



Crystal structure of *N*-carbamothioyl-2-methylbenzamide

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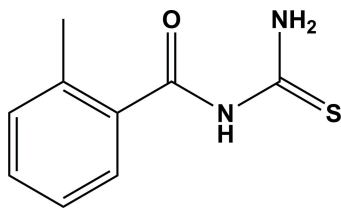
There are two molecules in the asymmetric unit of the title compound, $C_9H_{10}N_2OS$. In one, the dihedral angle between the aromatic ring and the carbamothioyl group is $52.31(7)^\circ$ and in the other it is $36.16(6)^\circ$. Each molecule features an intramolecular $N-H\cdots O$ hydrogen bond, which generates an $S(6)$ ring and the O and S atoms have an *anti* disposition. In the crystal, molecules are linked by $N-H\cdots S$ and $N-H\cdots O$ hydrogen bonds, generating separate $[130]$ and $[1\bar{3}0]$ infinite chains. Weak $C-H\cdots O$ and $C-H\cdots S$ interactions are also observed.

Keywords: crystal structure; benzamide; thiourea; hydrogen bonding.

CCDC reference: 1401733

1. Related literature

For related structures, see: Saeed & Flörke (2007); Shoukat *et al.* (2007); Hassan *et al.* (2008a,b,c); Ameram *et al.* (2015).



2. Experimental

2.1. Crystal data

$C_9H_{10}N_2OS$	$V = 3791.8(3) \text{ \AA}^3$
$M_r = 194.25$	$Z = 16$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 22.7886(12) \text{ \AA}$	$\mu = 0.30 \text{ mm}^{-1}$
$b = 7.1133(3) \text{ \AA}$	$T = 100 \text{ K}$
$c = 25.5388(13) \text{ \AA}$	$0.46 \times 0.33 \times 0.10 \text{ mm}$
$\beta = 113.664(3)^\circ$	

2.2. Data collection

Bruker APEX DUO CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2009)
 $T_{\min} = 0.814$, $T_{\max} = 0.872$

70711 measured reflections
5697 independent reflections
4862 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.110$
 $S = 1.10$
5697 reflections
261 parameters

H atoms treated by a mixture of
independent and constrained
refinement
 $\Delta\rho_{\text{max}} = 0.45 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1A-H1A\cdots S1A^i$	0.80 (2)	2.60 (2)	3.3227 (16)	151.2 (18)
$N1B-H1B\cdots S1B^{ii}$	0.84 (2)	2.65 (2)	3.4780 (14)	172 (2)
$N2A-H2A\cdots S1B^{iii}$	0.85 (2)	2.49 (2)	3.2945 (15)	157.8 (19)
$N2B-H2B\cdots O1B$	0.83 (2)	1.98 (2)	2.6404 (18)	136 (2)
$N2A-H3A\cdots O1A$	0.83 (2)	2.02 (2)	2.6515 (19)	133 (2)
$N2B-H3B\cdots S1A^{iii}$	0.89 (2)	2.49 (2)	3.3800 (14)	177 (2)
$C5B-H5BA\cdots O1A^{iv}$	0.95	2.45	3.3584 (19)	160
$C9B-H9BA\cdots S1A^i$	0.98	2.80	3.6946 (17)	152

Symmetry codes: (i) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z$; (ii) $-x + 1, -y + 1, -z$; (iii) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z$; (iv) $x + \frac{1}{2}, y + \frac{1}{2}, z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS2013* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7426).

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supporting information

Acta Cryst. (2015). E71, o425 [doi:10.1107/S2056989015009585]

Crystal structure of *N*-carbamothioyl-2-methylbenzamide

Farook Adam, Nadiah Ameram and Wai Mun Tan

S1. Introduction

In the crystal, molecules are linked by pairs of C=O—H hydrogen bonds with the methyl group from molecule (B) is facing the group from the molecule (A) forming slabs which is parallel to the benzene ring plane (A) as the bond of C6—C7 (A and B) can free to rotate.

S2. Experimental

The title compound (Fig. 1) is a benzoyl thiourea intermediate to a compound recently reported by us (Ameram *et al.*, 2015) and there is no substituent at the end of thioamide group.

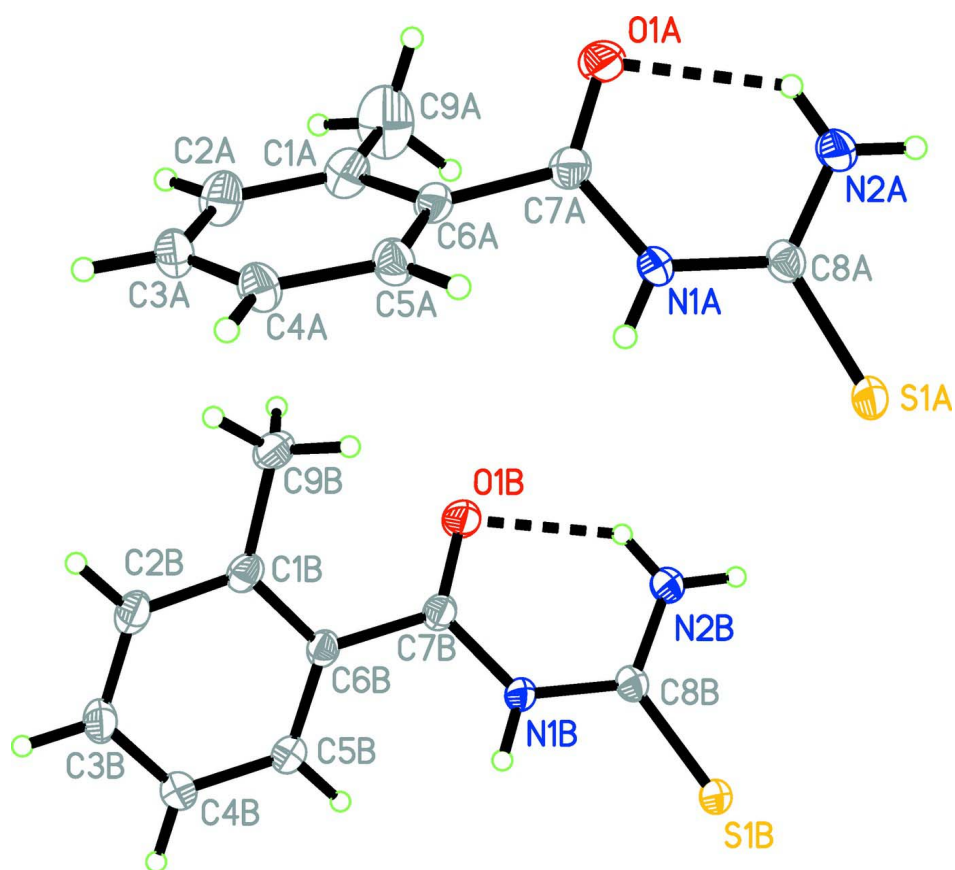
S2.1. Synthesis and crystallization

Freshly prepared substituted *o*-benzoyl chloride (13 mmol) was added dropwise to a stirred acetone solution (30 ml) of ammonium thiocyanate (13 mmol). The mixture was stirred for 10 min. A white side product which is ammonium chloride was filtered off. The compound was left at room temperature to crystallize, to yield colourless plates of the title compound.

S2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H-atoms on the N atoms were located in a difference-Fourier map and were freely refined. All other H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.96 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{aromatic C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

S3. Results and discussion

**Figure 1**

A view of the molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

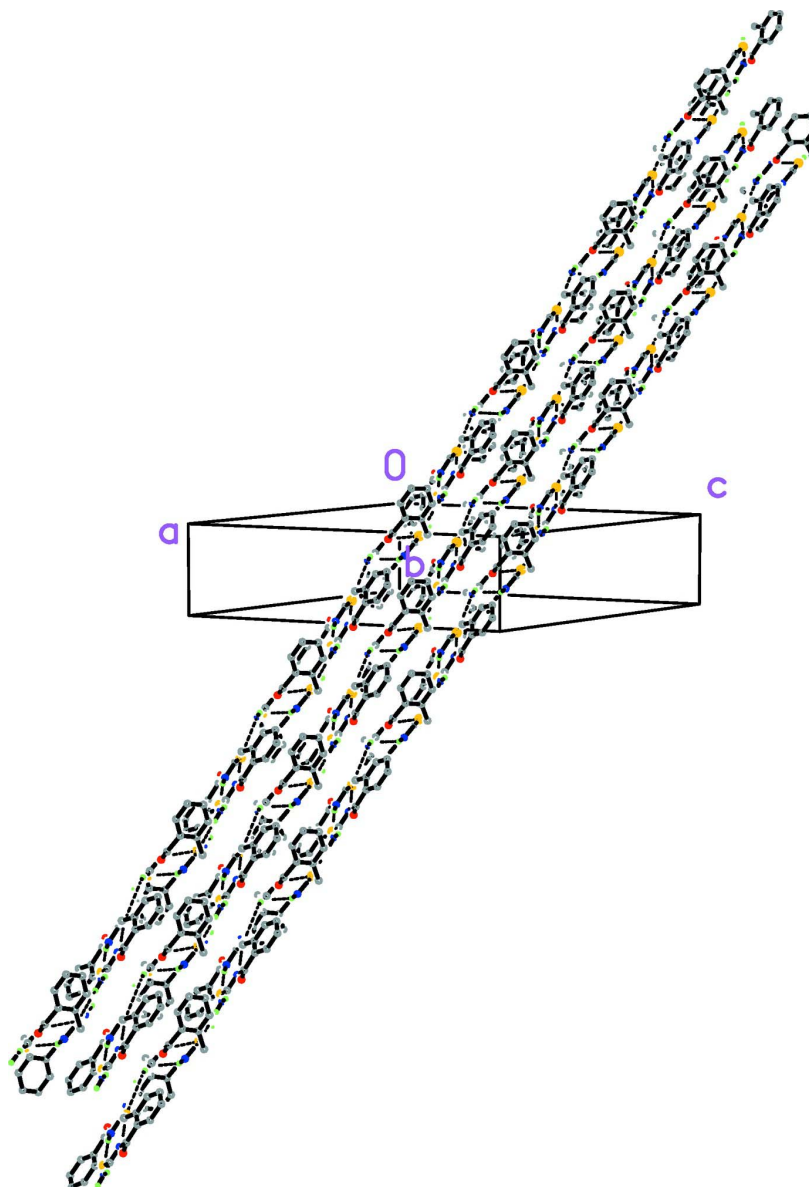


Figure 2

A view of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines (see Table 1 for details).

***N*-Carbamothioyl-2-methylbenzamide**

Crystal data

$C_9H_{10}N_2OS$

$M_r = 194.25$

Monoclinic, $C2/c$

$a = 22.7886$ (12) Å

$b = 7.1133$ (3) Å

$c = 25.5388$ (13) Å

$\beta = 113.664$ (3)°

$V = 3791.8$ (3) Å³

$Z = 16$

$F(000) = 1632$

$D_x = 1.361$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9948 reflections

$\theta = 3.0$ – 29.9°

$\mu = 0.30$ mm⁻¹

$T = 100$ K

Plate, colourless

$0.46 \times 0.33 \times 0.10$ mm

Data collection

Bruker APEX DUO CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2009)

$T_{\min} = 0.814$, $T_{\max} = 0.872$

70711 measured reflections

5697 independent reflections

4862 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\max} = 30.4^\circ$, $\theta_{\min} = 1.7^\circ$

$h = -32 \rightarrow 32$

$k = -10 \rightarrow 10$

$l = -36 \rightarrow 36$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.110$

$S = 1.10$

5697 reflections

261 parameters

0 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 4.2106P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.45 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1A	0.20453 (2)	0.37036 (5)	0.04623 (2)	0.02123 (9)
O1A	0.05447 (5)	0.09550 (16)	−0.11126 (5)	0.0285 (3)
N1A	0.15344 (6)	0.12795 (17)	−0.03834 (5)	0.0195 (2)
N2A	0.08336 (6)	0.3410 (2)	−0.02644 (7)	0.0264 (3)
C1A	0.12721 (8)	−0.1174 (2)	−0.16760 (7)	0.0255 (3)
C2A	0.14877 (8)	−0.2742 (2)	−0.18702 (7)	0.0290 (3)
H2AA	0.1428	−0.2801	−0.2260	0.035*
C3A	0.17880 (7)	−0.4224 (2)	−0.15103 (7)	0.0257 (3)
H3AA	0.1925	−0.5289	−0.1656	0.031*
C4A	0.18880 (7)	−0.4154 (2)	−0.09401 (7)	0.0239 (3)
H4AA	0.2096	−0.5165	−0.0692	0.029*
C5A	0.16820 (7)	−0.2595 (2)	−0.07329 (6)	0.0215 (3)
H5AA	0.1756	−0.2531	−0.0340	0.026*
C6A	0.13688 (7)	−0.11301 (19)	−0.10979 (6)	0.0190 (3)
C7A	0.11026 (7)	0.0452 (2)	−0.08773 (6)	0.0202 (3)
C8A	0.14215 (7)	0.27880 (19)	−0.00939 (6)	0.0186 (3)
C9A	0.09650 (12)	0.0421 (3)	−0.20800 (9)	0.0462 (5)
H9AA	0.1169	0.1608	−0.1906	0.069*
H9AB	0.0507	0.0472	−0.2159	0.069*
H9AC	0.1019	0.0222	−0.2438	0.069*
S1B	0.45007 (2)	0.73146 (5)	−0.00298 (2)	0.02408 (10)

O1B	0.31413 (5)	0.45230 (16)	−0.16642 (5)	0.0258 (2)
N1B	0.40643 (6)	0.47799 (17)	−0.08568 (5)	0.0187 (2)
N2B	0.33660 (6)	0.71847 (19)	−0.08869 (6)	0.0227 (3)
C1B	0.35431 (7)	0.0654 (2)	−0.17791 (6)	0.0199 (3)
C2B	0.38290 (8)	−0.0911 (2)	−0.19102 (6)	0.0240 (3)
H2BA	0.3574	−0.1983	−0.2076	0.029*
C3B	0.44736 (8)	−0.0943 (2)	−0.18057 (7)	0.0278 (3)
H3BA	0.4653	−0.2025	−0.1903	0.033*
C4B	0.48592 (7)	0.0595 (2)	−0.15600 (7)	0.0276 (3)
H4BA	0.5300	0.0586	−0.1496	0.033*
C5B	0.45933 (7)	0.2151 (2)	−0.14083 (6)	0.0231 (3)
H5BA	0.4856	0.3203	−0.1234	0.028*
C6B	0.39425 (7)	0.2184 (2)	−0.15102 (6)	0.0184 (3)
C7B	0.36692 (7)	0.3907 (2)	−0.13618 (6)	0.0190 (3)
C8B	0.39349 (6)	0.64135 (19)	−0.06277 (6)	0.0177 (3)
C9B	0.28310 (7)	0.0629 (2)	−0.19377 (7)	0.0244 (3)
H9BA	0.2741	0.1143	−0.1622	0.037*
H9BB	0.2674	−0.0667	−0.2014	0.037*
H9BC	0.2615	0.1396	−0.2281	0.037*
H1B	0.4428 (11)	0.433 (3)	−0.0664 (9)	0.038 (6)*
H3A	0.0543 (11)	0.291 (3)	−0.0542 (10)	0.039 (6)*
H1A	0.1904 (10)	0.102 (3)	−0.0300 (8)	0.028 (5)*
H3B	0.3275 (10)	0.827 (3)	−0.0763 (9)	0.037 (6)*
H2B	0.3111 (11)	0.667 (3)	−0.1184 (10)	0.039 (6)*
H2A	0.0765 (10)	0.437 (3)	−0.0096 (9)	0.038 (6)*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.02084 (16)	0.02238 (18)	0.01948 (17)	0.00473 (13)	0.00704 (13)	−0.00419 (13)
O1A	0.0193 (5)	0.0211 (5)	0.0368 (6)	0.0039 (4)	0.0025 (4)	−0.0060 (5)
N1A	0.0165 (5)	0.0181 (6)	0.0231 (6)	0.0031 (4)	0.0070 (5)	−0.0040 (5)
N2A	0.0192 (6)	0.0210 (6)	0.0374 (8)	0.0021 (5)	0.0098 (6)	−0.0096 (6)
C1A	0.0309 (8)	0.0211 (7)	0.0227 (7)	−0.0002 (6)	0.0089 (6)	0.0015 (6)
C2A	0.0364 (8)	0.0294 (8)	0.0220 (7)	0.0000 (7)	0.0127 (6)	−0.0030 (6)
C3A	0.0257 (7)	0.0225 (7)	0.0313 (8)	−0.0003 (6)	0.0140 (6)	−0.0073 (6)
C4A	0.0245 (7)	0.0184 (7)	0.0281 (8)	0.0049 (5)	0.0100 (6)	0.0013 (6)
C5A	0.0232 (7)	0.0197 (7)	0.0211 (7)	0.0037 (5)	0.0085 (5)	0.0004 (5)
C6A	0.0187 (6)	0.0152 (6)	0.0213 (7)	−0.0007 (5)	0.0062 (5)	−0.0021 (5)
C7A	0.0203 (6)	0.0143 (6)	0.0242 (7)	−0.0003 (5)	0.0070 (5)	−0.0004 (5)
C8A	0.0198 (6)	0.0153 (6)	0.0225 (7)	0.0004 (5)	0.0104 (5)	−0.0004 (5)
C9A	0.0681 (14)	0.0369 (10)	0.0309 (9)	0.0167 (10)	0.0169 (9)	0.0128 (8)
S1B	0.01921 (17)	0.02226 (18)	0.02552 (19)	0.00457 (13)	0.00349 (14)	−0.00916 (14)
O1B	0.0238 (5)	0.0242 (5)	0.0222 (5)	0.0056 (4)	0.0017 (4)	−0.0022 (4)
N1B	0.0178 (5)	0.0167 (5)	0.0182 (6)	0.0029 (4)	0.0035 (4)	−0.0036 (4)
N2B	0.0201 (6)	0.0209 (6)	0.0231 (6)	0.0052 (5)	0.0044 (5)	−0.0038 (5)
C1B	0.0230 (6)	0.0196 (7)	0.0142 (6)	−0.0007 (5)	0.0045 (5)	−0.0002 (5)
C2B	0.0297 (7)	0.0183 (7)	0.0200 (7)	−0.0002 (6)	0.0059 (6)	−0.0032 (5)

C3B	0.0304 (8)	0.0240 (7)	0.0248 (7)	0.0073 (6)	0.0068 (6)	−0.0060 (6)
C4B	0.0220 (7)	0.0303 (8)	0.0277 (8)	0.0038 (6)	0.0069 (6)	−0.0079 (6)
C5B	0.0223 (7)	0.0227 (7)	0.0216 (7)	−0.0004 (5)	0.0059 (5)	−0.0056 (6)
C6B	0.0215 (6)	0.0174 (6)	0.0147 (6)	0.0015 (5)	0.0056 (5)	−0.0012 (5)
C7B	0.0207 (6)	0.0171 (6)	0.0179 (6)	−0.0005 (5)	0.0063 (5)	−0.0020 (5)
C8B	0.0188 (6)	0.0155 (6)	0.0195 (6)	0.0015 (5)	0.0083 (5)	−0.0003 (5)
C9B	0.0227 (7)	0.0265 (8)	0.0216 (7)	−0.0043 (6)	0.0063 (6)	−0.0044 (6)

Geometric parameters (Å, °)

S1A—C8A	1.6858 (15)	S1B—C8B	1.6806 (14)
O1A—C7A	1.2215 (17)	O1B—C7B	1.2207 (17)
N1A—C7A	1.3818 (19)	N1B—C8B	1.3850 (18)
N1A—C8A	1.3845 (18)	N1B—C7B	1.3883 (18)
N1A—H1A	0.80 (2)	N1B—H1B	0.84 (2)
N2A—C8A	1.3083 (18)	N2B—C8B	1.3156 (18)
N2A—H3A	0.83 (2)	N2B—H3B	0.89 (2)
N2A—H2A	0.86 (2)	N2B—H2B	0.83 (2)
C1A—C2A	1.388 (2)	C1B—C2B	1.397 (2)
C1A—C6A	1.403 (2)	C1B—C6B	1.408 (2)
C1A—C9A	1.504 (2)	C1B—C9B	1.507 (2)
C2A—C3A	1.385 (2)	C2B—C3B	1.384 (2)
C2A—H2AA	0.9500	C2B—H2BA	0.9500
C3A—C4A	1.381 (2)	C3B—C4B	1.386 (2)
C3A—H3AA	0.9500	C3B—H3BA	0.9500
C4A—C5A	1.389 (2)	C4B—C5B	1.390 (2)
C4A—H4AA	0.9500	C4B—H4BA	0.9500
C5A—C6A	1.389 (2)	C5B—C6B	1.399 (2)
C5A—H5AA	0.9500	C5B—H5BA	0.9500
C6A—C7A	1.492 (2)	C6B—C7B	1.4909 (19)
C9A—H9AA	0.9800	C9B—H9BA	0.9800
C9A—H9AB	0.9800	C9B—H9BB	0.9800
C9A—H9AC	0.9800	C9B—H9BC	0.9800
C7A—N1A—C8A	126.92 (12)	C8B—N1B—C7B	126.81 (12)
C7A—N1A—H1A	115.6 (14)	C8B—N1B—H1B	113.6 (15)
C8A—N1A—H1A	115.7 (14)	C7B—N1B—H1B	119.6 (15)
C8A—N2A—H3A	119.9 (16)	C8B—N2B—H3B	120.3 (14)
C8A—N2A—H2A	118.2 (14)	C8B—N2B—H2B	117.4 (16)
H3A—N2A—H2A	122 (2)	H3B—N2B—H2B	122 (2)
C2A—C1A—C6A	117.74 (14)	C2B—C1B—C6B	117.41 (13)
C2A—C1A—C9A	119.66 (15)	C2B—C1B—C9B	118.81 (13)
C6A—C1A—C9A	122.58 (15)	C6B—C1B—C9B	123.77 (13)
C3A—C2A—C1A	121.71 (15)	C3B—C2B—C1B	121.89 (14)
C3A—C2A—H2AA	119.1	C3B—C2B—H2BA	119.1
C1A—C2A—H2AA	119.1	C1B—C2B—H2BA	119.1
C4A—C3A—C2A	120.05 (14)	C2B—C3B—C4B	120.35 (14)
C4A—C3A—H3AA	120.0	C2B—C3B—H3BA	119.8

C2A—C3A—H3AA	120.0	C4B—C3B—H3BA	119.8
C3A—C4A—C5A	119.48 (14)	C3B—C4B—C5B	119.14 (14)
C3A—C4A—H4AA	120.3	C3B—C4B—H4BA	120.4
C5A—C4A—H4AA	120.3	C5B—C4B—H4BA	120.4
C4A—C5A—C6A	120.29 (14)	C4B—C5B—C6B	120.64 (14)
C4A—C5A—H5AA	119.9	C4B—C5B—H5BA	119.7
C6A—C5A—H5AA	119.9	C6B—C5B—H5BA	119.7
C5A—C6A—C1A	120.71 (13)	C5B—C6B—C1B	120.48 (13)
C5A—C6A—C7A	119.33 (13)	C5B—C6B—C7B	119.09 (13)
C1A—C6A—C7A	119.88 (13)	C1B—C6B—C7B	120.34 (13)
O1A—C7A—N1A	122.93 (13)	O1B—C7B—N1B	122.28 (13)
O1A—C7A—C6A	122.40 (13)	O1B—C7B—C6B	122.72 (13)
N1A—C7A—C6A	114.67 (12)	N1B—C7B—C6B	115.00 (12)
N2A—C8A—N1A	117.98 (13)	N2B—C8B—N1B	118.11 (13)
N2A—C8A—S1A	123.67 (12)	N2B—C8B—S1B	122.68 (11)
N1A—C8A—S1A	118.34 (10)	N1B—C8B—S1B	119.21 (10)
C1A—C9A—H9AA	109.5	C1B—C9B—H9BA	109.5
C1A—C9A—H9AB	109.5	C1B—C9B—H9BB	109.5
H9AA—C9A—H9AB	109.5	H9BA—C9B—H9BB	109.5
C1A—C9A—H9AC	109.5	C1B—C9B—H9BC	109.5
H9AA—C9A—H9AC	109.5	H9BA—C9B—H9BC	109.5
H9AB—C9A—H9AC	109.5	H9BB—C9B—H9BC	109.5
C6A—C1A—C2A—C3A	0.1 (2)	C6B—C1B—C2B—C3B	−2.8 (2)
C9A—C1A—C2A—C3A	178.34 (18)	C9B—C1B—C2B—C3B	176.38 (14)
C1A—C2A—C3A—C4A	−0.9 (3)	C1B—C2B—C3B—C4B	0.5 (2)
C2A—C3A—C4A—C5A	0.4 (2)	C2B—C3B—C4B—C5B	1.4 (3)
C3A—C4A—C5A—C6A	1.0 (2)	C3B—C4B—C5B—C6B	−1.0 (2)
C4A—C5A—C6A—C1A	−1.9 (2)	C4B—C5B—C6B—C1B	−1.3 (2)
C4A—C5A—C6A—C7A	174.80 (13)	C4B—C5B—C6B—C7B	−177.71 (14)
C2A—C1A—C6A—C5A	1.3 (2)	C2B—C1B—C6B—C5B	3.2 (2)
C9A—C1A—C6A—C5A	−176.90 (17)	C9B—C1B—C6B—C5B	−175.98 (14)
C2A—C1A—C6A—C7A	−175.35 (14)	C2B—C1B—C6B—C7B	179.53 (13)
C9A—C1A—C6A—C7A	6.5 (2)	C9B—C1B—C6B—C7B	0.4 (2)
C8A—N1A—C7A—O1A	−2.2 (2)	C8B—N1B—C7B—O1B	−0.6 (2)
C8A—N1A—C7A—C6A	178.65 (13)	C8B—N1B—C7B—C6B	178.45 (13)
C5A—C6A—C7A—O1A	−126.72 (16)	C5B—C6B—C7B—O1B	139.95 (15)
C1A—C6A—C7A—O1A	50.0 (2)	C1B—C6B—C7B—O1B	−36.5 (2)
C5A—C6A—C7A—N1A	52.41 (18)	C5B—C6B—C7B—N1B	−39.13 (19)
C1A—C6A—C7A—N1A	−130.91 (15)	C1B—C6B—C7B—N1B	144.47 (13)
C7A—N1A—C8A—N2A	7.1 (2)	C7B—N1B—C8B—N2B	4.7 (2)
C7A—N1A—C8A—S1A	−173.59 (12)	C7B—N1B—C8B—S1B	−176.08 (12)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1A—H1A $\cdots$ S1A ⁱ	0.80 (2)	2.60 (2)	3.3227 (16)	151.2 (18)
N1B—H1B $\cdots$ S1B ⁱⁱ	0.84 (2)	2.65 (2)	3.4780 (14)	172 (2)

N2 <i>A</i> —H2 <i>A</i> ...S1 <i>B</i> ⁱⁱⁱ	0.85 (2)	2.49 (2)	3.2945 (15)	157.8 (19)
N2 <i>B</i> —H2 <i>B</i> ...O1 <i>B</i>	0.83 (2)	1.98 (2)	2.6404 (18)	136 (2)
N2 <i>A</i> —H3 <i>A</i> ...O1 <i>A</i>	0.83 (2)	2.02 (2)	2.6515 (19)	133 (2)
N2 <i>B</i> —H3 <i>B</i> ...S1 <i>A</i> ⁱⁱⁱ	0.89 (2)	2.49 (2)	3.3800 (14)	177 (2)
C5 <i>B</i> —H5 <i>B</i> <i>A</i> ...O1 <i>A</i> ^{iv}	0.95	2.45	3.3584 (19)	160
C9 <i>B</i> —H9 <i>B</i> <i>A</i> ...S1 <i>A</i> ⁱ	0.98	2.80	3.6946 (17)	152

Symmetry codes: (i) $-x+1/2, -y+1/2, -z$; (ii) $-x+1, -y+1, -z$; (iii) $-x+1/2, -y+3/2, -z$; (iv) $x+1/2, y+1/2, z$.