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Key indicators

Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.023
 wR factor = 0.046
Data-to-parameter ratio = 15.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Dichlorobis[1-methylimidazoline-2(3*H*)-thione]-cadmium(II)

In the title complex, $[\text{CdCl}_2(\text{C}_4\text{H}_6\text{N}_2\text{S})_2]$, the Cd atom has a distorted tetrahedral coordination geometry, with two Cl^- and two monodentate neutral thione ligands bonded through S. There are intramolecular $\text{N}-\text{H}\cdots\text{Cl}$ and intermolecular $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds, generating centrosymmetric dimers.

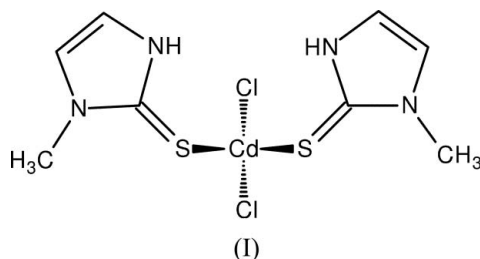
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Comment

Due to their relevance in biological systems, the use of heterocyclic thiones as ligands in transition metal complexes has attracted much attention in the recent past (Raper, 1994, 1997), because of the search for simple model compounds for metalloproteins. In view of this, Cu^{I} , Ag^{I} , Au^{I} , Hg^{II} and Cd^{II} complexes with thiones have been widely studied (Isab *et al.*, 2002, and references therein; Beheshti *et al.*, 2005).



The title compound, (I), is an unexpected product, obtained in an attempt to prepare a $\text{WS}_4(\text{CdCl}_2)(\text{Hmimt})_n$ complex [Hmimt = 1-methylimidazoline-2(3*H*)-thione]. The molecular structure of (I) is shown in Fig. 1, and selected bond lengths and angles are listed in Table 1. The Cd^{II} ion is coordinated by two Cl^- and two S-bonded monodentate Hmimt ligands, to give a distorted tetrahedral S_2Cl_2 donor set. The major distortions from regular tetrahedral geometry are an enlarged

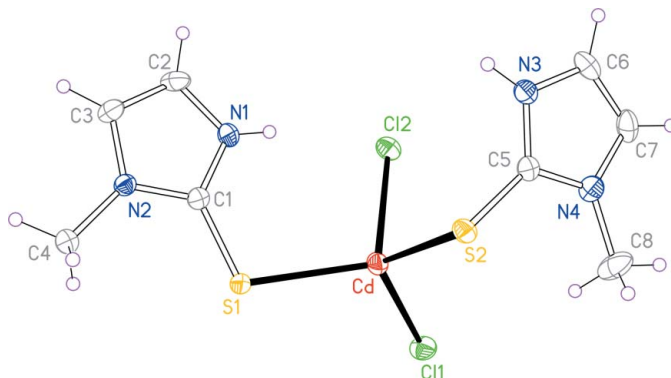


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids.

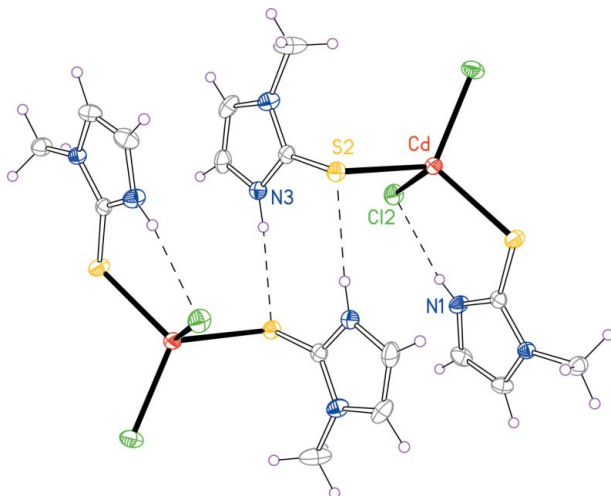


Figure 2
A centrosymmetric dimer in (I), formed by a pair of intermolecular N—H...S hydrogen bonds. All hydrogen bonds are shown as dashed lines. Unlabelled atoms are generated by the symmetry operation $(-x, 1 - y, 1 - z)$.

S—Cd—S angle and considerable variation in the four S—Cd—Cl angles. These are probably a result mainly of steric interactions.

The essentially planar Hmimt ligands are in their neutral thione form. Their geometry is typical of this ligand attached in a monodentate fashion through S to metal ions; the mean C=S bond length for almost 100 occurrences of this ligand in 39 crystal structures in the Cambridge Structural Database (version 5.26 with two updates, May 2005; Allen, 2002) is 1.718 Å, over a range of 1.684–1.750 Å with the omission of a few outliers, and compares with C=S bond lengths of 1.729 (3) and 1.733 (3) Å in (I). These bonds are thus lengthened and weakened on coordination, as expected, compared with their greater double-bond character in the uncomplexed ligand, which has a C=S bond length of 1.685 (2) Å (Raper *et al.*, 1983; Vampa *et al.*, 1995). The geometric results are in agreement with spectroscopic observations (see *Experimental* section).

The structure of (I) may be compared with those of other $[MX_2(\text{Hmimt})_2]$ complexes ($M = \text{Cd}$ or Hg , and $X = \text{Cl}$, Br or I). All of these have monomeric molecules with a distorted tetrahedral coordination geometry about the metal atom, and the variations in bond lengths and angles can be readily understood in terms of the sizes of the metal and halogen atoms. None of the other complexes is isomorphous with (I). Indeed, all five known structures have different space groups and packing arrangements (Bell *et al.*, 2000, 2004; Pavlović *et al.*, 2000). The bromo analogue of (I) has an unusual structure, with six molecules in the asymmetric unit and a high degree of pseudo-symmetry (Bell *et al.*, 2004).

The N—H groups of the two Hmimt ligands in (I) engage in hydrogen bonds. One of these is intramolecular, to atom Cl2, and presumably contributes to the lengthening of this Cd—Cl bond relative to the other. The other hydrogen bond is intermolecular, to the S atom of an adjacent Hmimt ligand, and generates centrosymmetric dimers (Fig. 2 and Table 2).

Experimental

$\text{CdCl}_2 \cdot \text{H}_2\text{O}$ (1.12 g, 5.56 mmol) was added to a suspension of $(\text{NH}_4)_2[\text{WS}_4]$ (0.967 g, 2.78 mmol) in acetone (70 ml) and the mixture was stirred for 1 h. Hmimt (0.71 g, 6.22 mmol) was added to this solution and the mixture was stirred for another 4 h at room temperature. The mixture was centrifuged and the yellow supernatant liquid was decanted and evaporated to dryness in a vacuum. The residue was washed with diethyl ether (2×5 ml) and *n*-pentane (2×5 ml) to remove any unreacted Hmimt, and dried in a vacuum to give an orange–yellow powder. Both IR [$\nu(\text{W—S}) = 441 \text{ cm}^{-1}$, $\nu(\text{C=S}) = 506 \text{ cm}^{-1}$ and $\nu(\text{N—H}) = 3133 \text{ cm}^{-1}$] and UV–vis $\lambda_{\text{max}} = 430, 374, 315$ and 273 nm spectra of the product confirmed the presence of WS_4 and S-bonded Hmimt ligands. In the solid state, the complex is air-stable and can be stored for months in a desiccator, but it decomposed slowly when diethyl ether was diffused slowly into an acetone solution of the product over 3 d at room temperature, resulting in the formation of pale-yellow crystals with an empirical formula $\text{C}_8\text{H}_{12}\text{CdCl}_2\text{N}_4\text{S}_2$, as confirmed by X-ray crystallography. The air-stable crystals of this compound are insoluble in common organic solvents, but soluble in solvents with pronounced donor properties, such as dimethyl sulfoxide and dimethylformamide. ^1H NMR ($\text{DMSO-}d_6$, 298 K, δ , p.p.m.): 12.01 (s, NH), 6.98 (s, CH), 6.80 (s, CH), 3.32 (s, NCH_3); ^{13}C NMR ($\text{DMSO-}d_6$, 298 K, δ , p.p.m.): 160.52 (C1/5), 120.05 and 114.62 (C2/6 and C3/7), 33.99 (C4/8) (see Fig. 1 for atom numbering). In the NMR spectra of the complex, the ligand signals are shifted down-field from their positions in the spectra of the free ligand (Casa *et al.*, 1996), suggesting that, in $\text{DMSO-}d_6$, the ligand remains coordinated to the metal. The absence of a weak S—H signal of the thiol form of the ligand in the ^1H NMR spectrum of the complex confirms that coordination of Hmimt in $\text{DMSO-}d_6$ solution, as in the solid state, takes place only through the S atom, the Hmimt ligands being in the neutral thione form.

Crystal data

$[\text{CdCl}_2(\text{C}_4\text{H}_6\text{N}_2\text{S})_2]$	$D_x = 1.897 \text{ Mg m}^{-3}$
$M_r = 411.64$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 22587 reflections
$a = 9.6464$ (8) Å	$\theta = 2.5\text{--}25.0^\circ$
$b = 7.6262$ (8) Å	$\mu = 2.16 \text{ mm}^{-1}$
$c = 19.7151$ (8) Å	$T = 150$ (2) K
$\beta = 96.485$ (6)°	Block, pale yellow
$V = 1441.1$ (2) Å ³	$0.36 \times 0.32 \times 0.28 \text{ mm}$
$Z = 4$	

Data collection

Nonius KappaCCD area-detector diffractometer	2518 independent reflections
φ and ω scans	2115 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$R_{\text{int}} = 0.058$
$T_{\text{min}} = 0.481$, $T_{\text{max}} = 0.549$	$\theta_{\text{max}} = 25.0^\circ$
22587 measured reflections	$h = -11 \rightarrow 11$
	$k = -9 \rightarrow 9$
	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.016P)^2 + 0.9012P]$
$R[F^2 > 2\sigma(F^2)] = 0.023$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.046$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$
2518 reflections	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$
163 parameters	Extinction correction: SHELXTL (Sheldrick, 2001)
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.0027 (3)

Table 1

Selected geometric parameters (Å, °).

Cd—Cl1	2.4410 (7)	Cd—S2	2.5663 (7)
Cd—Cl2	2.5175 (7)	S1—C1	1.729 (3)
Cd—S1	2.5392 (7)	S2—C5	1.733 (3)
Cl1—Cd—Cl2	104.43 (2)	Cl2—Cd—S2	97.66 (2)
Cl1—Cd—S1	111.60 (2)	S1—Cd—S2	117.32 (2)
Cl1—Cd—S2	116.52 (2)	Cd—S1—C1	107.78 (9)
Cl2—Cd—S1	106.84 (2)	Cd—S2—C5	102.85 (9)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...Cl2	0.80 (3)	2.41 (3)	3.204 (3)	168 (3)
N3—H3...S2 ⁱ	0.88 (3)	2.49 (3)	3.358 (3)	173 (3)

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

All H atoms were located in a difference map. Those bonded to N were refined with unconstrained coordinates and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. Other H atoms were refined as riding with idealized geometries, including free rotation of methyl groups about the C—C bonds (C—H = 0.95–0.98 Å), with the constraint $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$ applied.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *EVALCCD* (Duisenberg *et al.*, 2003); data reduction: *EVALCCD*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001);

program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Dichlorobis[1-methylimidazoline-2(3*H*)-thione]cadmium(II)

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Dichlorobis[1-methylimidazoline-2(3*H*)-thione]cadmium(II)*Crystal data*

[CdCl₂(C₄H₆N₂S)₂]

M_r = 411.64

Monoclinic, *P*2₁/*c*

Hall symbol: -*P* 2ybc

a = 9.6464 (8) Å

b = 7.6262 (8) Å

c = 19.7151 (8) Å

β = 96.485 (6)°

V = 1441.1 (2) Å³

Z = 4

F(000) = 808

D_x = 1.897 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 23643 reflections

θ = 2.5–25.0°

μ = 2.16 mm⁻¹

T = 150 K

Block, pale yellow

0.36 × 0.32 × 0.28 mm

Data collection

Nonius KappaCCD area-detector
diffractometer

Radiation source: sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 2002)

T_{min} = 0.481, *T_{max}* = 0.549

22587 measured reflections

2518 independent reflections

2115 reflections with *I* > 2σ(*I*)

R_{int} = 0.058

θ_{\max} = 25.0°, θ_{\min} = 4.9°

h = -11→11

k = -9→9

l = -23→23

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.023

wR(*F*²) = 0.046

S = 1.05

2518 reflections

163 parameters

0 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/[σ²(*F_o*²) + (0.016*P*)² + 0.9012*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.001

Δρ_{max} = 0.36 e Å⁻³

Δρ_{min} = -0.32 e Å⁻³

Extinction correction: SHELXTL (Sheldrick,
2001), *F_c** = *kF_c*[1 + 0.001*xF_c*²λ³/sin(2θ)]^{-1/4}

Extinction coefficient: 0.0027 (3)

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

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{iso}</i> */ <i>U_{eq}</i>
Cd	0.305327 (19)	0.40552 (3)	0.413963 (10)	0.01882 (9)

Cl1	0.41103 (7)	0.42594 (9)	0.30744 (3)	0.02480 (17)
Cl2	0.11347 (7)	0.18284 (9)	0.38971 (3)	0.02436 (17)
S1	0.47501 (7)	0.28210 (9)	0.50996 (3)	0.02039 (17)
C1	0.3861 (3)	0.1299 (3)	0.55362 (13)	0.0159 (6)
N1	0.2581 (2)	0.0623 (3)	0.53657 (12)	0.0206 (6)
H1	0.211 (3)	0.084 (4)	0.5012 (16)	0.025*
N2	0.4360 (2)	0.0558 (3)	0.61350 (11)	0.0165 (5)
C2	0.2271 (3)	-0.0553 (4)	0.58620 (14)	0.0246 (7)
H2	0.1434	-0.1210	0.5863	0.030*
C3	0.3374 (3)	-0.0588 (3)	0.63401 (14)	0.0216 (6)
H3A	0.3463	-0.1272	0.6745	0.026*
C4	0.5738 (3)	0.0896 (4)	0.65069 (14)	0.0216 (6)
H4A	0.6455	0.0766	0.6196	0.032*
H4B	0.5914	0.0056	0.6883	0.032*
H4C	0.5766	0.2091	0.6690	0.032*
S2	0.15259 (7)	0.66470 (9)	0.44266 (3)	0.01838 (17)
C5	-0.0033 (3)	0.6253 (3)	0.39218 (13)	0.0165 (6)
N3	-0.1171 (2)	0.5455 (3)	0.41061 (12)	0.0205 (5)
H3	-0.119 (3)	0.495 (4)	0.4504 (16)	0.025*
N4	-0.0372 (2)	0.6812 (3)	0.32768 (11)	0.0202 (5)
C6	-0.2242 (3)	0.5515 (4)	0.35804 (15)	0.0255 (7)
H6	-0.3154	0.5045	0.3583	0.031*
C7	-0.1741 (3)	0.6372 (4)	0.30602 (15)	0.0257 (7)
H7	-0.2236	0.6624	0.2627	0.031*
C8	0.0581 (3)	0.7743 (4)	0.28699 (15)	0.0351 (8)
H8A	0.0866	0.8854	0.3093	0.053*
H8B	0.0105	0.7978	0.2413	0.053*
H8C	0.1407	0.7017	0.2832	0.053*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd	0.01600 (12)	0.02447 (13)	0.01584 (13)	0.00119 (9)	0.00109 (8)	0.00265 (9)
Cl1	0.0252 (4)	0.0334 (4)	0.0164 (4)	-0.0041 (3)	0.0050 (3)	0.0002 (3)
Cl2	0.0185 (4)	0.0279 (4)	0.0256 (4)	-0.0043 (3)	-0.0022 (3)	0.0001 (3)
S1	0.0164 (3)	0.0233 (4)	0.0205 (4)	-0.0050 (3)	-0.0019 (3)	0.0071 (3)
C1	0.0173 (14)	0.0131 (15)	0.0177 (15)	0.0013 (11)	0.0031 (11)	-0.0008 (11)
N1	0.0180 (13)	0.0261 (15)	0.0164 (13)	-0.0042 (10)	-0.0041 (10)	0.0018 (10)
N2	0.0173 (12)	0.0156 (12)	0.0166 (13)	-0.0011 (9)	0.0021 (10)	0.0010 (9)
C2	0.0217 (16)	0.0268 (17)	0.0263 (17)	-0.0099 (12)	0.0067 (13)	-0.0010 (13)
C3	0.0258 (16)	0.0209 (16)	0.0189 (15)	-0.0055 (12)	0.0056 (13)	0.0015 (12)
C4	0.0195 (15)	0.0253 (16)	0.0194 (15)	-0.0028 (13)	-0.0009 (12)	0.0026 (12)
S2	0.0159 (3)	0.0204 (4)	0.0182 (4)	-0.0020 (3)	-0.0012 (3)	-0.0011 (3)
C5	0.0183 (14)	0.0138 (15)	0.0173 (15)	0.0018 (11)	0.0014 (11)	-0.0024 (11)
N3	0.0170 (13)	0.0255 (14)	0.0192 (13)	0.0018 (10)	0.0022 (11)	0.0028 (10)
N4	0.0234 (13)	0.0196 (13)	0.0165 (13)	-0.0046 (10)	-0.0026 (10)	-0.0011 (10)
C6	0.0154 (15)	0.0305 (18)	0.0291 (17)	0.0025 (12)	-0.0037 (13)	-0.0036 (13)
C7	0.0272 (16)	0.0229 (17)	0.0241 (16)	0.0031 (13)	-0.0098 (13)	0.0002 (13)

C8 0.0445 (19) 0.041 (2) 0.0185 (17) -0.0199 (16) -0.0006 (14) 0.0072 (14)

Geometric parameters (Å, °)

Cd—C11	2.4410 (7)	C4—H4B	0.980
Cd—C12	2.5175 (7)	C4—H4C	0.980
Cd—S1	2.5392 (7)	S2—C5	1.733 (3)
Cd—S2	2.5663 (7)	C5—N3	1.341 (3)
S1—C1	1.729 (3)	C5—N4	1.346 (3)
C1—N1	1.345 (3)	N3—H3	0.88 (3)
C1—N2	1.348 (3)	N3—C6	1.379 (4)
N1—H1	0.80 (3)	N4—C7	1.383 (4)
N1—C2	1.385 (4)	N4—C8	1.469 (4)
N2—C3	1.386 (3)	C6—H6	0.950
N2—C4	1.466 (3)	C6—C7	1.351 (4)
C2—H2	0.950	C7—H7	0.950
C2—C3	1.340 (4)	C8—H8A	0.980
C3—H3A	0.950	C8—H8B	0.980
C4—H4A	0.980	C8—H8C	0.980
C11—Cd—C12	104.43 (2)	H4A—C4—H4B	109.5
C11—Cd—S1	111.60 (2)	H4A—C4—H4C	109.5
C11—Cd—S2	116.52 (2)	H4B—C4—H4C	109.5
C12—Cd—S1	106.84 (2)	Cd—S2—C5	102.85 (9)
C12—Cd—S2	97.66 (2)	S2—C5—N3	127.4 (2)
S1—Cd—S2	117.32 (2)	S2—C5—N4	126.1 (2)
Cd—S1—C1	107.78 (9)	N3—C5—N4	106.3 (2)
S1—C1—N1	128.8 (2)	C5—N3—H3	123.1 (19)
S1—C1—N2	124.7 (2)	C5—N3—C6	110.4 (2)
N1—C1—N2	106.6 (2)	H3—N3—C6	126.5 (19)
C1—N1—H1	123 (2)	C5—N4—C7	109.6 (2)
C1—N1—C2	109.7 (2)	C5—N4—C8	124.7 (2)
H1—N1—C2	127 (2)	C7—N4—C8	125.7 (2)
C1—N2—C3	109.3 (2)	N3—C6—H6	126.7
C1—N2—C4	125.3 (2)	N3—C6—C7	106.5 (3)
C3—N2—C4	125.3 (2)	H6—C6—C7	126.7
N1—C2—H2	126.5	N4—C7—C6	107.1 (3)
N1—C2—C3	107.0 (2)	N4—C7—H7	126.4
H2—C2—C3	126.5	C6—C7—H7	126.4
N2—C3—C2	107.4 (2)	N4—C8—H8A	109.5
N2—C3—H3A	126.3	N4—C8—H8B	109.5
C2—C3—H3A	126.3	N4—C8—H8C	109.5
N2—C4—H4A	109.5	H8A—C8—H8B	109.5
N2—C4—H4B	109.5	H8A—C8—H8C	109.5
N2—C4—H4C	109.5	H8B—C8—H8C	109.5
C11—Cd—S1—C1	-136.06 (9)	C11—Cd—S2—C5	79.26 (10)
C12—Cd—S1—C1	-22.49 (10)	C12—Cd—S2—C5	-31.11 (9)

S2—Cd—S1—C1	85.76 (10)	S1—Cd—S2—C5	-144.60 (9)
Cd—S1—C1—N1	10.0 (3)	Cd—S2—C5—N3	96.2 (2)
Cd—S1—C1—N2	-169.9 (2)	Cd—S2—C5—N4	-89.2 (2)
S1—C1—N1—C2	-179.8 (2)	S2—C5—N3—C6	175.1 (2)
N2—C1—N1—C2	0.1 (3)	N4—C5—N3—C6	-0.4 (3)
S1—C1—N2—C3	179.65 (19)	S2—C5—N4—C7	-175.0 (2)
S1—C1—N2—C4	-1.0 (4)	S2—C5—N4—C8	5.2 (4)
N1—C1—N2—C3	-0.3 (3)	N3—C5—N4—C7	0.6 (3)
N1—C1—N2—C4	179.0 (2)	N3—C5—N4—C8	-179.2 (3)
C1—N1—C2—C3	0.1 (3)	C5—N3—C6—C7	0.1 (3)
N1—C2—C3—N2	-0.3 (3)	N3—C6—C7—N4	0.3 (3)
C1—N2—C3—C2	0.4 (3)	C5—N4—C7—C6	-0.5 (3)
C4—N2—C3—C2	-179.0 (2)	C8—N4—C7—C6	179.3 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...C12	0.80 (3)	2.41 (3)	3.204 (3)	168 (3)
N3—H3...S2 ⁱ	0.88 (3)	2.49 (3)	3.358 (3)	173 (3)

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