	0.1256 (2)	0.0483 (10)
H23	0.9192	0.6181	0.1100	0.058*
C24	0.7163 (5)	0.4590 (4)	0.0644 (2)	0.0409 (9)
C25	0.5894 (5)	0.3676 (4)	0.0844 (2)	0.0462 (10)
H25	0.5103	0.3019	0.0418	0.055*
C26	0.5824 (5)	0.3758 (4)	0.1701 (2)	0.0436 (9)
H26	0.4955	0.3157	0.1851	0.052*
C27	0.6992 (5)	0.4782 (3)	0.3278 (2)	0.0339 (8)
C31	0.9354 (5)	0.2001 (3)	0.2088 (2)	0.0357 (8)
C32	1.0135 (5)	0.2538 (4)	0.1488 (2)	0.0475 (10)
H32	1.1044	0.3294	0.1666	0.057*
C33	0.9584 (6)	0.1967 (4)	0.0623 (3)	0.0544 (11)
H33	1.0099	0.2339	0.0218	0.065*
C34	0.8269 (6)	0.0847 (4)	0.0378 (2)	0.0492 (10)
C35	0.7478 (6)	0.0278 (4)	0.0956 (3)	0.0634 (12)
H35	0.6596	−0.0492	0.0777	0.076*
C36	0.8020 (6)	0.0875 (4)	0.1808 (3)	0.0554 (11)
H36	0.7471	0.0511	0.2207	0.067*
C37	0.9909 (5)	0.2639 (3)	0.3028 (2)	0.0368 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Cd	0.03806 (15)	0.02893 (14)	0.02221 (14)	−0.00009 (10)	0.00893 (10)	0.00328 (10)
O1	0.0354 (12)	0.0313 (12)	0.0234 (12)	−0.0019 (10)	0.0074 (10)	0.0001 (10)
O2	0.0371 (14)	0.0617 (17)	0.0345 (14)	0.0039 (12)	0.0113 (11)	−0.0015 (12)
O21	0.0548 (16)	0.0443 (15)	0.0226 (13)	−0.0031 (12)	0.0102 (11)	0.0050 (11)
O22	0.0441 (14)	0.0511 (15)	0.0238 (13)	−0.0024 (12)	0.0107 (11)	−0.0014 (12)
O23	0.096 (2)	0.102 (3)	0.0470 (19)	0.004 (2)	0.0346 (18)	0.0315 (19)
O24	0.147 (3)	0.094 (3)	0.0289 (18)	−0.008 (2)	0.028 (2)	−0.0048 (18)
O31	0.0586 (17)	0.0476 (16)	0.0267 (14)	−0.0062 (13)	−0.0004 (12)	0.0037 (12)
O32	0.0660 (18)	0.0468 (15)	0.0332 (15)	−0.0044 (13)	0.0203 (13)	−0.0017 (12)
O33	0.095 (3)	0.097 (3)	0.058 (2)	−0.017 (2)	0.0033 (19)	−0.040 (2)
O34	0.132 (3)	0.101 (3)	0.0348 (19)	0.017 (2)	0.015 (2)	−0.0051 (19)
N11	0.0427 (17)	0.0273 (14)	0.0219 (15)	0.0031 (12)	0.0078 (13)	0.0015 (12)
N12	0.077 (2)	0.050 (2)	0.0205 (16)	−0.0115 (17)	0.0068 (16)	−0.0017 (14)
N13	0.0339 (15)	0.0330 (15)	0.0227 (15)	0.0032 (12)	0.0087 (12)	0.0063 (12)
N14	0.065 (2)	0.0427 (18)	0.0246 (16)	−0.0062 (15)	0.0155 (15)	0.0041 (14)
N21	0.066 (2)	0.073 (3)	0.0280 (19)	0.018 (2)	0.0177 (17)	0.0140 (19)
N31	0.070 (3)	0.082 (3)	0.037 (2)	0.019 (2)	0.006 (2)	−0.014 (2)
S11	0.0512 (6)	0.0347 (5)	0.0402 (6)	−0.0036 (4)	0.0019 (5)	−0.0038 (4)
S12	0.0630 (6)	0.0451 (5)	0.0279 (5)	−0.0006 (5)	0.0185 (5)	0.0108 (4)
C11	0.0358 (19)	0.0293 (18)	0.0302 (19)	0.0040 (14)	0.0086 (15)	0.0061 (15)
C12	0.044 (2)	0.038 (2)	0.043 (2)	−0.0046 (16)	0.0094 (18)	0.0060 (17)
C13	0.044 (2)	0.0265 (18)	0.031 (2)	0.0039 (15)	0.0044 (16)	0.0007 (15)
C14	0.0351 (19)	0.0304 (18)	0.0302 (19)	0.0032 (14)	0.0104 (15)	0.0067 (15)
C15	0.050 (2)	0.038 (2)	0.037 (2)	−0.0031 (17)	0.0166 (18)	0.0098 (17)
C16	0.041 (2)	0.0330 (18)	0.0225 (18)	0.0066 (15)	0.0111 (15)	0.0087 (15)
C21	0.0342 (18)	0.0354 (19)	0.0247 (18)	0.0072 (15)	0.0082 (15)	0.0042 (15)
C22	0.049 (2)	0.046 (2)	0.028 (2)	−0.0026 (17)	0.0129 (17)	0.0010 (17)
C23	0.057 (2)	0.054 (2)	0.036 (2)	−0.0010 (19)	0.0230 (19)	0.0121 (19)
C24	0.054 (2)	0.050 (2)	0.0256 (19)	0.0143 (18)	0.0184 (17)	0.0105 (17)
C25	0.060 (2)	0.046 (2)	0.0240 (19)	−0.0029 (18)	0.0064 (18)	0.0024 (17)
C26	0.050 (2)	0.050 (2)	0.0257 (19)	−0.0037 (18)	0.0128 (17)	0.0079 (17)
C27	0.0358 (19)	0.042 (2)	0.0234 (18)	0.0071 (16)	0.0071 (15)	0.0066 (16)
C31	0.0357 (19)	0.039 (2)	0.0279 (19)	0.0058 (15)	0.0035 (15)	0.0001 (15)
C32	0.055 (2)	0.044 (2)	0.033 (2)	−0.0054 (18)	0.0081 (18)	0.0003 (17)
C33	0.074 (3)	0.053 (3)	0.033 (2)	0.007 (2)	0.013 (2)	0.0062 (19)
C34	0.057 (2)	0.053 (2)	0.028 (2)	0.012 (2)	−0.0003 (18)	−0.0077 (18)
C35	0.066 (3)	0.058 (3)	0.047 (3)	−0.014 (2)	0.007 (2)	−0.007 (2)
C36	0.065 (3)	0.049 (2)	0.039 (2)	−0.010 (2)	0.013 (2)	−0.0036 (19)
C37	0.039 (2)	0.037 (2)	0.030 (2)	0.0069 (16)	0.0046 (16)	0.0017 (16)

Geometric parameters (Å, °)

Cd—O1	2.294 (2)	S11—C13	1.734 (3)
Cd—O1^{i}	2.393 (2)	S12—C15	1.717 (4)
Cd—O2	2.250 (2)	S12—C16	1.740 (3)
Cd—O21	2.313 (2)	C11—C12	1.340 (5)
Cd—N11	2.266 (3)	C11—C14	1.468 (5)
Cd—N13	2.344 (2)	C12—H12	0.9300
O1—H1A	0.8319	C14—C15	1.347 (5)

O1—H1B	0.8843	C15—H15	0.9300
O2—H2A	0.8386	C21—C26	1.379 (5)
O2—H2B	0.8316	C21—C22	1.388 (5)
O21—C27	1.267 (4)	C21—C27	1.516 (4)
O22—C27	1.244 (4)	C22—C23	1.367 (5)
O23—N21	1.216 (4)	C22—H22	0.9300
O24—N21	1.200 (4)	C23—C24	1.370 (5)
O31—C37	1.263 (4)	C23—H23	0.9300
O32—C37	1.239 (4)	C24—C25	1.368 (5)
O33—N31	1.213 (5)	C25—C26	1.386 (5)
O34—N31	1.223 (5)	C25—H25	0.9300
N11—C13	1.306 (4)	C26—H26	0.9300
N11—C11	1.391 (4)	C31—C32	1.377 (5)
N12—C13	1.331 (4)	C31—C36	1.377 (5)
N12—H12A	0.8599	C31—C37	1.510 (5)
N12—H12B	0.8876	C32—C33	1.383 (5)
N13—C16	1.309 (4)	C32—H32	0.9300
N13—C14	1.395 (4)	C33—C34	1.365 (5)
N14—C16	1.342 (4)	C33—H33	0.9300
N14—H14A	0.8607	C34—C35	1.366 (6)
N14—H14B	0.8708	C35—C36	1.374 (5)
N21—C24	1.473 (4)	C35—H35	0.9300
N31—C34	1.472 (5)	C36—H36	0.9300
S11—C12	1.720 (4)		
O2—Cd—N11	103.40 (9)	N12—C13—S11	122.6 (3)
O2—Cd—O1	91.73 (8)	C15—C14—N13	115.3 (3)
N11—Cd—O1	164.40 (8)	C15—C14—C11	125.7 (3)
O2—Cd—O21	88.97 (9)	N13—C14—C11	118.9 (3)
N11—Cd—O21	90.87 (9)	C14—C15—S12	110.4 (3)
O1—Cd—O21	85.56 (8)	C14—C15—H15	124.8
O2—Cd—N13	96.10 (9)	S12—C15—H15	124.8
N11—Cd—N13	74.66 (9)	N13—C16—N14	125.9 (3)
O1—Cd—N13	107.87 (8)	N13—C16—S12	113.9 (2)
O21—Cd—N13	165.41 (9)	N14—C16—S12	120.1 (2)
O2—Cd—O1^{i}	166.01 (8)	C26—C21—C22	118.9 (3)
N11—Cd—O1^{i}	90.59 (8)	C26—C21—C27	121.0 (3)
O1—Cd—O1^{i}	74.30 (8)	C22—C21—C27	120.0 (3)
O21—Cd—O1^{i}	90.54 (8)	C23—C22—C21	120.8 (3)
N13—Cd—O1^{i}	87.80 (8)	C23—C22—H22	119.6
Cd—O1—Cd^{i}	105.70 (8)	C21—C22—H22	119.6
Cd—O1—H1A	108.5	C22—C23—C24	118.8 (3)
Cd^{i}—O1—H1A	100.5	C22—C23—H23	120.6
Cd—O1—H1B	116.5	C24—C23—H23	120.6
Cd^{i}—O1—H1B	116.7	C25—C24—C23	122.5 (3)
H1A—O1—H1B	107.5	C25—C24—N21	117.9 (3)
Cd—O2—H2A	118.1	C23—C24—N21	119.7 (3)
Cd—O2—H2B	125.5	C24—C25—C26	118.0 (3)

H2A—O2—H2B	110.8	C24—C25—H25	121.0
C27—O21—Cd	126.5 (2)	C26—C25—H25	121.0
C13—N11—C11	111.2 (3)	C21—C26—C25	120.9 (3)
C13—N11—Cd	133.0 (2)	C21—C26—H26	119.5
C11—N11—Cd	115.3 (2)	C25—C26—H26	119.5
C13—N12—H12A	119.8	O22—C27—O21	125.5 (3)
C13—N12—H12B	118.4	O22—C27—C21	118.2 (3)
H12A—N12—H12B	121.4	O21—C27—C21	116.4 (3)
C16—N13—C14	110.8 (3)	C32—C31—C36	118.4 (3)
C16—N13—Cd	136.9 (2)	C32—C31—C37	121.1 (3)
C14—N13—Cd	112.3 (2)	C36—C31—C37	120.4 (3)
C16—N14—H14A	119.9	C31—C32—C33	120.9 (3)
C16—N14—H14B	117.0	C31—C32—H32	119.6
H14A—N14—H14B	120.8	C33—C32—H32	119.6
O24—N21—O23	122.2 (4)	C34—C33—C32	118.6 (4)
O24—N21—C24	119.1 (4)	C34—C33—H33	120.7
O23—N21—C24	118.6 (4)	C32—C33—H33	120.7
O33—N31—O34	123.3 (4)	C33—C34—C35	122.2 (4)
O33—N31—C34	118.8 (4)	C33—C34—N31	119.0 (4)
O34—N31—C34	117.8 (4)	C35—C34—N31	118.8 (4)
C12—S11—C13	89.26 (17)	C34—C35—C36	118.2 (4)
C15—S12—C16	89.57 (16)	C34—C35—H35	120.9
C12—C11—N11	114.9 (3)	C36—C35—H35	120.9
C12—C11—C14	127.1 (3)	C35—C36—C31	121.7 (4)
N11—C11—C14	118.0 (3)	C35—C36—H36	119.1
C11—C12—S11	110.8 (3)	C31—C36—H36	119.1
C11—C12—H12	124.6	O32—C37—O31	125.6 (3)
S11—C12—H12	124.6	O32—C37—C31	118.0 (3)
N11—C13—N12	123.5 (3)	O31—C37—C31	116.3 (3)
N11—C13—S11	113.9 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O22	0.83	1.90	2.662 (3)	151
O1—H1B···O31^{ii}	0.88	1.66	2.522 (3)	164
O2—H2A···O32	0.84	1.83	2.650 (4)	164
O2—H2B···O22^{ii}	0.83	1.95	2.766 (3)	165
N12—H12A···O33^{iii}	0.86	2.45	3.164 (4)	141
N12—H12A···O34^{iii}	0.86	2.35	3.192 (5)	165
N12—H12B···O21	0.89	2.07	2.901 (4)	156
N14—H14A···O24^{iv}	0.86	2.54	3.292 (4)	147
N14—H14B···O31^{ii}	0.87	2.19	3.014 (4)	158

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

Fig. 1

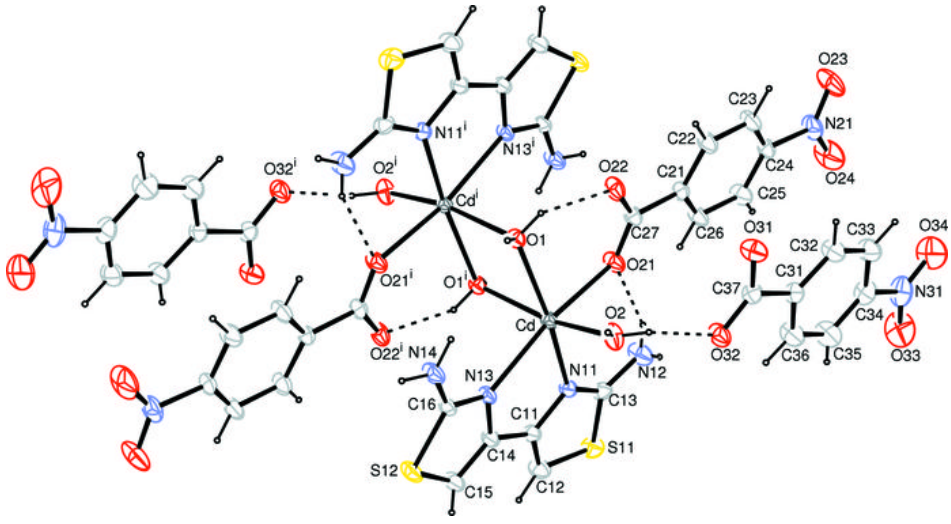
O23
C23
N21
C22
C24
O24
C21
C25
O22
O32i
O2i
N11i
N13i
Cdi
C27
C26
O31
C33
O34
C32
C31
O1
O21
C37
N31
O21i
O1i
Cd
O2
C34
O22i
N14
N13
N11
N12
O32
C36
C35
O33
C16
C11
C13
C14
S11
S12
C15
C12

Fig. 2