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Bis(*N*-benzyl-*N*-methyldithiocarbamato-$\kappa^2 S,S'$)-(pyridine-κN)cadmium(II)

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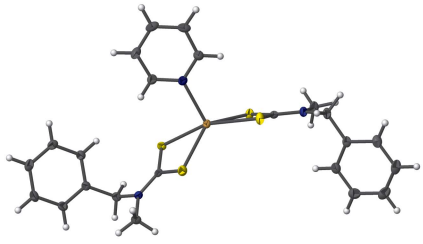
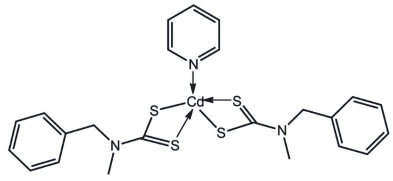
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Cd(C_9H_{10}NS_2)_2(C_5H_5N)]$, features a five-coordinate Cd^{II} atom, being coordinated by two nearly symmetrically chelating dithiocarbamate ligands and a pyridine N atom. The resulting NS_4 donor set defines a distorted coordination geometry tending toward square pyramidal. In the molecular packing, centrosymmetric ten-membered $\{\cdots HCNCS\}_2$ synthons arise as a result of methylene-C—H$\cdots$S interactions. These are connected into layers parallel to $(10\bar{2})$ *via* weak methyl-C—H$\cdots\pi$(phenyl) interactions.

3D view



Chemical scheme



Structure description

Binary cadmium dithiocarbamates self-assemble *via* secondary Cd$\cdots$S interactions in their crystal structures (Tiekink, 2003) but, the addition of base can disrupt these arrangements. A practical application of this is that the compounds become more suitable as synthetic precursors for the generation of CdS nanoparticles (Ehsan *et al.*, 2012; Tan *et al.* 2013; Mlowe *et al.*, 2014). It was in this connection that the title compound was synthesized.

The cadmium atom in $Cd[S_2CNMe(CH_2Ph)]_2(NC_5H_5)$, Fig. 1, is chelated by two almost symmetrically chelating dithiocarbamate ligands and the pyridine-N atom. The near equivalence in the Cd—S bond lengths [*i.e.* Cd—S1–S4 = 2.5868 (5), 2.6421 (5), 2.5908 (4) and 2.6473 (5) Å, respectively] is reflected in the experimental equivalence in the associated C—S bond lengths that span the narrow range 1.7191 (17) —1.7284 (16) Å. The dihedral angle between the chelate rings is 43.36 (3)°, and the dihedral angles formed between the S1- and S3-chelate rings and the least-squares plane through the pyridine ring are 75.55 (6) and 75.99 (6)°, indicating that the pyridine molecule is symmetrically

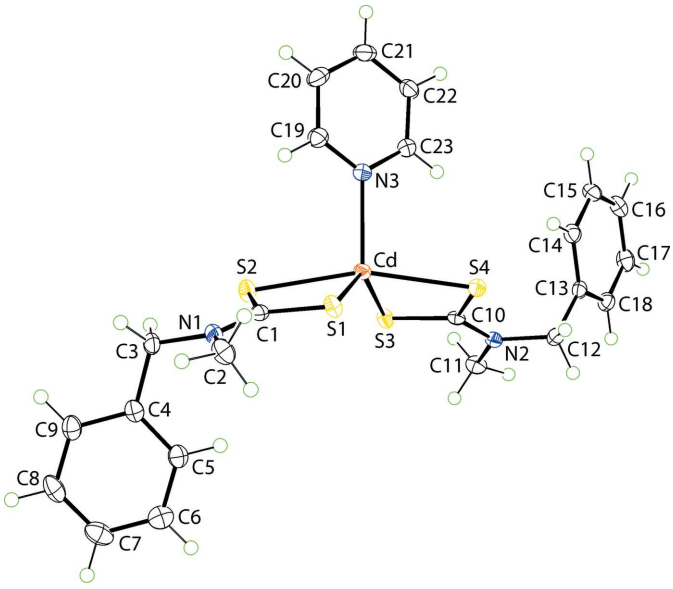


Figure 1
The molecular structure of $Cd[S_2CNMe(CH_2Ph)]_2(NC_5H_5)$ showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

disposed with respect to each chelate ring. An indicator of coordination geometry in five-coordinate structures is the value of τ (Addison *et al.*, 1984). In the present structure τ computes to 0.41 which is nearer to an ideal square pyramidal geometry (τ = 0) than to an ideal trigonal bipyramidal geometry with τ = 1.0. The presence acute ligand bite angles [*i.e.* S1—Cd—S2 is 69.295 (13)° and S3—Cd—S4 is 69.094 (13)°] is partially responsible for the observed distortion. The gross structural features just described, match literature precedents (Wei *et al.* 2005; Ehsan *et al.*, 2012; Mlowe *et al.*, 2014).

The most prominent feature of the molecular packing is the formation of supramolecular layers parallel to $(10\bar{2})$, Fig. 2. Thus, centrosymmetrically related molecules are connected *via* methylene-C—H···S interactions (Table 1) resulting in ten-membered $\{\cdots HCNCS\}_2$ synthons. The dimers are connected into a two-dimensional array *via* methyl-C—H···π(phenyl) interactions.

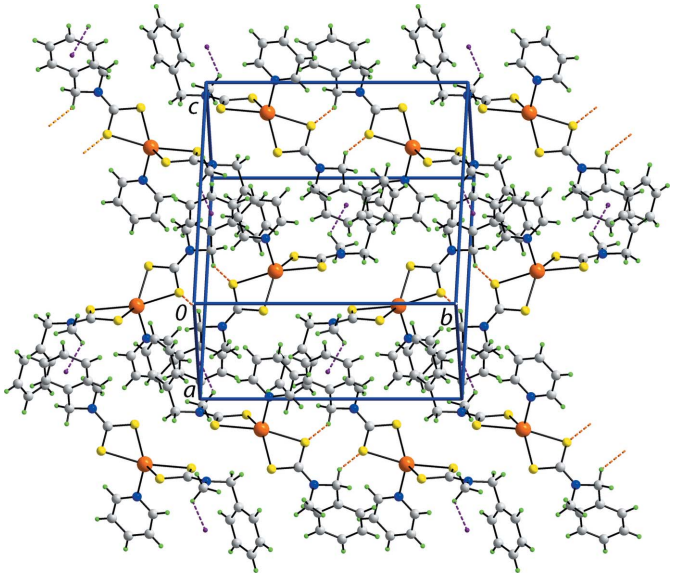


Figure 2
A view of the supramolecular layer parallel to $(10\bar{2})$ in the crystal structure of the title compound. The layers are sustained by C—H···S and C—H···π interactions, shown as orange and purple dashed lines, respectively.

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

*Cg*1 is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···S2^{i}	0.99	2.79	3.5926 (17)	138
C11—H11*C*···*Cg*1^{ii}	0.98	2.91	3.3715 (18)	110

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

Synthesis and crystallization

Sodium *N*-benzyl, *N*-methyldithiocarbamate (2.00 g, 9.13 mmol) was dissolved in acetone (25 mL) and placed in a 250 mL round-bottom flask fitted with a dropping funnel, reflux condenser and an inert gas line. $Cd(NO_3)_2{\cdot}3H_2O$ (1.32 g, 4.54 mmol) was added, and the milky-white solution was stirred for 30 min. At this point, pyridine (30 mL) was

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd(C_9H_{10}NS_2)_2(C_5H_5N)]$
M_r	584.10
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, *b*, *c* (Å)	8.9361 (6), 14.832 (1), 18.9680 (13)
β (°)	101.613 (1)
V (Å^3)	2462.6 (3)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	1.24
Crystal size (mm)	0.40 × 0.40 × 0.40
Data collection	
Diffractometer	Bruker SMART APEX diffractometer
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.636, 0.636
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30058, 5650, 5201
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.020, 0.051, 1.04
No. of reflections	5650
No. of parameters	282
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.31

Computer programs: *APEX2* (Bruker, 2009), *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006), *publCIF* (Westrip, 2010).

added to give a clear and colourless solution, and stirring was continued for a further 1 h. Filtration and slow evaporation of the reaction mixture afforded the title compound, $Cd[S_2CNMe(CH_2Ph)]_2(NC_5H_5)$, as colourless crystals. Yield 87%, M.p. 135°C. Anal. calc. for $C_{23}H_{25}CdN_3S_4$ (MW 584.10): C 47.25, H 4.28, N 7.19, S 21.91; found C 46.54, H 5.25, N 7.74, S 23.31%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.40 [*s*, 6H, $2(CH_3)$], 5.19 [*s*, 4H, $2(CH_2)$], 7.25–7.37 p.p.m. [complex pattern, 10H, aromatic $2(C_6H_5)$], 7.48–9.03 [complex pattern, 5H, C_5H_5N]. TGA: 84–138°C (5.2% wt. loss); 138–156°C (2.9%); 146–210°C (5.5%); 210–260°C (1.1%); 260–400°C (59.1%) 26.2% residue. calc. for CdS, 24.7%.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x152429 [doi:10.1107/S2414314615024293]

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Crystal data

$[Cd(C_9H_{10}NS_2)_2(C_5H_5N)]$
M_r = 584.10
Monoclinic, $P2_1/n$
a = 8.9361 (6) Å
b = 14.832 (1) Å
c = 18.9680 (13) Å
β = 101.613 (1)°
V = 2462.6 (3) Å^3
Z = 4
$F(000)$ = 1184
D_x = 1.575 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9940 reflections
θ = 4.7–56.6°
μ = 1.24 mm^{-1}
T = 100 K
Block, yellow
0.40 × 0.40 × 0.40 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.636, T_{max} = 0.636
30058 measured reflections
5650 independent reflections
5201 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 27.5°, θ_{min} = 1.8°
h = −11→11
k = −19→19
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.051
S = 1.04
5650 reflections
282 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 1.412P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd	0.22879 (2)	0.27114 (2)	0.48001 (2)	0.01746 (4)
S1	0.11972 (5)	0.22882 (3)	0.34732 (2)	0.01997 (9)
S2	0.11154 (5)	0.10701 (3)	0.47097 (2)	0.02111 (9)
S3	0.12935 (5)	0.33548 (3)	0.58899 (2)	0.01989 (9)
S4	0.25719 (4)	0.44878 (3)	0.48621 (2)	0.01675 (8)
N1	−0.01535 (16)	0.06902 (9)	0.33438 (7)	0.0186 (3)
N2	0.14132 (15)	0.51358 (9)	0.59553 (7)	0.0156 (3)
N3	0.48097 (16)	0.23716 (9)	0.51799 (8)	0.0183 (3)
C1	0.06310 (17)	0.12864 (11)	0.38019 (9)	0.0166 (3)
C2	−0.0497 (2)	0.08587 (13)	0.25657 (9)	0.0251 (4)
H2A	−0.1229	0.1356	0.2458	0.038*
H2B	−0.0938	0.0314	0.2313	0.038*
H2C	0.0445	0.1018	0.2406	0.038*
C3	−0.07418 (19)	−0.01537 (11)	0.35810 (9)	0.0213 (3)
H3A	−0.0305	−0.0243	0.4099	0.026*
H3B	−0.0398	−0.0661	0.3314	0.026*
C4	−0.24685 (19)	−0.01729 (11)	0.34673 (8)	0.0192 (3)
C5	−0.3330 (2)	0.06057 (12)	0.34563 (9)	0.0222 (3)
H5	−0.2831	0.1174	0.3523	0.027*
C6	−0.4916 (2)	0.05665 (13)	0.33482 (10)	0.0269 (4)
H6	−0.5495	0.1106	0.3335	0.032*
C7	−0.5647 (2)	−0.02603 (15)	0.32604 (10)	0.0301 (4)
H7	−0.6730	−0.0290	0.3186	0.036*
C8	−0.4798 (2)	−0.10468 (13)	0.32808 (10)	0.0281 (4)
H8	−0.5298	−0.1615	0.3225	0.034*
C9	−0.3221 (2)	−0.10036 (12)	0.33824 (9)	0.0232 (4)
H9	−0.2646	−0.1544	0.3395	0.028*
C10	0.17278 (17)	0.44101 (11)	0.56036 (8)	0.0151 (3)
C11	0.06478 (19)	0.50691 (12)	0.65699 (9)	0.0208 (3)
H11A	−0.0390	0.4836	0.6406	0.031*
H11B	0.0599	0.5667	0.6783	0.031*
H11C	0.1224	0.4660	0.6931	0.031*
C12	0.18704 (19)	0.60540 (11)	0.57864 (9)	0.0187 (3)
H12A	0.1029	0.6481	0.5808	0.022*
H12B	0.2070	0.6067	0.5292	0.022*
C13	0.32917 (18)	0.63419 (11)	0.63151 (9)	0.0168 (3)
C14	0.47127 (19)	0.59832 (11)	0.62688 (9)	0.0199 (3)
H14	0.4793	0.5574	0.5893	0.024*
C15	0.60061 (19)	0.62210 (12)	0.67682 (9)	0.0221 (3)
H15	0.6968	0.5972	0.6734	0.026*
C16	0.5905 (2)	0.68217 (12)	0.73185 (9)	0.0235 (4)
H16	0.6795	0.6983	0.7660	0.028*
C17	0.4501 (2)	0.71837 (12)	0.73662 (10)	0.0241 (4)
H17	0.4427	0.7598	0.7740	0.029*
C18	0.3198 (2)	0.69417 (11)	0.68669 (9)	0.0206 (3)

H18	0.2237	0.7189	0.6904	0.025*
C19	0.5383 (2)	0.15745 (12)	0.50318 (9)	0.0223 (3)
H19	0.4710	0.1136	0.4776	0.027*
C20	0.6921 (2)	0.13664 (13)	0.52385 (10)	0.0255 (4)
H20	0.7297	0.0799	0.5121	0.031*
C21	0.7892 (2)	0.19962 (13)	0.56167 (10)	0.0255 (4)
H21	0.8952	0.1872	0.5761	0.031*
C22	0.7303 (2)	0.28154 (12)	0.57855 (10)	0.0240 (4)
H22	0.7949	0.3255	0.6056	0.029*
C23	0.57606 (19)	0.29799 (12)	0.55539 (9)	0.0211 (3)
H23	0.5360	0.3544	0.5664	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd	0.01342 (6)	0.01678 (7)	0.02104 (7)	−0.00078 (4)	0.00073 (4)	−0.00360 (4)
S1	0.0214 (2)	0.0189 (2)	0.01913 (19)	−0.00597 (16)	0.00304 (15)	0.00025 (15)
S2	0.0254 (2)	0.01795 (19)	0.01831 (19)	−0.00568 (16)	0.00052 (16)	0.00007 (15)
S3	0.02097 (19)	0.01831 (19)	0.0215 (2)	−0.00438 (15)	0.00700 (16)	0.00030 (16)
S4	0.01800 (18)	0.01699 (19)	0.01633 (18)	0.00039 (14)	0.00602 (14)	−0.00006 (14)
N1	0.0186 (7)	0.0169 (7)	0.0195 (7)	−0.0030 (5)	0.0019 (5)	−0.0024 (5)
N2	0.0136 (6)	0.0177 (7)	0.0157 (6)	−0.0006 (5)	0.0035 (5)	−0.0013 (5)
N3	0.0158 (7)	0.0186 (7)	0.0201 (7)	0.0001 (5)	0.0024 (5)	0.0002 (5)
C1	0.0129 (7)	0.0167 (8)	0.0203 (8)	0.0011 (6)	0.0036 (6)	−0.0021 (6)
C2	0.0276 (9)	0.0283 (9)	0.0188 (8)	−0.0064 (7)	0.0033 (7)	−0.0054 (7)
C3	0.0225 (8)	0.0141 (8)	0.0253 (9)	−0.0027 (6)	0.0000 (7)	−0.0022 (6)
C4	0.0229 (8)	0.0193 (8)	0.0145 (7)	−0.0036 (6)	0.0017 (6)	0.0003 (6)
C5	0.0255 (9)	0.0206 (8)	0.0206 (8)	−0.0025 (7)	0.0047 (7)	−0.0014 (7)
C6	0.0276 (9)	0.0312 (10)	0.0230 (9)	0.0029 (8)	0.0081 (7)	0.0012 (7)
C7	0.0228 (9)	0.0444 (12)	0.0239 (9)	−0.0064 (8)	0.0063 (7)	0.0046 (8)
C8	0.0310 (10)	0.0298 (10)	0.0229 (9)	−0.0140 (8)	0.0038 (7)	0.0033 (7)
C9	0.0294 (9)	0.0193 (8)	0.0197 (8)	−0.0039 (7)	0.0021 (7)	0.0015 (7)
C10	0.0101 (7)	0.0186 (8)	0.0153 (7)	−0.0003 (6)	−0.0002 (5)	−0.0006 (6)
C11	0.0196 (8)	0.0266 (9)	0.0175 (8)	−0.0003 (7)	0.0070 (6)	−0.0047 (7)
C12	0.0197 (8)	0.0162 (8)	0.0197 (8)	0.0026 (6)	0.0024 (6)	0.0005 (6)
C13	0.0192 (8)	0.0134 (7)	0.0180 (7)	−0.0003 (6)	0.0046 (6)	0.0022 (6)
C14	0.0215 (8)	0.0182 (8)	0.0214 (8)	−0.0018 (6)	0.0076 (6)	−0.0013 (6)
C15	0.0176 (8)	0.0242 (9)	0.0255 (9)	−0.0019 (7)	0.0070 (7)	0.0022 (7)
C16	0.0231 (8)	0.0259 (9)	0.0213 (8)	−0.0089 (7)	0.0038 (7)	0.0002 (7)
C17	0.0308 (9)	0.0206 (8)	0.0219 (8)	−0.0052 (7)	0.0079 (7)	−0.0058 (7)
C18	0.0222 (8)	0.0164 (8)	0.0243 (8)	0.0010 (6)	0.0075 (7)	−0.0009 (7)
C19	0.0214 (8)	0.0219 (9)	0.0240 (8)	0.0012 (7)	0.0053 (7)	−0.0027 (7)
C20	0.0243 (9)	0.0246 (9)	0.0293 (9)	0.0081 (7)	0.0096 (7)	0.0019 (7)
C21	0.0155 (8)	0.0308 (9)	0.0304 (10)	0.0036 (7)	0.0054 (7)	0.0094 (8)
C22	0.0174 (8)	0.0233 (9)	0.0294 (9)	−0.0040 (7)	0.0000 (7)	0.0042 (7)
C23	0.0183 (8)	0.0186 (8)	0.0254 (9)	0.0004 (6)	0.0023 (7)	0.0008 (7)

Geometric parameters (Å, º)

Cd—N3	2.2799 (14)	C7—H7	0.9500
Cd—S1	2.5868 (5)	C8—C9	1.384 (3)
Cd—S3	2.5908 (4)	C8—H8	0.9500
Cd—S2	2.6421 (5)	C9—H9	0.9500
Cd—S4	2.6473 (5)	C11—H11A	0.9800
S1—C1	1.7262 (17)	C11—H11B	0.9800
S2—C1	1.7191 (17)	C11—H11C	0.9800
S3—C10	1.7264 (17)	C12—C13	1.513 (2)
S4—C10	1.7284 (16)	C12—H12A	0.9900
N1—C1	1.335 (2)	C12—H12B	0.9900
N1—C3	1.463 (2)	C13—C18	1.389 (2)
N1—C2	1.467 (2)	C13—C14	1.396 (2)
N2—C10	1.326 (2)	C14—C15	1.385 (2)
N2—C11	1.469 (2)	C14—H14	0.9500
N2—C12	1.475 (2)	C15—C16	1.389 (2)
N3—C23	1.340 (2)	C15—H15	0.9500
N3—C19	1.340 (2)	C16—C17	1.384 (3)
C2—H2A	0.9800	C16—H16	0.9500
C2—H2B	0.9800	C17—C18	1.392 (2)
C2—H2C	0.9800	C17—H17	0.9500
C3—C4	1.515 (2)	C18—H18	0.9500
C3—H3A	0.9900	C19—C20	1.386 (2)
C3—H3B	0.9900	C19—H19	0.9500
C4—C5	1.386 (2)	C20—C21	1.375 (3)
C4—C9	1.397 (2)	C20—H20	0.9500
C5—C6	1.392 (3)	C21—C22	1.387 (3)
C5—H5	0.9500	C21—H21	0.9500
C6—C7	1.384 (3)	C22—C23	1.381 (2)
C6—H6	0.9500	C22—H22	0.9500
C7—C8	1.388 (3)	C23—H23	0.9500
N3—Cd—S1	114.12 (4)	C7—C8—H8	120.0
N3—Cd—S3	107.77 (4)	C8—C9—C4	120.63 (17)
S1—Cd—S3	137.998 (15)	C8—C9—H9	119.7
N3—Cd—S2	99.83 (4)	C4—C9—H9	119.7
S1—Cd—S2	69.295 (13)	N2—C10—S3	119.60 (12)
S3—Cd—S2	101.303 (14)	N2—C10—S4	121.79 (12)
N3—Cd—S4	97.24 (4)	S3—C10—S4	118.61 (9)
S1—Cd—S4	107.379 (13)	N2—C11—H11A	109.5
S3—Cd—S4	69.094 (13)	N2—C11—H11B	109.5
S2—Cd—S4	162.384 (14)	H11A—C11—H11B	109.5
C1—S1—Cd	86.44 (6)	N2—C11—H11C	109.5
C1—S2—Cd	84.82 (6)	H11A—C11—H11C	109.5
C10—S3—Cd	87.02 (5)	H11B—C11—H11C	109.5
C10—S4—Cd	85.19 (6)	N2—C12—C13	110.41 (13)
C1—N1—C3	122.72 (14)	N2—C12—H12A	109.6

C1—N1—C2	121.19 (14)	C13—C12—H12A	109.6
C3—N1—C2	116.08 (13)	N2—C12—H12B	109.6
C10—N2—C11	121.63 (14)	C13—C12—H12B	109.6
C10—N2—C12	122.96 (13)	H12A—C12—H12B	108.1
C11—N2—C12	115.34 (13)	C18—C13—C14	119.01 (15)
C23—N3—C19	118.46 (15)	C18—C13—C12	120.71 (15)
C23—N3—Cd	119.97 (11)	C14—C13—C12	120.24 (15)
C19—N3—Cd	121.57 (11)	C15—C14—C13	120.30 (16)
N1—C1—S2	121.43 (12)	C15—C14—H14	119.8
N1—C1—S1	119.26 (12)	C13—C14—H14	119.8
S2—C1—S1	119.30 (9)	C14—C15—C16	120.40 (16)
N1—C2—H2A	109.5	C14—C15—H15	119.8
N1—C2—H2B	109.5	C16—C15—H15	119.8
H2A—C2—H2B	109.5	C17—C16—C15	119.65 (16)
N1—C2—H2C	109.5	C17—C16—H16	120.2
H2A—C2—H2C	109.5	C15—C16—H16	120.2
H2B—C2—H2C	109.5	C16—C17—C18	120.03 (16)
N1—C3—C4	113.03 (14)	C16—C17—H17	120.0
N1—C3—H3A	109.0	C18—C17—H17	120.0
C4—C3—H3A	109.0	C13—C18—C17	120.60 (16)
N1—C3—H3B	109.0	C13—C18—H18	119.7
C4—C3—H3B	109.0	C17—C18—H18	119.7
H3A—C3—H3B	107.8	N3—C19—C20	122.40 (16)
C5—C4—C9	118.70 (16)	N3—C19—H19	118.8
C5—C4—C3	122.22 (15)	C20—C19—H19	118.8
C9—C4—C3	119.08 (15)	C21—C20—C19	118.82 (17)
C4—C5—C6	120.89 (16)	C21—C20—H20	120.6
C4—C5—H5	119.6	C19—C20—H20	120.6
C6—C5—H5	119.6	C20—C21—C22	119.14 (16)
C7—C6—C5	119.79 (18)	C20—C21—H21	120.4
C7—C6—H6	120.1	C22—C21—H21	120.4
C5—C6—H6	120.1	C23—C22—C21	118.80 (17)
C6—C7—C8	119.95 (18)	C23—C22—H22	120.6
C6—C7—H7	120.0	C21—C22—H22	120.6
C8—C7—H7	120.0	N3—C23—C22	122.35 (16)
C9—C8—C7	120.04 (17)	N3—C23—H23	118.8
C9—C8—H8	120.0	C22—C23—H23	118.8

C3—N1—C1—S2	4.2 (2)	Cd—S3—C10—N2	177.56 (12)
C2—N1—C1—S2	−176.90 (12)	Cd—S3—C10—S4	−2.63 (8)
C3—N1—C1—S1	−176.86 (12)	Cd—S4—C10—N2	−177.61 (13)
C2—N1—C1—S1	2.0 (2)	Cd—S4—C10—S3	2.58 (8)
Cd—S2—C1—N1	−177.38 (13)	C10—N2—C12—C13	−100.13 (17)
Cd—S2—C1—S1	3.67 (9)	C11—N2—C12—C13	76.79 (17)
Cd—S1—C1—N1	177.29 (13)	N2—C12—C13—C18	−103.51 (17)
Cd—S1—C1—S2	−3.74 (9)	N2—C12—C13—C14	74.33 (19)
C1—N1—C3—C4	111.20 (17)	C18—C13—C14—C15	0.2 (2)
C2—N1—C3—C4	−67.76 (19)	C12—C13—C14—C15	−177.64 (15)

N1—C3—C4—C5	−27.0 (2)	C13—C14—C15—C16	−0.3 (3)
N1—C3—C4—C9	154.03 (15)	C14—C15—C16—C17	0.0 (3)
C9—C4—C5—C6	−1.3 (3)	C15—C16—C17—C18	0.4 (3)
C3—C4—C5—C6	179.78 (16)	C14—C13—C18—C17	0.1 (2)
C4—C5—C6—C7	0.9 (3)	C12—C13—C18—C17	177.98 (15)
C5—C6—C7—C8	0.0 (3)	C16—C17—C18—C13	−0.4 (3)
C6—C7—C8—C9	−0.6 (3)	C23—N3—C19—C20	−1.3 (3)
C7—C8—C9—C4	0.2 (3)	Cd—N3—C19—C20	177.92 (13)
C5—C4—C9—C8	0.7 (3)	N3—C19—C20—C21	0.8 (3)
C3—C4—C9—C8	179.71 (16)	C19—C20—C21—C22	0.6 (3)
C11—N2—C10—S3	−2.3 (2)	C20—C21—C22—C23	−1.4 (3)
C12—N2—C10—S3	174.39 (11)	C19—N3—C23—C22	0.5 (3)
C11—N2—C10—S4	177.86 (11)	Cd—N3—C23—C22	−178.80 (13)
C12—N2—C10—S4	−5.4 (2)	C21—C22—C23—N3	0.9 (3)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···S2^{i}	0.99	2.79	3.5926 (17)	138
C11—H11*C*···*Cg*1^{ii}	0.98	2.91	3.3715 (18)	110

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