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

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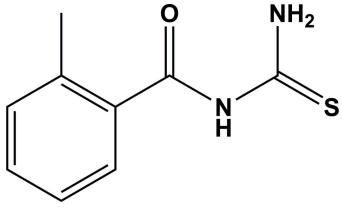
There are two molecules in the asymmetric unit of the title compound, $C_9H_{10}N_2OS$. In one, the dihedral angle between the aromatic ring and the carbamothioyl group is 52.31 (7)° and in the other it is 36.16 (6)°. Each molecule features an intramolecular N—H···O hydrogen bond, which generates an *S*(6) ring and the O and S atoms have an *anti* disposition. In the crystal, molecules are linked by N—H···S and N—H···O hydrogen bonds, generating separate [130] and [1$\bar{3}$0] infinite chains. Weak C—H···O and C—H···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.* (2008*a*,*b*,*c*); Ameram *et al.* (2015).




## 2. Experimental

### 2.1. 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) Å$^3$
$Z$ = 16
Mo $K\alpha$ radiation
$\mu$ = 0.30 mm$^{-1}$
$T$ = 100 K
0.46 × 0.33 × 0.10 mm

### 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 $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.45 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1$A$—H1$A$···S1$A^{i}$ | 0.80 (2) | 2.60 (2) | 3.3227 (16) | 151.2 (18) |
| N1$B$—H1$B$···S1$B^{ii}$ | 0.84 (2) | 2.65 (2) | 3.4780 (14) | 172 (2) |
| N2$A$—H2$A$···S1$B^{iii}$ | 0.85 (2) | 2.49 (2) | 3.2945 (15) | 157.8 (19) |
| N2$B$—H2$B$···O1$B$ | 0.83 (2) | 1.98 (2) | 2.6404 (18) | 136 (2) |
| N2$A$—H3$A$···O1$A$ | 0.83 (2) | 2.02 (2) | 2.6515 (19) | 133 (2) |
| N2$B$—H3$B$···S1$A^{iii}$ | 0.89 (2) | 2.49 (2) | 3.3800 (14) | 177 (2) |
| C5$B$—H5$BA$···O1$A^{iv}$ | 0.95 | 2.45 | 3.3584 (19) | 160 |
| C9$B$—H9$BA$···S1$A^{i}$ | 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).

## Acknowledgements

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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). E**71**, 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 $U_{iso}$(H) = 1.2$U_{eq}$(aromatic C) or 1.5$U_{eq}$(methyl C).

## S3. Results and discussion

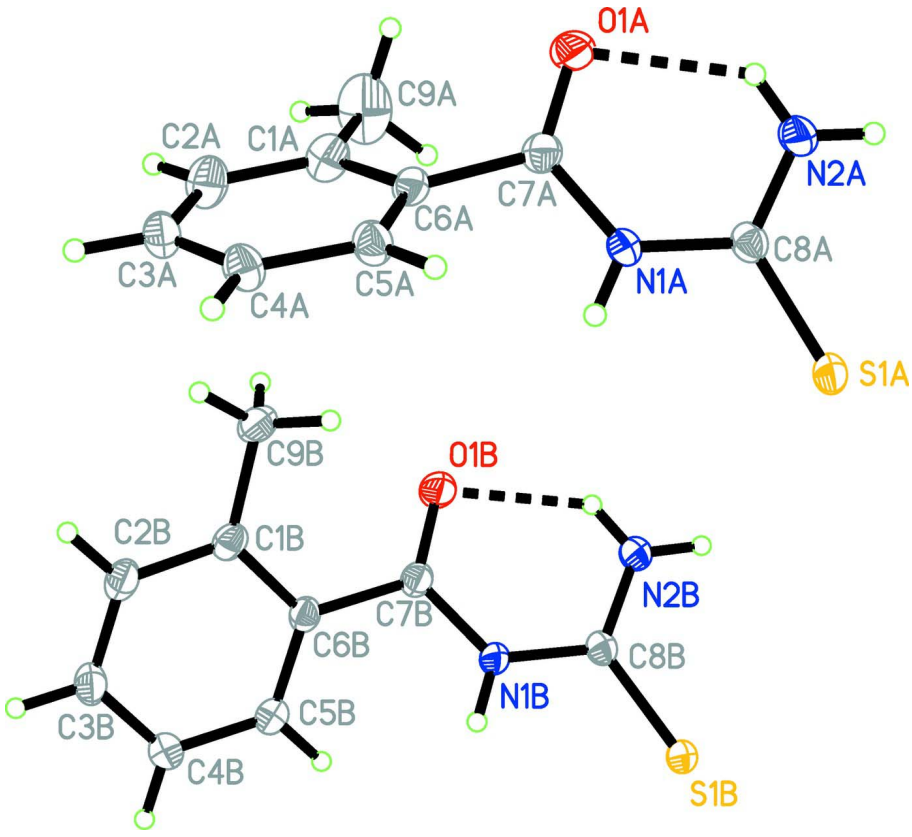


**Figure 1**

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

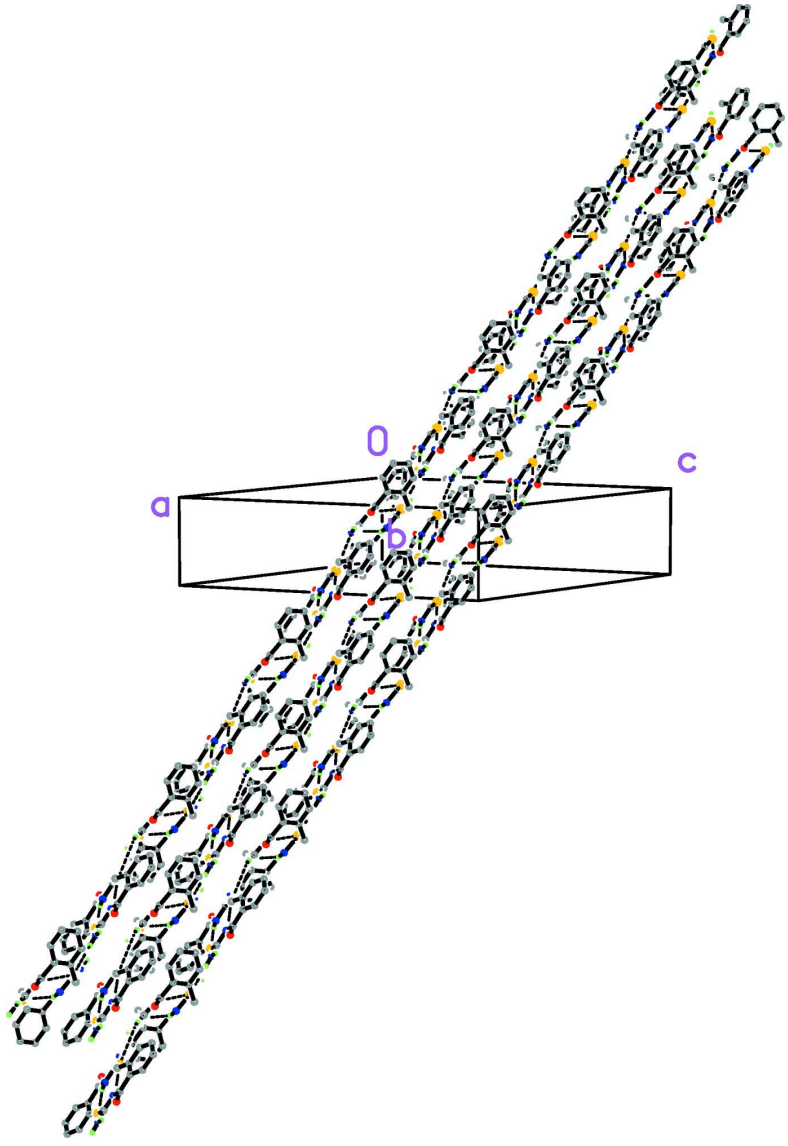


**Figure 2**

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
$\beta = 113.664\ (3)°$
$V = 3791.8\ (3)$ Å$^3$
$Z = 16$
$F(000) = 1632$
$D_x = 1.361$ 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 × 0.33 × 0.10 mm

*Data collection*

Bruker APEX DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ 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 $I > 2\sigma(I)$
$R_{int}$ = 0.051
$\theta_{max}$ = 30.4°, $\theta_{min}$ = 1.7°
$h$ = −32→32
$k$ = −10→10
$l$ = −36→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 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

*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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1*A*—H1*A*···S1*A*$^{i}$ | 0.80 (2) | 2.60 (2) | 3.3227 (16) | 151.2 (18) |
| N1*B*—H1*B*···S1*B*$^{ii}$ | 0.84 (2) | 2.65 (2) | 3.4780 (14) | 172 (2) |

| | | | | |
|---|---|---|---|---|
| N2*A*—H2*A*···S1*B*$^{iii}$ | 0.85 (2) | 2.49 (2) | 3.2945 (15) | 157.8 (19) |
| N2*B*—H2*B*···O1*B* | 0.83 (2) | 1.98 (2) | 2.6404 (18) | 136 (2) |
| N2*A*—H3*A*···O1*A* | 0.83 (2) | 2.02 (2) | 2.6515 (19) | 133 (2) |
| N2*B*—H3*B*···S1*A*$^{iii}$ | 0.89 (2) | 2.49 (2) | 3.3800 (14) | 177 (2) |
| C5*B*—H5*BA*···O1*A*$^{iv}$ | 0.95 | 2.45 | 3.3584 (19) | 160 |
| C9*B*—H9*BA*···S1*A*$^{i}$ | 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) $x+1/2, y+1/2, z$.