Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[2-(benzimidazol-2-ylsulfanyl)-acetato]bis(2,2′-bipyridine)cadmium(II)

Lin Cheng,* Yan-Yan Sun, Jian-Quan Wang and Ya-Wen Zhang

School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, People's Republic of China
Correspondence e-mail: cep02chl@yahoo.com.cn

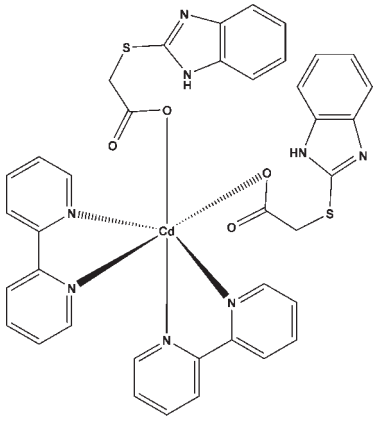
Received 3 July 2009; accepted 29 September 2009

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.030; wR factor = 0.069; data-to-parameter ratio = 14.2.

In the structure of the title compound, $[Cd(C_9H_7N_2O_2S)_2(C_{10}H_8N_2)_2]$, the complex molecules are located on a crystallographic twofold rotation axis and the Cd^{II} ion is octahedrally coordinated by two chelating 2,2′-bipyridine ligands and two O atoms from the carboxylate groups of two 2-(benzimidazol-2-ylsulfanyl)acetate ligands. The two carboxylate ligands adopt a *cis* configuration with respect to each other. Within each of these ligands, the imidazole fragments are bent back in a loop towards the acetyl groups, forming intramolecular N—H···O hydrogen bonds, which help to stablilize the mononuclear complex. Adjacent molecules are further linked by weak C—H···O hydrogen bonds, resulting in a chain along the *c* axis.

Related literature

For related structures, see: Matthews *et al.* (1998); Cheng *et al.* (2009).



Experimental

Crystal data

$[Cd(C_9H_7N_2O_2S)_2(C_{10}H_8N_2)_2]$
M_r = 839.25
Monoclinic, $C2/c$
a = 26.733 (2) Å
b = 9.3043 (8) Å
c = 16.4220 (14) Å
β = 120.2540 (10)°
V = 3528.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 295 K
0.20 × 0.18 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
T_{min} = 0.858, T_{max} = 0.911
9308 measured reflections
3460 independent reflections
2946 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.069
S = 1.05
3460 reflections
244 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2C···O2	0.80 (2)	1.96 (2)	2.708 (3)	156 (2)
C11—H11A···O1^{i}	0.93	2.29	3.179 (3)	161

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Program for Young Excellent Talents at Southeast University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2228).

References

Bruker (2000). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cheng, L., Sun, Y.-Y., Zhang, Y.-W. & Wang, J.-Q. (2009). *Acta Cryst.* E**65**, m34.
Matthews, C. J., Heath, S. L., Elsegood, M. R. J., Clegg, W., Leese, T. A. & Lockhart, J. C. (1998). *J. Chem. Soc. Dalton Trans.* pp. 1973–1977.
Sheldrick, G. M. (2000). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2009). E**65**, m1356 [**doi:10.1107/S1600536809039592**]

Bis[2-(benzimidazol-2-ylsulfanyl)acetato]bis(2,2'-bipyridine)cadmium(II)

L. Cheng, Y.-Y. Sun, J.-Q. Wang and Y.-W. Zhang

Comment

Recently, the photophysical properties of coordination compounds of d_{10} monovalent ions of the coinage metals have attracted considerable attention. Meanwhile, benzimidazole compounds and thioether carboxylates have been widely used to construct many interesting coordination compounds. However, such compounds formed by bifunctional ligands with both benzimidazole and thioether carboxylate groups have only been rarely reported (Cheng *et al.* 2009, Matthews *et al.* 1998). Herein, we present the synthesis and structural characterization of a new coordination compound of a d_{10} mononuclear complex $Cd(Hbia)_2(2,2'\text{-bipy})_2$ (H*2*bia = 2-(1*H*-benzo[*d*]imidazol-2-ylthio)acetic acid; 2,2'-bipy = 2,2'-bipyridine) with the bifunctional ligand H*2*bia.

In the structure of the title compound the complex is located on a crystallographic two fold rotation axis with one Cd^{II} cation, one Hbia and one chelating 2,2'-bipy ligand in the asymmetric unit. The Cd^{II} ion displays a distorted octahedral geometry, being surrounded by two chelating 2,2'-bipy ligands with Cd—N coordinating distances of 2.342 (2) and 2.378 (2) Å and two oxygen atoms coming from the carboxylates of two Hbia ligands, respectively, with the distance involving O atoms and Cd being 2.275 (2) Å. The angles around Cd are in the range of 69.50 (8)–158.51 (8) °. Meanwhile, the two carboxylate ligands are related by a two fold rotation axis and adopt a *cis*- configuration with respect to each other. Within each of these ligands the imidazole fragments are bent back in a loop towards the acetyl groups to form intramolecular N—H···O hydrogen bonds which help to stablilize the mononuclear complex (table 1). The N···O distance between N2 of the imidazole and the coordinated O atom O2 is 2.708 (3) Å. Adjacent molecules are further linked together by C—H···O hydrogen bonding between the uncoordinated oxygen atoms and the carbon atoms of 2,2'-bipyridine ($C11\cdots O1^{ii}$ 3.180 (4) Å. symmetry code: ^{ii}, -*x*, 1-*y*, 1-*z*), resulting in a one-dimensional hydrogen bonded chain.

Experimental

A mixture of H*2*bia (0.0208 g, 0.1 mmol), 2,2'-bipy (0.0156 g, 0.1 mmol), $Cd(NO_3)_2.6H_2O$ (0.0345 g, 0.1 mmol) and H_2O (8 ml) was heated in a 15-ml Teflon-lined autoclave at 363 K for 5 days, followed by slow cooling (5 K h^{-1}) to room temperature. The resulting mixture was washed with water, and colorless block crystals were collected and dried in air [yield 91% (76.3 mg) based on Cd(II)].

Refinement

The H atom bonded to the N atom was located in a difference map and was freely refined without use of restraints. All other H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.97 Å and with U_{iso}(H) = 1.2 U_{eq}(C).

Figures

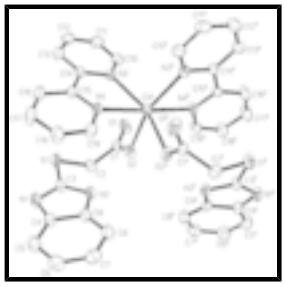


Fig. 1. Structure of the title compound with 30% thermal ellipsoids. Symmetry code: i: -*x*, *y*, 1/2-*z*. Hydrogen atoms are omitted for clarity.

Fig. 2. The one-dimensional hydrogen bonding chain of the title compound.

Bis[2-(benzimidazol-2-ylsulfanyl)acetato]bis(2,2'-bipyridine)cadmium(II)

Crystal data

$[Cd(C_9H_7N_2O_2S)_2(C_{10}H_8N_2)_2]$	F_{000} = 1704
M_r = 839.25	D_x = 1.580 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 783 reflections
a = 26.733 (2) Å	θ = 2.4–28.0º
b = 9.3043 (8) Å	μ = 0.79 mm^{-1}
c = 16.4220 (14) Å	*T* = 295 K
β = 120.2540 (10)º	Block, colorless
V = 3528.3 (5) Å^3	0.20 × 0.18 × 0.12 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	3460 independent reflections
Radiation source: fine-focus sealed tube	2946 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 295 K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 2000)	*h* = −32→30
T_{min} = 0.858, T_{max} = 0.911	*k* = −11→11
9308 measured reflections	*l* = −20→19

Refinement

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

$R[F^2 > 2\sigma(F^2)] = 0.030$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.069$	$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 1.2632P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
3460 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
244 parameters	$\Delta\rho_{min} = -0.47$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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}
Cd1	0.0000	0.27478 (3)	0.2500	0.03543 (10)
S1	0.15271 (3)	0.05110 (8)	0.52528 (4)	0.04872 (19)
C1	0.03416 (10)	0.1120 (3)	0.43699 (17)	0.0373 (6)
C2	0.08216 (10)	0.0184 (3)	0.51125 (16)	0.0415 (6)
H2A	0.0721	−0.0817	0.4945	0.050*
H2B	0.0843	0.0346	0.5713	0.050*
C3	0.15201 (10)	−0.0542 (3)	0.43638 (16)	0.0388 (6)
C4	0.17937 (11)	−0.1829 (3)	0.35876 (17)	0.0413 (6)
C5	0.20952 (13)	−0.2670 (3)	0.3279 (2)	0.0540 (7)
H5A	0.2493	−0.2809	0.3653	0.065*
C6	0.17850 (13)	−0.3294 (3)	0.2399 (2)	0.0567 (7)
H6A	0.1979	−0.3860	0.2179	0.068*
C7	0.11932 (13)	−0.3099 (3)	0.1835 (2)	0.0561 (8)
H7A	0.1000	−0.3523	0.1242	0.067*
C8	0.08838 (13)	−0.2290 (3)	0.2134 (2)	0.0524 (7)
H8A	0.0486	−0.2163	0.1759	0.063*
C9	0.11938 (10)	−0.1676 (3)	0.30194 (16)	0.0385 (6)
C10	0.03449 (11)	0.5176 (3)	0.4126 (2)	0.0494 (7)
H10A	−0.0049	0.5104	0.3915	0.059*
C11	0.06748 (12)	0.6067 (3)	0.4870 (2)	0.0539 (7)
H11A	0.0511	0.6576	0.5166	0.065*
C12	0.12519 (12)	0.6190 (3)	0.5169 (2)	0.0526 (7)
H12A	0.1485	0.6799	0.5667	0.063*

C13	0.14864 (11)	0.5405 (3)	0.47287 (18)	0.0456 (6)
H13A	0.1878	0.5479	0.4924	0.055*
C14	0.11277 (9)	0.4506 (2)	0.39904 (16)	0.0336 (5)
C15	0.13512 (9)	0.3589 (3)	0.35035 (16)	0.0339 (5)
C16	0.19346 (11)	0.3488 (3)	0.3800 (2)	0.0542 (7)
H16A	0.2203	0.4034	0.4307	0.065*
C17	0.21161 (12)	0.2577 (3)	0.3340 (2)	0.0634 (9)
H17A	0.2508	0.2496	0.3537	0.076*
C18	0.17124 (11)	0.1788 (3)	0.2589 (2)	0.0525 (7)
H18A	0.1824	0.1166	0.2266	0.063*
C19	0.11432 (11)	0.1940 (3)	0.23272 (18)	0.0454 (7)
H19A	0.0869	0.1410	0.1817	0.055*
N1	0.19912 (8)	−0.1097 (2)	0.44392 (15)	0.0478 (5)
N2	0.10299 (9)	−0.0851 (2)	0.35415 (14)	0.0410 (5)
N3	0.05612 (8)	0.4404 (2)	0.36884 (14)	0.0390 (5)
N4	0.09607 (8)	0.2814 (2)	0.27686 (14)	0.0360 (5)
O1	0.01181 (8)	0.2029 (2)	0.46217 (13)	0.0559 (5)
O2	0.02068 (7)	0.08785 (18)	0.35135 (11)	0.0422 (4)
H2C	0.0731 (11)	−0.046 (3)	0.3391 (17)	0.040 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02273 (14)	0.04258 (17)	0.03763 (15)	0.000	0.01272 (11)	0.000
S1	0.0323 (3)	0.0634 (5)	0.0415 (4)	0.0011 (3)	0.0120 (3)	−0.0134 (3)
C1	0.0281 (12)	0.0453 (15)	0.0395 (14)	0.0012 (11)	0.0178 (11)	0.0034 (12)
C2	0.0437 (14)	0.0473 (16)	0.0351 (13)	0.0069 (12)	0.0211 (12)	0.0061 (11)
C3	0.0293 (13)	0.0463 (15)	0.0354 (13)	0.0004 (11)	0.0123 (11)	−0.0007 (11)
C4	0.0352 (13)	0.0485 (16)	0.0412 (14)	0.0000 (11)	0.0199 (12)	0.0005 (12)
C5	0.0413 (16)	0.067 (2)	0.0592 (18)	0.0054 (13)	0.0293 (15)	−0.0053 (15)
C6	0.0614 (19)	0.0594 (19)	0.0638 (19)	0.0036 (15)	0.0424 (17)	−0.0084 (16)
C7	0.064 (2)	0.0568 (19)	0.0482 (17)	−0.0032 (15)	0.0289 (15)	−0.0110 (14)
C8	0.0430 (16)	0.0599 (18)	0.0452 (16)	0.0030 (13)	0.0154 (13)	−0.0044 (14)
C9	0.0357 (13)	0.0404 (14)	0.0376 (13)	0.0031 (11)	0.0170 (11)	0.0038 (11)
C10	0.0418 (15)	0.0446 (16)	0.0701 (18)	0.0026 (12)	0.0344 (14)	−0.0066 (14)
C11	0.0633 (19)	0.0424 (16)	0.0722 (19)	0.0020 (14)	0.0462 (17)	−0.0104 (15)
C12	0.0540 (17)	0.0482 (17)	0.0573 (17)	−0.0067 (13)	0.0293 (15)	−0.0161 (14)
C13	0.0363 (14)	0.0483 (16)	0.0512 (15)	−0.0059 (12)	0.0213 (12)	−0.0138 (13)
C14	0.0288 (12)	0.0340 (13)	0.0379 (13)	0.0002 (10)	0.0167 (11)	0.0002 (10)
C15	0.0275 (12)	0.0379 (14)	0.0362 (13)	−0.0033 (10)	0.0160 (10)	−0.0032 (11)
C16	0.0296 (13)	0.070 (2)	0.0594 (17)	−0.0091 (13)	0.0196 (13)	−0.0281 (15)
C17	0.0293 (14)	0.088 (2)	0.073 (2)	−0.0054 (14)	0.0259 (15)	−0.0318 (18)
C18	0.0393 (15)	0.0666 (19)	0.0589 (17)	−0.0006 (13)	0.0302 (14)	−0.0177 (15)
C19	0.0373 (14)	0.0567 (18)	0.0443 (15)	−0.0087 (12)	0.0220 (12)	−0.0163 (13)
N1	0.0295 (11)	0.0618 (15)	0.0459 (13)	0.0042 (10)	0.0144 (10)	−0.0054 (11)
N2	0.0281 (11)	0.0496 (14)	0.0393 (12)	0.0059 (10)	0.0126 (10)	−0.0043 (10)
N3	0.0297 (11)	0.0404 (12)	0.0491 (12)	0.0008 (9)	0.0215 (10)	−0.0055 (10)
N4	0.0267 (10)	0.0443 (12)	0.0366 (11)	−0.0027 (9)	0.0156 (9)	−0.0065 (9)

O1	0.0470 (11)	0.0704 (14)	0.0491 (11)	0.0212 (10)	0.0234 (9)	−0.0027 (10)
O2	0.0393 (9)	0.0521 (11)	0.0332 (9)	0.0121 (8)	0.0168 (8)	0.0054 (8)

Geometric parameters (Å, °)

Cd1—O2^{i}	2.2746 (16)	C8—H8A	0.9300
Cd1—O2	2.2746 (16)	C9—N2	1.376 (3)
Cd1—N3	2.342 (2)	C10—N3	1.336 (3)
Cd1—N3^{i}	2.3417 (19)	C10—C11	1.369 (4)
Cd1—N4^{i}	2.3775 (19)	C10—H10A	0.9300
Cd1—N4	2.3775 (19)	C11—C12	1.368 (4)
S1—C3	1.750 (2)	C11—H11A	0.9300
S1—C2	1.807 (2)	C12—C13	1.381 (3)
C1—O1	1.221 (3)	C12—H12A	0.9300
C1—O2	1.284 (3)	C13—C14	1.385 (3)
C1—C2	1.521 (3)	C13—H13A	0.9300
C2—H2A	0.9700	C14—N3	1.338 (3)
C2—H2B	0.9700	C14—C15	1.485 (3)
C3—N1	1.308 (3)	C15—N4	1.340 (3)
C3—N2	1.357 (3)	C15—C16	1.383 (3)
C4—C5	1.389 (4)	C16—C17	1.375 (4)
C4—N1	1.398 (3)	C16—H16A	0.9300
C4—C9	1.398 (3)	C17—C18	1.373 (4)
C5—C6	1.381 (4)	C17—H17A	0.9300
C5—H5A	0.9300	C18—C19	1.364 (3)
C6—C7	1.385 (4)	C18—H18A	0.9300
C6—H6A	0.9300	C19—N4	1.335 (3)
C7—C8	1.378 (4)	C19—H19A	0.9300
C7—H7A	0.9300	N2—H2C	0.80 (2)
C8—C9	1.383 (4)		
O2^{i}—Cd1—O2	80.25 (8)	N2—C9—C4	105.0 (2)
O2^{i}—Cd1—N3	158.50 (6)	C8—C9—C4	122.5 (2)
O2—Cd1—N3	94.35 (7)	N3—C10—C11	123.2 (2)
O2^{i}—Cd1—N3^{i}	94.35 (7)	N3—C10—H10A	118.4
O2—Cd1—N3^{i}	158.50 (6)	C11—C10—H10A	118.4
N3—Cd1—N3^{i}	97.71 (10)	C12—C11—C10	118.3 (2)
O2^{i}—Cd1—N4^{i}	92.44 (6)	C12—C11—H11A	120.9
O2—Cd1—N4^{i}	89.84 (6)	C10—C11—H11A	120.9
N3—Cd1—N4^{i}	108.43 (7)	C11—C12—C13	119.7 (3)
N3^{i}—Cd1—N4^{i}	69.49 (6)	C11—C12—H12A	120.1
O2^{i}—Cd1—N4	89.84 (6)	C13—C12—H12A	120.1
O2—Cd1—N4	92.44 (6)	C12—C13—C14	118.8 (2)
N3—Cd1—N4	69.49 (6)	C12—C13—H13A	120.6
N3^{i}—Cd1—N4	108.43 (7)	C14—C13—H13A	120.6
N4^{i}—Cd1—N4	177.01 (10)	N3—C14—C13	121.5 (2)
C3—S1—C2	103.15 (12)	N3—C14—C15	116.5 (2)

O1—C1—O2	125.2 (2)	C13—C14—C15	122.0 (2)
O1—C1—C2	118.9 (2)	N4—C15—C16	120.6 (2)
O2—C1—C2	115.8 (2)	N4—C15—C14	116.84 (19)
C1—C2—S1	114.25 (17)	C16—C15—C14	122.5 (2)
C1—C2—H2A	108.7	C17—C16—C15	119.7 (2)
S1—C2—H2A	108.7	C17—C16—H16A	120.1
C1—C2—H2B	108.7	C15—C16—H16A	120.1
S1—C2—H2B	108.7	C18—C17—C16	119.2 (3)
H2A—C2—H2B	107.6	C18—C17—H17A	120.4
N1—C3—N2	114.3 (2)	C16—C17—H17A	120.4
N1—C3—S1	122.47 (18)	C19—C18—C17	118.3 (2)
N2—C3—S1	123.23 (18)	C19—C18—H18A	120.8
C5—C4—N1	130.0 (2)	C17—C18—H18A	120.8
C5—C4—C9	119.7 (2)	N4—C19—C18	123.2 (2)
N1—C4—C9	110.2 (2)	N4—C19—H19A	118.4
C6—C5—C4	117.8 (3)	C18—C19—H19A	118.4
C6—C5—H5A	121.1	C3—N1—C4	103.73 (19)
C4—C5—H5A	121.1	C3—N2—C9	106.7 (2)
C5—C6—C7	121.7 (3)	C3—N2—H2C	121.9 (18)
C5—C6—H6A	119.1	C9—N2—H2C	130.3 (18)
C7—C6—H6A	119.1	C10—N3—C14	118.6 (2)
C8—C7—C6	121.5 (3)	C10—N3—Cd1	122.20 (16)
C8—C7—H7A	119.3	C14—N3—Cd1	119.05 (15)
C6—C7—H7A	119.3	C19—N4—C15	119.0 (2)
C7—C8—C9	116.8 (3)	C19—N4—Cd1	122.67 (16)
C7—C8—H8A	121.6	C15—N4—Cd1	117.36 (14)
C9—C8—H8A	121.6	C1—O2—Cd1	119.90 (16)
N2—C9—C8	132.4 (2)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2C···O2	0.80 (2)	1.96 (2)	2.708 (3)	156 (2)
C11—H11A···O1^{ii}	0.93	2.29	3.179 (3)	161

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

Fig. 1

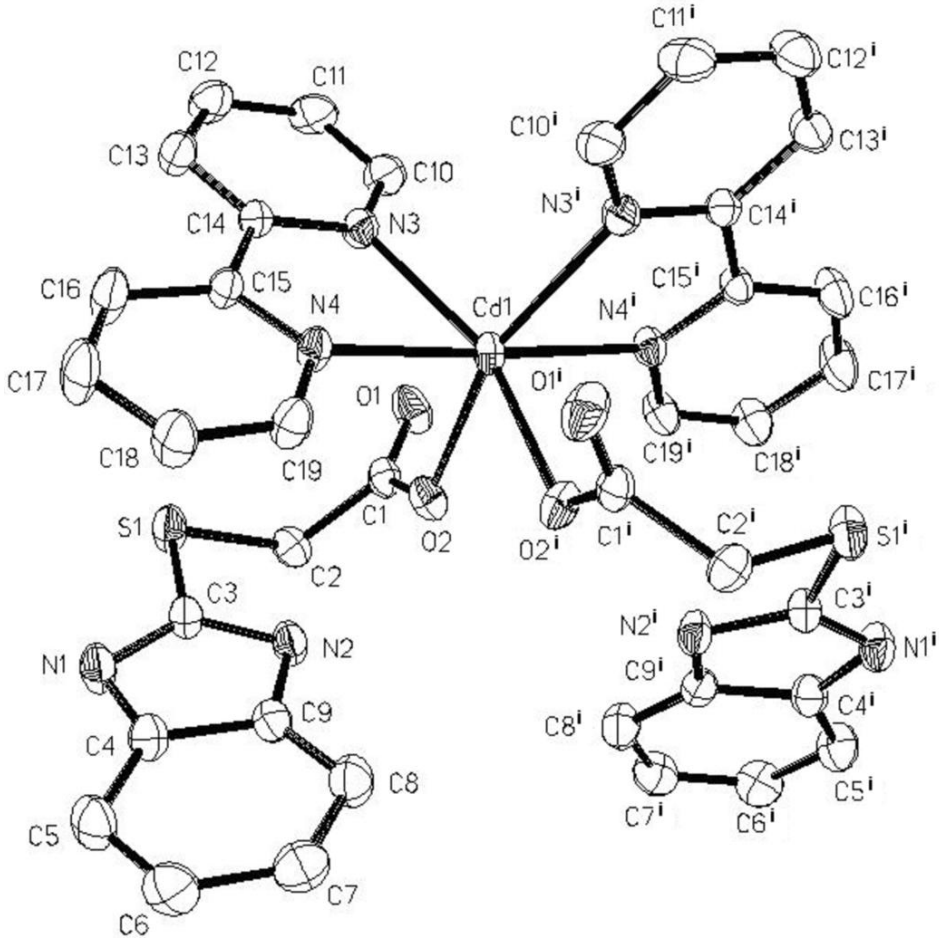

C11i
C12
C11
C12i
C10i
C13
C10
C13i
N3i
C14
N3
C14i
C16
C15
N4
Cd1
N4i
C15i
C16i
C17
O1
O1i
C17i
C18
C19
C19i
C18i
S1
C1
O2
O2i
C1i
C2i
S1i
C2
C3
C3i
N2i
N1
N2
N1i
C9i
C9
C4i
C4
C8i
C8
C5
C5i
C7i
C6i
C7
C6

Fig. 2