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2-Amino-4,5-dihydro-1*H*-imidazol-3-ium 7,8-dihydroimidazo[1,2-c][1,3,5]thiadiazine-2,4(6*H*)-dithione(1−) dimethylformamide disolvate

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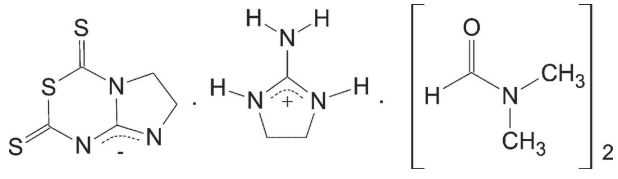
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.088; data-to-parameter ratio = 15.3.

The structure of the title compound, $C_5H_4N_3S_3^-\cdot C_3H_8N_3^+\cdot 2C_3H_7NO$, has been determined from a non-merohedral twin. The asymmetric unit consists of a heterocyclic anion, a guanidinium-type cation and two dimethylformamide solvent molecules. The three C—N bond lengths in the guanidinium fragment range from 1.315 (3) to 1.342 (3) Å, the shortest bond being to the exocyclic amino group. The anion and cation are connected *via* a pair of N—H···N hydrogen bonds and the two solvent molecules are linked to this ion pair *via* N—H···O hydrogen bonds.

Related literature

For synthesis and crystallographic data reported earlier for the title compound, see Saczewski *et al.* (2003). For related literature, see: Allen (2002); Cooper *et al.* (2002); Farrugia (1999).



Experimental

Crystal data

$C_3H_8N_3^+\cdot C_5H_4N_3S_3^-\cdot 2C_3H_7NO$
M_r = 434.61
Triclinic, $P\overline{1}$
a = 6.8301 (7) Å
b = 12.1321 (14) Å
c = 12.9487 (10) Å
α = 79.232 (7)°
β = 89.907 (7)°
γ = 82.125 (7)°
V = 1043.82 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 120 (2) K
0.60 × 0.20 × 0.10 mm

Data collection

Kuma KM-4-CCD κ-geometry diffractometer
Absorption correction: none
8801 measured reflections
4006 independent reflections
3627 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.088
S = 1.12
4006 reflections
261 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1B—H1B···N7A	0.81 (3)	2.11 (3)	2.916 (3)	178 (3)
N3B—H3B···O1D	0.81 (3)	2.07 (3)	2.806 (3)	153 (2)
N6B—H6BB···N1A	0.81 (3)	2.14 (3)	2.952 (3)	173 (3)
N6B—H6BA···O1C	0.85 (2)	1.98 (3)	2.827 (3)	174 (3)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *Stereochemical Workstation Operation Manual* (Siemens, 1989) and *Mercury* (Version 1.4; Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2169).

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supplementary materials

Acta Cryst. (2007). E**63**, o3329 [**doi:10.1107/S1600536807030590**]

2-Amino-4,5-dihydro-1*H*-imidazol-3-ium 7,8-dihydroimidazo[1,2-*c*][1,3,5]thiadiazine-2,4(6*H*)-dithione(1-) dimethylformamide disolvate

M. Gdaniec, J. Saczewski and F. Saczewski

Comment

In course of our research on the reactivity of 2-hydroxylamino-4,5-dihydroimidazolium-*O*-sulfonate, it was reacted with carbon disulfide in aqueous NaOH, forming, unexpectedly, the salt of 2-aminoimidazoline and 7,8-dihydroimidazo [1,2-*c*][1,3,5]thiadiazine-2,4(6*H*)-dithione (Saczewski *et al.*, 2003). The crystal structure of (I) has been solved based on diffraction data collected for a twinned specimen. The structure was refined to a R1 factor = 0.20 but twinning was not taken into account, neither at the data processing stage nor during refinement. The structure just served to confirm the connectivity of atoms deduced from spectroscopic methods. When we noticed that this is the first crystal structure of a 2-aminoimdazoline in the Cambridge Structural Databank (Allen, 2002) we decided to refine this structure taking twinning into account. Here, we present the structure of (I) refined as a nonmerohedral twin.

The asymmetric unit is shown in Fig. 1. The cation and anion are linked *via* two N—H···N hydrogen bonds into an ionic pair and the two solvate molecule are joined *via* N—H···O interactions to the cation, thus forming discrete hydrogen-bonded assemblies. The five-membered ring of the 2-aminoimidazolinium cation, with the largest endocyclic torsion angle of 15.8 (2)°, forms a slightly puckered half-chair. The three C—N bonds of the guanidinium fragment in the cation range from 1.315 (3) to 1.342 (3) Å, with the shortest bond being to the exocyclic amino group and the longest to the ring N3 atom exhibiting slightly pyramidal sp^2 hybridization. Deprotonation has an enormous influence on the geometry of the 7,8-dihydroimidazo[1,2-*c*][1,3,5]thiadiazine-2,4(6*H*)dithione molecule. For example, in the neutral form, with the acidic proton bonded to N7A (Saczewski *et al.*, 2003), the endocyclic bond angle at this atom is 113.72(16.)° whereas in the ionic form this angle is much smaller, 108.93 (17)°. Bond lengths are also strongly altered and, for example, the N1A—C6A bond length changes from 1.323 (2) in the neutral acid to 1.373 (3) Å in the anion.

Experimental

The title compound was prepared according to the known procedure (Saczewski *et al.*, 2003). Crystals for X-ray analysis were obtained by recrystallization from a dimethylformamide solution of (I).

Refinement

The twin matrix, 1 0 0 0.475 − 1 0 0.003 0 − 1, corresponding to 180° rotation about [100] direct lattice direction has been determined with the program ROTAX (Cooper *et al.*, 2002). For the refinement with the *SHELXL97* program (Sheldrick, 1997), the reflection data file was prepared in the HKLF 5 format using the 'Make HKLF5' function of the *WinGX* program (Farrugia, 1999). The overlapping reflections and those belonging to only one twin domain are used in the refinement (HKLF 5 format of *SHELXL*). Those which were excluded, 250 reflections, are partial overlaps which could not be integrated properly at the data processing stage.

The H atoms of the N—H groups were freely refined. The H atoms bonded to C atoms were placed at calculated positions, with C—H = 0.95–0.99 Å, and refined as riding on their parent atoms, with U_{iso}(H) = x U_{eq}(C), where x = 1.5 for the H atoms from methyl groups and x = 1.2 for the remaining H atoms.

Figures

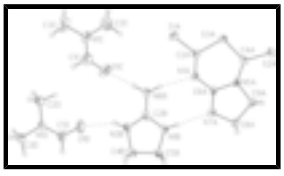


Fig. 1. Asymmetric unit of (I) showing atom labelling scheme and displacement ellipsoids shown at the 50% probability level. Hydrogen bonds are shown as dashed lines.

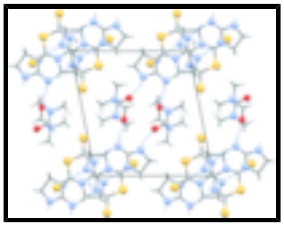


Fig. 2. Crystal packing shown down the *a*-axis. Hydrogen bonds are shown as dashed lines.

2-Amino-4,5-dihydro-1*H*-imidazol-3-ium 7,8-dihydroimidazo[1,2-*c*][1,3,5]thiadiazine-2,4(6*H*)-dithione(1-) dimethylformamide disolvate

Crystal data

$C_3H_8N_3^+·C_5H_4N_3S_3^-·2C_3H_7NO$	Z = 2
M_r = 434.61	F_{000} = 460
Triclinic, $P\bar{1}$	D_x = 1.383 Mg m^{-3}
Hall symbol: -P 1	Melting point: 447 K
a = 6.8301 (7) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
b = 12.1321 (14) Å	Cell parameters from 2455 reflections
c = 12.9487 (10) Å	θ = 4.0–25.0º
α = 79.232 (7)º	μ = 0.38 mm^{-1}
β = 89.907 (7)º	T = 120 (2) K
γ = 82.125 (7)º	Prism, yellow
V = 1043.82 (18) Å^3	0.60 × 0.20 × 0.10 mm

Data collection

Kuma KM-4-CCD κ-geometry diffractometer	3627 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.035
Monochromator: graphite	θ_{max} = 26.5º
T = 120(2) K	θ_{min} = 4.2º
ω scans	h = −8→8
Absorption correction: none	k = −15→15
8801 measured reflections	l = −16→16

4006 independent reflections

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.037$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.088$	$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2 + 0.3779P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} < 0.001$
4006 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
261 parameters	$\Delta\rho_{min} = -0.28$ 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 $F^2 > 2$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}
S1A	0.74388 (10)	−0.03696 (5)	0.69870 (4)	0.02750 (15)
S2A	0.73548 (10)	−0.34589 (5)	1.09680 (5)	0.02675 (15)
N1A	0.7458 (3)	0.01169 (14)	0.88951 (13)	0.0205 (4)
C2A	0.7457 (3)	−0.06552 (17)	0.83134 (16)	0.0194 (4)
S3A	0.74710 (10)	−0.21218 (4)	0.88413 (4)	0.02568 (15)
C4A	0.7430 (3)	−0.22047 (17)	1.02092 (17)	0.0199 (5)
N5A	0.7464 (3)	−0.12406 (14)	1.05684 (13)	0.0192 (4)
C6A	0.7493 (3)	−0.01300 (17)	0.99742 (16)	0.0190 (4)
N7A	0.7534 (3)	0.06311 (14)	1.05371 (13)	0.0224 (4)
C8A	0.7578 (4)	0.00908 (18)	1.16541 (16)	0.0222 (5)
H8B	0.6442	0.0435	1.2016	0.027*
H8A	0.8815	0.0187	1.2004	0.027*
C9A	0.7465 (4)	−0.11769 (17)	1.16928 (16)	0.0224 (5)
H9B	0.8624	−0.1660	1.2074	0.027*
H9A	0.6240	−0.1401	1.2028	0.027*
N1B	0.7728 (3)	0.28829 (16)	0.93022 (15)	0.0236 (4)
H1B	0.765 (4)	0.227 (2)	0.965 (2)	0.027 (7)*

C2B	0.7435 (3)	0.31567 (17)	0.82677 (18)	0.0224 (5)
N3B	0.7231 (3)	0.42843 (15)	0.79407 (16)	0.0263 (5)
H3B	0.750 (4)	0.456 (2)	0.735 (2)	0.020 (6)*
C4B	0.7636 (4)	0.48437 (18)	0.88018 (18)	0.0280 (5)
H4BA	0.6611	0.5497	0.8833	0.034*
H4BB	0.8950	0.5105	0.8738	0.034*
C5B	0.7578 (4)	0.38891 (18)	0.97749 (18)	0.0266 (5)
H5BA	0.8704	0.3851	1.0267	0.032*
H5BB	0.6325	0.3996	1.0152	0.032*
N6B	0.7384 (3)	0.24212 (17)	0.76439 (17)	0.0275 (5)
H6BB	0.742 (4)	0.177 (2)	0.794 (2)	0.032 (7)*
H6BA	0.717 (4)	0.2707 (19)	0.700 (2)	0.020 (6)*
O1C	0.6385 (3)	0.33821 (18)	0.55175 (14)	0.0496 (5)
N1C	0.6926 (3)	0.29562 (18)	0.38911 (15)	0.0336 (5)
C1C	0.6495 (4)	0.3658 (2)	0.4563 (2)	0.0388 (6)
H1CA	0.6252	0.4445	0.4274	0.047*
C2C	0.7292 (5)	0.1734 (2)	0.4252 (2)	0.0477 (7)
H2CA	0.7208	0.1559	0.5019	0.072*
H2CB	0.8614	0.1441	0.4045	0.072*
H2CC	0.6301	0.1379	0.3934	0.072*
C3C	0.7023 (5)	0.3360 (3)	0.2762 (2)	0.0536 (8)
H3CA	0.6770	0.4190	0.2610	0.080*
H3CB	0.6024	0.3056	0.2397	0.080*
H3CC	0.8340	0.3106	0.2521	0.080*
O1D	0.8400 (3)	0.58284 (15)	0.62367 (14)	0.0491 (5)
N1D	0.8126 (3)	0.72687 (15)	0.48209 (14)	0.0252 (4)
C1D	0.8103 (4)	0.6845 (2)	0.58456 (18)	0.0330 (6)
H1D	0.7839	0.7366	0.6310	0.040*
C2D	0.8469 (4)	0.65334 (19)	0.40540 (19)	0.0325 (6)
H2DA	0.8733	0.5742	0.4419	0.049*
H2DB	0.9610	0.6726	0.3632	0.049*
H2DC	0.7296	0.6635	0.3593	0.049*
C3D	0.7716 (5)	0.84823 (19)	0.44212 (18)	0.0374 (7)
H3DA	0.7507	0.8883	0.5012	0.056*
H3DB	0.6526	0.8647	0.3967	0.056*
H3DC	0.8839	0.8734	0.4016	0.056*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0346 (4)	0.0317 (3)	0.0166 (3)	−0.0039 (3)	0.0002 (3)	−0.0062 (2)
S2A	0.0287 (3)	0.0186 (3)	0.0310 (3)	−0.0042 (2)	0.0013 (2)	0.0009 (2)
N1A	0.0238 (11)	0.0208 (8)	0.0162 (8)	−0.0017 (8)	−0.0001 (8)	−0.0026 (7)
C2A	0.0159 (12)	0.0216 (10)	0.0201 (10)	−0.0011 (9)	−0.0014 (9)	−0.0030 (8)
S3A	0.0347 (4)	0.0194 (3)	0.0233 (3)	−0.0025 (2)	−0.0010 (2)	−0.0058 (2)
C4A	0.0134 (12)	0.0206 (10)	0.0248 (11)	−0.0019 (8)	−0.0021 (9)	−0.0021 (8)
N5A	0.0210 (10)	0.0190 (8)	0.0159 (8)	0.0007 (7)	−0.0003 (7)	−0.0016 (6)
C6A	0.0191 (11)	0.0187 (10)	0.0170 (9)	0.0005 (8)	0.0001 (9)	0.0000 (8)

N7A	0.0285 (11)	0.0222 (9)	0.0168 (8)	−0.0033 (8)	−0.0006 (8)	−0.0043 (7)
C8A	0.0243 (13)	0.0270 (11)	0.0163 (10)	−0.0043 (10)	0.0006 (9)	−0.0059 (8)
C9A	0.0233 (13)	0.0248 (11)	0.0179 (10)	−0.0011 (9)	−0.0005 (9)	−0.0022 (8)
N1B	0.0294 (12)	0.0172 (9)	0.0232 (9)	−0.0038 (8)	0.0002 (8)	−0.0006 (8)
C2B	0.0174 (12)	0.0193 (10)	0.0290 (11)	−0.0008 (9)	0.0029 (9)	−0.0022 (9)
N3B	0.0334 (13)	0.0183 (9)	0.0262 (10)	−0.0053 (8)	0.0057 (9)	−0.0003 (8)
C4B	0.0313 (14)	0.0182 (10)	0.0343 (13)	−0.0034 (9)	0.0017 (11)	−0.0046 (9)
C5B	0.0284 (14)	0.0236 (11)	0.0286 (12)	−0.0027 (10)	0.0007 (10)	−0.0075 (9)
N6B	0.0377 (13)	0.0207 (10)	0.0237 (10)	−0.0047 (9)	0.0026 (9)	−0.0030 (8)
O1C	0.0513 (14)	0.0707 (14)	0.0281 (10)	−0.0133 (11)	−0.0030 (9)	−0.0089 (9)
N1C	0.0322 (13)	0.0425 (12)	0.0232 (10)	−0.0066 (10)	−0.0023 (9)	0.0024 (9)
C1C	0.0346 (17)	0.0461 (15)	0.0365 (14)	−0.0132 (13)	−0.0034 (13)	−0.0041 (12)
C2C	0.047 (2)	0.0425 (15)	0.0499 (17)	−0.0003 (14)	0.0001 (15)	−0.0027 (13)
C3C	0.053 (2)	0.074 (2)	0.0271 (13)	−0.0011 (17)	−0.0008 (14)	0.0007 (13)
O1D	0.0645 (15)	0.0369 (10)	0.0366 (10)	−0.0008 (10)	0.0105 (10)	0.0126 (8)
N1D	0.0314 (12)	0.0224 (9)	0.0207 (9)	−0.0032 (8)	0.0014 (9)	−0.0016 (7)
C1D	0.0376 (16)	0.0335 (12)	0.0251 (12)	−0.0045 (11)	0.0047 (11)	0.0013 (10)
C2D	0.0391 (16)	0.0282 (12)	0.0300 (12)	−0.0010 (11)	0.0039 (12)	−0.0073 (10)
C3D	0.063 (2)	0.0230 (11)	0.0244 (12)	−0.0014 (12)	−0.0032 (13)	−0.0034 (9)

Geometric parameters (Å, °)

S1A—C2A	1.687 (2)	C5B—H5BA	0.9900
S2A—C4A	1.657 (2)	C5B—H5BB	0.9900
N1A—C2A	1.307 (3)	N6B—H6BB	0.81 (3)
N1A—C6A	1.373 (3)	N6B—H6BA	0.85 (2)
C2A—S3A	1.782 (2)	O1C—C1C	1.224 (3)
S3A—C4A	1.756 (2)	N1C—C1C	1.333 (3)
C4A—N5A	1.340 (3)	N1C—C2C	1.456 (3)
N5A—C6A	1.424 (3)	N1C—C3C	1.457 (3)
N5A—C9A	1.472 (3)	C1C—H1CA	0.9500
C6A—N7A	1.282 (3)	C2C—H2CA	0.9800
N7A—C8A	1.471 (2)	C2C—H2CB	0.9800
C8A—C9A	1.542 (3)	C2C—H2CC	0.9800
C8A—H8B	0.9900	C3C—H3CA	0.9800
C8A—H8A	0.9900	C3C—H3CB	0.9800
C9A—H9B	0.9900	C3C—H3CC	0.9800
C9A—H9A	0.9900	O1D—C1D	1.232 (3)
N1B—C2B	1.327 (3)	N1D—C1D	1.331 (3)
N1B—C5B	1.456 (3)	N1D—C2D	1.452 (3)
N1B—H1B	0.81 (3)	N1D—C3D	1.455 (3)
C2B—N6B	1.315 (3)	C1D—H1D	0.9500
C2B—N3B	1.342 (3)	C2D—H2DA	0.9800
N3B—C4B	1.455 (3)	C2D—H2DB	0.9800
N3B—H3B	0.81 (3)	C2D—H2DC	0.9800
C4B—C5B	1.548 (3)	C3D—H3DA	0.9800
C4B—H4BA	0.9900	C3D—H3DB	0.9800
C4B—H4BB	0.9900	C3D—H3DC	0.9800
C2A—N1A—C6A	123.01 (17)	C4B—C5B—H5BA	111.3

N1A—C2A—S1A	123.67 (16)	N1B—C5B—H5BB	111.3
N1A—C2A—S3A	123.39 (15)	C4B—C5B—H5BB	111.3
S1A—C2A—S3A	112.95 (12)	H5BA—C5B—H5BB	109.2
C4A—S3A—C2A	104.71 (10)	C2B—N6B—H6BB	115.3 (19)
N5A—C4A—S2A	124.40 (16)	C2B—N6B—H6BA	115.2 (16)
N5A—C4A—S3A	117.30 (15)	H6BB—N6B—H6BA	129 (2)
S2A—C4A—S3A	118.30 (12)	C1C—N1C—C2C	121.3 (2)
C4A—N5A—C6A	128.01 (17)	C1C—N1C—C3C	122.3 (2)
C4A—N5A—C9A	123.64 (17)	C2C—N1C—C3C	116.4 (2)
C6A—N5A—C9A	108.35 (16)	O1C—C1C—N1C	126.0 (3)
N7A—C6A—N1A	122.48 (18)	O1C—C1C—H1CA	117.0
N7A—C6A—N5A	114.00 (18)	N1C—C1C—H1CA	117.0
N1A—C6A—N5A	123.52 (18)	N1C—C2C—H2CA	109.5
C6A—N7A—C8A	108.93 (17)	N1C—C2C—H2CB	109.5
N7A—C8A—C9A	106.84 (16)	H2CA—C2C—H2CB	109.5
N7A—C8A—H8B	110.4	N1C—C2C—H2CC	109.5
C9A—C8A—H8B	110.4	H2CA—C2C—H2CC	109.5
N7A—C8A—H8A	110.4	H2CB—C2C—H2CC	109.5
C9A—C8A—H8A	110.4	N1C—C3C—H3CA	109.5
H8B—C8A—H8A	108.6	N1C—C3C—H3CB	109.5
N5A—C9A—C8A	101.81 (15)	H3CA—C3C—H3CB	109.5
N5A—C9A—H9B	111.4	N1C—C3C—H3CC	109.5
C8A—C9A—H9B	111.4	H3CA—C3C—H3CC	109.5
N5A—C9A—H9A	111.4	H3CB—C3C—H3CC	109.5
C8A—C9A—H9A	111.4	C1D—N1D—C2D	121.24 (19)
H9B—C9A—H9A	109.3	C1D—N1D—C3D	121.4 (2)
C2B—N1B—C5B	111.22 (18)	C2D—N1D—C3D	117.33 (18)
C2B—N1B—H1B	124.7 (18)	O1D—C1D—N1D	124.8 (2)
C5B—N1B—H1B	121.5 (18)	O1D—C1D—H1D	117.6
N6B—C2B—N1B	124.5 (2)	N1D—C1D—H1D	117.6
N6B—C2B—N3B	124.5 (2)	N1D—C2D—H2DA	109.5
N1B—C2B—N3B	111.0 (2)	N1D—C2D—H2DB	109.5
C2B—N3B—C4B	110.62 (19)	H2DA—C2D—H2DB	109.5
C2B—N3B—H3B	120.9 (17)	N1D—C2D—H2DC	109.5
C4B—N3B—H3B	119.5 (18)	H2DA—C2D—H2DC	109.5
N3B—C4B—C5B	102.30 (17)	H2DB—C2D—H2DC	109.5
N3B—C4B—H4BA	111.3	N1D—C3D—H3DA	109.5
C5B—C4B—H4BA	111.3	N1D—C3D—H3DB	109.5
N3B—C4B—H4BB	111.3	H3DA—C3D—H3DB	109.5
C5B—C4B—H4BB	111.3	N1D—C3D—H3DC	109.5
H4BA—C4B—H4BB	109.2	H3DA—C3D—H3DC	109.5
N1B—C5B—C4B	102.14 (18)	H3DB—C3D—H3DC	109.5
N1B—C5B—H5BA	111.3		

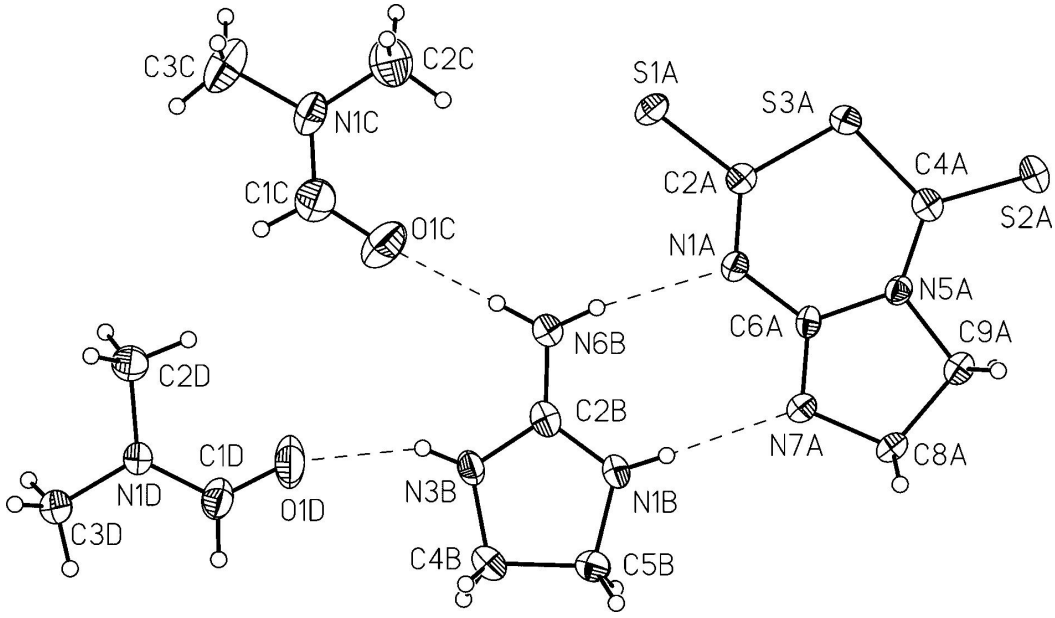
C6A—N1A—C2A—S1A	−179.33 (17)	N5A—C6A—N7A—C8A	1.1 (3)
C6A—N1A—C2A—S3A	0.8 (3)	C6A—N7A—C8A—C9A	−2.4 (3)
N1A—C2A—S3A—C4A	1.3 (2)	C4A—N5A—C9A—C8A	178.2 (2)
S1A—C2A—S3A—C4A	−178.67 (13)	C6A—N5A—C9A—C8A	−2.1 (2)
C2A—S3A—C4A—N5A	−2.1 (2)	N7A—C8A—C9A—N5A	2.6 (2)
C2A—S3A—C4A—S2A	177.92 (14)	C5B—N1B—C2B—N6B	−176.4 (2)

S2A—C4A—N5A—C6A	−178.78 (18)	C5B—N1B—C2B—N3B	4.6 (3)
S3A—C4A—N5A—C6A	1.2 (3)	N6B—C2B—N3B—C4B	−172.0 (2)
S2A—C4A—N5A—C9A	0.9 (3)	N1B—C2B—N3B—C4B	7.0 (3)
S3A—C4A—N5A—C9A	−179.10 (17)	C2B—N3B—C4B—C5B	−14.5 (3)
C2A—N1A—C6A—N7A	178.6 (2)	C2B—N1B—C5B—C4B	−13.1 (3)
C2A—N1A—C6A—N5A	−2.2 (4)	N3B—C4B—C5B—N1B	15.8 (2)
C4A—N5A—C6A—N7A	−179.6 (2)	C2C—N1C—C1C—O1C	1.0 (5)
C9A—N5A—C6A—N7A	0.7 (3)	C3C—N1C—C1C—O1C	179.9 (3)
C4A—N5A—C6A—N1A	1.1 (4)	C2D—N1D—C1D—O1D	1.5 (4)
C9A—N5A—C6A—N1A	−178.6 (2)	C3D—N1D—C1D—O1D	178.6 (3)
N1A—C6A—N7A—C8A	−179.6 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1B—H1B···N7A	0.81 (3)	2.11 (3)	2.916 (3)	178 (3)
N3B—H3B···O1D	0.81 (3)	2.07 (3)	2.806 (3)	153 (2)
N6B—H6BB···N1A	0.81 (3)	2.14 (3)	2.952 (3)	173 (3)
N6B—H6BA···O1C	0.85 (2)	1.98 (3)	2.827 (3)	174 (3)

Fig. 1


C3C
C2C
N1C
C1C
O1C
S1A
S3A
C4A
C2A
S2A
N1A
N5A
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C9A
N6B
C2D
C2B
C1D
N7A
C8A
N1D
O1D
N3B
N1B
C3D
C4B
C5B

Fig. 2