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## Structure Reports

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## 1-Methyl-3-phenylimidazolidine-2-thione

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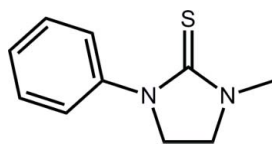
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.033;  $wR$  factor = 0.090; data-to-parameter ratio = 16.6.

The asymmetric unit of the title cyclic thiourea derivative,  $\text{C}_{10}\text{H}_{12}\text{N}_2\text{S}$ , comprises two molecules, each of which has a twist about the  $\text{CH}_2-\text{CH}_2$  bond within the five-membered ring. The major difference between the independent molecules is manifested in the relative orientations of the five- and six-membered rings [dihedral angles between the least-squares planes =  $28.03$  (11) and  $41.54$  (11) $^\circ$ ]. A network of  $\text{C}-\text{H}\cdots\pi$  interactions consolidates the three-dimensional crystal packing.

## Related literature

For the biological activity of phosphinegold(I) species of related molecules, see: Henderson *et al.* (2006). For the structure of dimethyl-2-imidazolidinethione, see: Chieh & Cheung (1983).



## Experimental

## Crystal data

$\text{C}_{10}\text{H}_{12}\text{N}_2\text{S}$	$V = 1922.12$ (6) Å <sup>3</sup>
$M_r = 192.28$	$Z = 8$
Orthorhombic, $P2_12_12_1$	Cu $K\alpha$ radiation
$a = 7.5159$ (1) Å	$\mu = 2.59$ mm <sup>-1</sup>
$b = 14.0478$ (3) Å	$T = 100$ K
$c = 18.2050$ (3) Å	$0.20 \times 0.10 \times 0.05$ mm

## Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector  
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)  
 $T_{\min} = 0.427$ ,  $T_{\max} = 1.000$

7245 measured reflections  
3955 independent reflections  
3814 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$   
 $wR(F^2) = 0.090$   
 $S = 1.08$   
3955 reflections  
238 parameters  
H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.39$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983),  
1665 Friedel pairs  
Absolute structure parameter:  
0.117 (14)

Table 1

Hydrogen-bond geometry (Å,  $^\circ$ ).

Cg1 and Cg2 are the centroids of the C5–C10 and C15–C20 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C11–H11C $\cdots$ Cg1 <sup>i</sup>	0.98	2.96	3.759 (2)	140
C19–H19 $\cdots$ Cg1 <sup>ii</sup>	0.95	2.85	3.612 (2)	138
C6–H6 $\cdots$ Cg2 <sup>iii</sup>	0.95	2.89	3.719 (2)	147
C17–H17 $\cdots$ Cg2 <sup>iv</sup>	0.95	2.76	3.577 (2)	144

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

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), Gans & Shalloway (2001) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5384).

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## supporting information

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## 1-Methyl-3-phenylimidazolidine-2-thione

Nabihah Al Muna Mohd Nor, Zanariah Abdullah, Seik Weng Ng and Edward R. T. Tiekink

### S1. Structural commentary

In connection with studies of the biological activities of phosphine gold(I) species of functionalized thiourea derivatives (Henderson *et al.*, 2006), the title compound, (I), was synthesised. The crystallographic asymmetric unit contains two independent molecules, Fig. 1. Each molecule is twisted about the CH<sub>2</sub>—CH<sub>2</sub> bond. From the overlay diagram of the S1-containing molecule with the inverted S2-containing molecule, Fig. 2, only a small difference in the relative orientations of the phenyl groups is noted, as quantified in the C2—N2—C5—C10 and C12—N4—C15—C20 torsion angles of 35.6 (3) and -42.8 (3)°, respectively. The twisted conformation in (I) contrasts the near planar structure of the dimethyl-2-imidazolidinethione derivative (Chieh & Cheung, 1983).

The three-dimensional crystal packing is sustained by C—H··· $\pi$  interactions, Table 1, involving phenyl- and methyl-H interacting with each of the phenyl rings, with each ring accepting two interactions, Fig. 3.

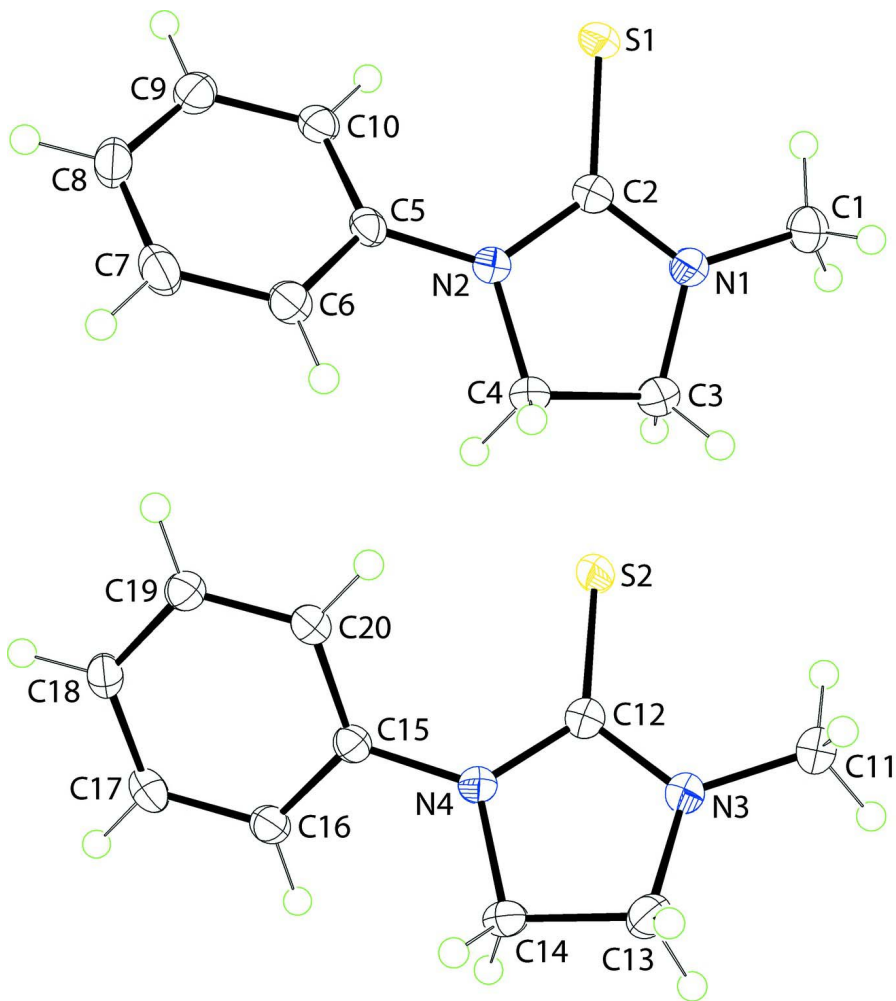
### S2. Synthesis and crystallization

The title compound, (I), was prepared in two steps. 2-Methylamino ethanol (10 mmol, 0.82 ml) was dissolved in absolute ethanol (5 ml). Phenyl isothiocyanate (10.1 mmol, 1.24 ml) was added drop wise to the solution over 30 mins. The solution changed from colourless to light-yellow and left to stir for 3 h. Distilled water was added to the mixture resulting in a white precipitate. The precipitate was filtered off and washed with distilled water and a small amount of diethyl ether. Yield: 90% (1.8923 g, 8.9981 mmol) of white powder. The crystals are obtained from slow evaporation of this powder in absolute ethanol. M.pt: 375.8–376.0 K. This powder was subsequently used in the next reaction.

1-(2-Hydroxyethyl)-1-methyl-3-phenylthiourea (9.03 mmol, 1.8963 g) was dissolved in dry THF (7 ml). Sodium hydride (9 mmol, 0.36 g) in dry THF (6 ml) was added drop wise at room temperature, under nitrogen and with stirring for 1 h. The solvent was removed and the white powder was washed with diethyl ether, and taken up in DMSO (4 ml). Phenyl isothiocyanate (4 mmol, 0.48 ml) was added drop wise to the solution. The mixture was heated at 323 K and stirred for 5 h. A clear yellow solution was observed which was cooled to room temperature. Cold distilled water was added with further stirring for 30 min. whereupon a yellow precipitate formed. The precipitate was filtered off and washed with water and hexane. Yield: 71% (0.5469 g, 2.8443 mmol) of a white powder. Crystals were obtained by slow evaporation from its absolute ethanol solution; M.pt: 404.7–404.9 K. IR ( $\nu_{\max}$ , cm<sup>-1</sup>): 2977 and 2899 (CH<sub>2</sub>), 1085 (C=S), 1613, 1598 and 1565 (aromatic C=C). <sup>1</sup>H NMR (CDCl<sub>3</sub>):  $\delta$  3.42 (*d*, CH<sub>3</sub>, 6.76 Hz), 3.64 (*t*, CH<sub>2</sub>, 4.12 Hz), 3.92 (*t*, CH<sub>2</sub>, 4.32 Hz), 7.13 (*t*, aromatic-H, 7.24 Hz), 7.31 (*t*, aromatic-H, 7.38 Hz), 7.39 (*d*, aromatic-H, 7.80 Hz) ppm.

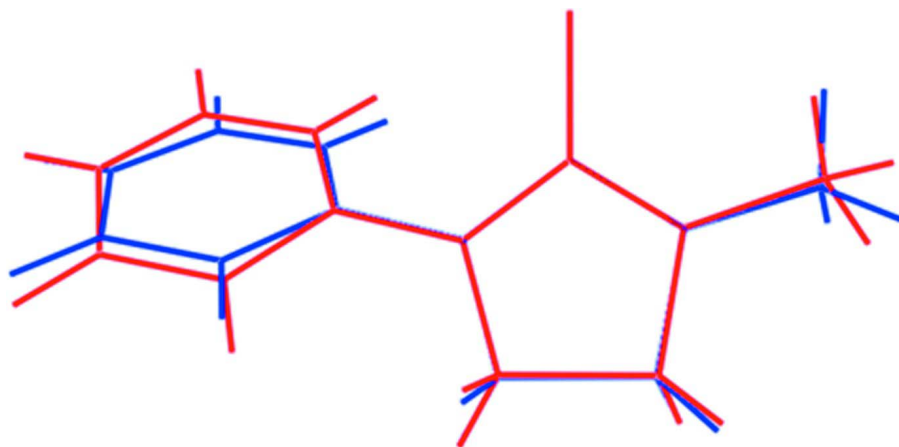
### S3. Refinement

The C-bound H atoms were geometrically placed (C—H = 0.93–0.98 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$ . Owing to poor agreement, two reflections, *i.e.* (2 0 1) and (4 0 1), were omitted from the final cycles of refinement. The studied crystal is a racemic twin with the minor component being 0.117 (14).



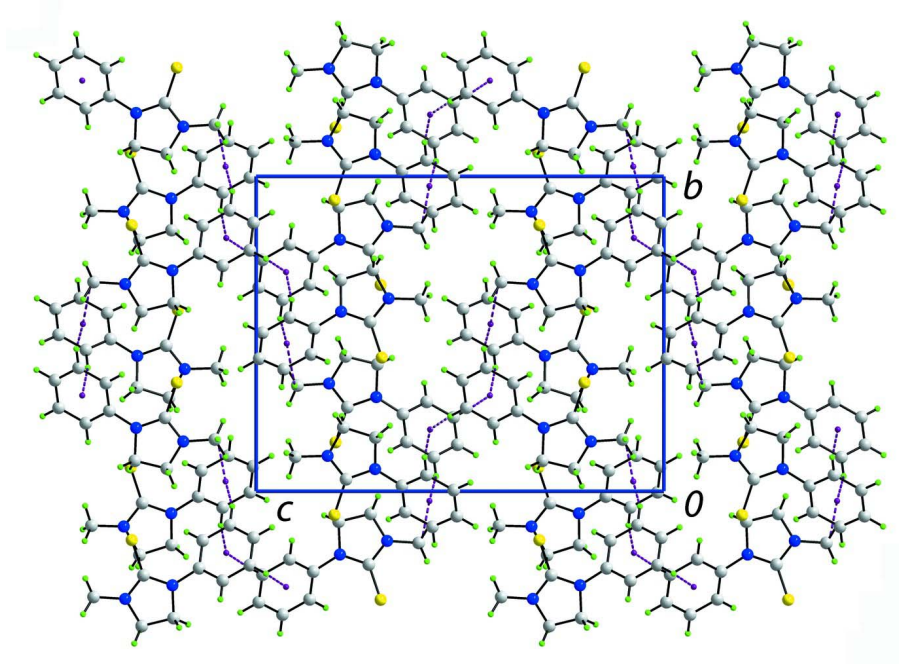
**Figure 1**

The molecular structure of the two independent molecules comprising the asymmetric unit in (I), showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.



**Figure 2**

Overlay diagram of the S1-containing (red image) and inverted S2-containing (blue) molecules drawn so that the heteroatoms overlap.



**Figure 3**

A view of the unit-cell contents of (I) in projection down the *a* axis. The C—H... $\pi$  interactions are shown as purple dashed lines.

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#### *Crystal data*

$C_{10}H_{12}N_2S$

$M_r = 192.28$

Orthorhombic,  $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 7.5159 (1) \text{ \AA}$

$b = 14.0478 (3) \text{ \AA}$

$c = 18.2050 (3) \text{ \AA}$

$V = 1922.12 (6) \text{ \AA}^3$

$Z = 8$

$F(000) = 816$

$D_x = 1.329 \text{ Mg m}^{-3}$   
 Cu  $K\alpha$  radiation,  $\lambda = 1.54184 \text{ \AA}$   
 Cell parameters from 3909 reflections  
 $\theta = 4.0\text{--}76.3^\circ$

$\mu = 2.59 \text{ mm}^{-1}$   
 $T = 100 \text{ K}$   
 Prism, colourless  
 $0.20 \times 0.10 \times 0.05 \text{ mm}$

*Data collection*

Agilent SuperNova Dual  
 diffractometer with an Atlas detector  
 Radiation source: SuperNova (Cu) X-ray  
 Source  
 Mirror monochromator  
 Detector resolution:  $10.4041 \text{ pixels mm}^{-1}$   
 $\omega$  scan  
 Absorption correction: multi-scan  
 (CrysAlis PRO; Agilent, 2013)

$T_{\min} = 0.427$ ,  $T_{\max} = 1.000$   
 7245 measured reflections  
 3955 independent reflections  
 3814 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$   
 $\theta_{\max} = 76.5^\circ$ ,  $\theta_{\min} = 4.0^\circ$   
 $h = -9 \rightarrow 9$   
 $k = -16 \rightarrow 17$   
 $l = -22 \rightarrow 22$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.033$   
 $wR(F^2) = 0.090$   
 $S = 1.08$   
 3955 reflections  
 238 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-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.4944P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.39 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.26 \text{ e \AA}^{-3}$   
 Absolute structure: Flack (1983), 1665 Friedel  
 pairs  
 Absolute structure parameter: 0.117 (14)

*Special details*

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.95401 (6)	0.92442 (3)	0.80811 (2)	0.02271 (12)
N1	0.9949 (2)	1.11210 (11)	0.82471 (8)	0.0216 (3)
N2	0.9877 (2)	1.07023 (11)	0.70835 (8)	0.0185 (3)
C1	0.9816 (3)	1.10938 (15)	0.90394 (10)	0.0291 (4)
H1A	0.9392	1.0465	0.9194	0.044*
H1B	0.8978	1.1583	0.9205	0.044*
H1C	1.0989	1.1215	0.9255	0.044*
C2	0.9780 (3)	1.03784 (13)	0.77947 (10)	0.0188 (4)
C3	1.0070 (3)	1.20270 (13)	0.78616 (10)	0.0229 (4)
H3A	1.1056	1.2422	0.8055	0.027*

H3B	0.8943	1.2389	0.7896	0.027*
C4	1.0434 (3)	1.17071 (13)	0.70745 (10)	0.0212 (4)
H4A	0.9724	1.2081	0.6719	0.025*
H4B	1.1711	1.1768	0.6951	0.025*
C5	0.9852 (2)	1.01694 (13)	0.64236 (9)	0.0185 (4)
C6	1.0800 (3)	1.05145 (13)	0.58225 (10)	0.0228 (4)
H6	1.1489	1.1078	0.5869	0.027*
C7	1.0738 (3)	1.00333 (15)	0.51530 (11)	0.0275 (4)
H7	1.1380	1.0275	0.4744	0.033*
C8	0.9753 (3)	0.92088 (14)	0.50772 (10)	0.0278 (4)
H8	0.9729	0.8878	0.4622	0.033*
C9	0.8798 (3)	0.88714 (14)	0.56760 (11)	0.0253 (4)
H9	0.8117	0.8305	0.5626	0.030*
C10	0.8816 (3)	0.93438 (13)	0.63471 (10)	0.0211 (4)
H10	0.8137	0.9111	0.6749	0.025*
S2	1.01213 (7)	0.84486 (3)	0.30525 (2)	0.02324 (12)
N4	0.9717 (2)	0.70117 (11)	0.20545 (8)	0.0194 (3)
N3	0.9499 (2)	0.65787 (11)	0.32123 (8)	0.0217 (3)
C11	0.9083 (3)	0.66426 (14)	0.39877 (10)	0.0261 (4)
H11A	0.9590	0.7230	0.4190	0.039*
H11B	0.9588	0.6093	0.4245	0.039*
H11C	0.7789	0.6649	0.4053	0.039*
C12	0.9758 (3)	0.73296 (13)	0.27636 (9)	0.0184 (4)
C13	0.9028 (3)	0.57188 (14)	0.28070 (10)	0.0250 (4)
H13A	0.7737	0.5585	0.2843	0.030*
H13B	0.9700	0.5161	0.2989	0.030*
C14	0.9557 (3)	0.59672 (12)	0.20238 (10)	0.0216 (4)
H14A	1.0703	0.5667	0.1888	0.026*
H14B	0.8631	0.5768	0.1669	0.026*
C15	0.9922 (3)	0.75522 (13)	0.13998 (9)	0.0180 (4)
C16	1.0888 (3)	0.71622 (13)	0.08195 (10)	0.0212 (4)
H16	1.1459	0.6564	0.0877	0.025*
C17	1.1016 (3)	0.76506 (14)	0.01552 (10)	0.0231 (4)
H17	1.1672	0.7381	-0.0239	0.028*
C18	1.0197 (3)	0.85249 (13)	0.00654 (9)	0.0209 (4)
H18	1.0286	0.8854	-0.0389	0.025*
C19	0.9240 (3)	0.89183 (13)	0.06463 (10)	0.0206 (4)
H19	0.8682	0.9520	0.0588	0.025*
C20	0.9095 (2)	0.84342 (13)	0.13122 (10)	0.0189 (3)
H20	0.8436	0.8704	0.1705	0.023*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0319 (2)	0.0178 (2)	0.0185 (2)	-0.00049 (17)	0.00129 (18)	0.00386 (16)
N1	0.0280 (8)	0.0183 (7)	0.0184 (7)	0.0008 (7)	0.0005 (6)	-0.0005 (6)
N2	0.0212 (7)	0.0165 (7)	0.0177 (7)	0.0001 (6)	-0.0003 (6)	0.0007 (6)
C1	0.0415 (12)	0.0270 (10)	0.0188 (9)	0.0019 (9)	0.0025 (9)	-0.0023 (7)

C2	0.0175 (9)	0.0191 (9)	0.0197 (8)	0.0014 (7)	0.0017 (7)	0.0011 (6)
C3	0.0269 (9)	0.0189 (9)	0.0229 (8)	0.0002 (7)	-0.0001 (8)	-0.0004 (7)
C4	0.0261 (9)	0.0172 (8)	0.0204 (8)	-0.0032 (7)	-0.0013 (7)	0.0016 (7)
C5	0.0210 (9)	0.0191 (8)	0.0156 (8)	0.0053 (7)	-0.0016 (7)	0.0017 (6)
C6	0.0259 (10)	0.0220 (9)	0.0205 (9)	0.0009 (8)	0.0006 (8)	0.0021 (7)
C7	0.0341 (11)	0.0316 (10)	0.0167 (8)	0.0056 (9)	0.0023 (8)	0.0034 (7)
C8	0.0380 (11)	0.0275 (10)	0.0180 (8)	0.0081 (9)	-0.0046 (8)	-0.0043 (7)
C9	0.0297 (10)	0.0208 (9)	0.0253 (9)	0.0023 (8)	-0.0070 (8)	-0.0011 (8)
C10	0.0232 (9)	0.0193 (9)	0.0208 (9)	0.0008 (7)	-0.0030 (7)	0.0034 (7)
S2	0.0349 (3)	0.0177 (2)	0.0172 (2)	-0.00294 (18)	0.00142 (19)	-0.00212 (15)
N4	0.0246 (8)	0.0157 (7)	0.0180 (7)	-0.0010 (6)	-0.0006 (7)	-0.0006 (6)
N3	0.0273 (8)	0.0191 (7)	0.0187 (7)	-0.0009 (6)	0.0012 (6)	0.0009 (6)
C11	0.0337 (10)	0.0246 (9)	0.0199 (9)	0.0006 (9)	0.0021 (8)	0.0033 (7)
C12	0.0159 (8)	0.0199 (8)	0.0193 (8)	0.0001 (7)	-0.0005 (7)	0.0007 (6)
C13	0.0317 (10)	0.0198 (9)	0.0237 (9)	-0.0036 (8)	-0.0036 (8)	0.0034 (7)
C14	0.0262 (9)	0.0149 (8)	0.0238 (9)	-0.0007 (7)	0.0014 (8)	-0.0012 (7)
C15	0.0189 (8)	0.0177 (8)	0.0174 (8)	-0.0008 (7)	-0.0014 (7)	-0.0015 (6)
C16	0.0233 (9)	0.0202 (9)	0.0199 (9)	0.0026 (7)	-0.0026 (7)	-0.0029 (7)
C17	0.0239 (9)	0.0282 (10)	0.0173 (8)	0.0013 (8)	0.0015 (8)	-0.0048 (7)
C18	0.0234 (9)	0.0238 (9)	0.0156 (8)	-0.0025 (8)	-0.0006 (7)	0.0011 (7)
C19	0.0227 (9)	0.0189 (8)	0.0201 (8)	0.0013 (7)	-0.0025 (7)	-0.0006 (7)
C20	0.0193 (8)	0.0194 (8)	0.0181 (8)	-0.0005 (7)	0.0009 (7)	-0.0022 (7)

*Geometric parameters (Å, °)*

S1—C2	1.6861 (18)	S2—C12	1.6800 (19)
N1—C2	1.335 (2)	N4—C12	1.366 (2)
N1—C1	1.446 (2)	N4—C15	1.422 (2)
N1—C3	1.456 (2)	N4—C14	1.473 (2)
N2—C2	1.374 (2)	N3—C12	1.348 (2)
N2—C5	1.416 (2)	N3—C11	1.449 (2)
N2—C4	1.472 (2)	N3—C13	1.459 (2)
C1—H1A	0.9800	C11—H11A	0.9800
C1—H1B	0.9800	C11—H11B	0.9800
C1—H1C	0.9800	C11—H11C	0.9800
C3—C4	1.526 (2)	C13—C14	1.521 (3)
C3—H3A	0.9900	C13—H13A	0.9900
C3—H3B	0.9900	C13—H13B	0.9900
C4—H4A	0.9900	C14—H14A	0.9900
C4—H4B	0.9900	C14—H14B	0.9900
C5—C6	1.393 (3)	C15—C16	1.394 (3)
C5—C10	1.404 (3)	C15—C20	1.395 (3)
C6—C7	1.395 (3)	C16—C17	1.394 (3)
C6—H6	0.9500	C16—H16	0.9500
C7—C8	1.381 (3)	C17—C18	1.384 (3)
C7—H7	0.9500	C17—H17	0.9500
C8—C9	1.389 (3)	C18—C19	1.393 (3)
C8—H8	0.9500	C18—H18	0.9500



C9—C10	1.390 (3)	C19—C20	1.394 (2)
C9—H9	0.9500	C19—H19	0.9500
C10—H10	0.9500	C20—H20	0.9500
C2—N1—C1	126.02 (17)	C12—N4—C15	127.96 (16)
C2—N1—C3	113.05 (15)	C12—N4—C14	111.30 (15)
C1—N1—C3	120.53 (16)	C15—N4—C14	120.60 (15)
C2—N2—C5	128.59 (15)	C12—N3—C11	124.96 (16)
C2—N2—C4	110.05 (15)	C12—N3—C13	112.11 (15)
C5—N2—C4	120.09 (15)	C11—N3—C13	119.44 (16)
N1—C1—H1A	109.5	N3—C11—H11A	109.5
N1—C1—H1B	109.5	N3—C11—H11B	109.5
H1A—C1—H1B	109.5	H11A—C11—H11B	109.5
N1—C1—H1C	109.5	N3—C11—H11C	109.5
H1A—C1—H1C	109.5	H11A—C11—H11C	109.5
H1B—C1—H1C	109.5	H11B—C11—H11C	109.5
N1—C2—N2	108.51 (16)	N3—C12—N4	108.27 (16)
N1—C2—S1	123.89 (14)	N3—C12—S2	124.46 (14)
N2—C2—S1	127.58 (14)	N4—C12—S2	127.25 (14)
N1—C3—C4	101.90 (14)	N3—C13—C14	102.74 (15)
N1—C3—H3A	111.4	N3—C13—H13A	111.2
C4—C3—H3A	111.4	C14—C13—H13A	111.2
N1—C3—H3B	111.4	N3—C13—H13B	111.2
C4—C3—H3B	111.4	C14—C13—H13B	111.2
H3A—C3—H3B	109.3	H13A—C13—H13B	109.1
N2—C4—C3	102.76 (15)	N4—C14—C13	102.37 (15)
N2—C4—H4A	111.2	N4—C14—H14A	111.3
C3—C4—H4A	111.2	C13—C14—H14A	111.3
N2—C4—H4B	111.2	N4—C14—H14B	111.3
C3—C4—H4B	111.2	C13—C14—H14B	111.3
H4A—C4—H4B	109.1	H14A—C14—H14B	109.2
C6—C5—C10	119.56 (17)	C16—C15—C20	119.62 (17)
C6—C5—N2	118.41 (17)	C16—C15—N4	118.81 (16)
C10—C5—N2	121.91 (16)	C20—C15—N4	121.47 (16)
C5—C6—C7	120.06 (19)	C17—C16—C15	120.01 (17)
C5—C6—H6	120.0	C17—C16—H16	120.0
C7—C6—H6	120.0	C15—C16—H16	120.0
C8—C7—C6	120.76 (19)	C18—C17—C16	120.58 (18)
C8—C7—H7	119.6	C18—C17—H17	119.7
C6—C7—H7	119.6	C16—C17—H17	119.7
C7—C8—C9	119.00 (18)	C17—C18—C19	119.48 (17)
C7—C8—H8	120.5	C17—C18—H18	120.3
C9—C8—H8	120.5	C19—C18—H18	120.3
C8—C9—C10	121.45 (19)	C18—C19—C20	120.44 (17)
C8—C9—H9	119.3	C18—C19—H19	119.8
C10—C9—H9	119.3	C20—C19—H19	119.8
C9—C10—C5	119.15 (18)	C19—C20—C15	119.87 (17)
C9—C10—H10	120.4	C19—C20—H20	120.1



C5—C10—H10	120.4	C15—C20—H20	120.1
C1—N1—C2—N2	176.14 (19)	C11—N3—C12—N4	-166.37 (18)
C3—N1—C2—N2	3.5 (2)	C13—N3—C12—N4	-7.7 (2)
C1—N1—C2—S1	-5.2 (3)	C11—N3—C12—S2	15.2 (3)
C3—N1—C2—S1	-177.86 (15)	C13—N3—C12—S2	173.80 (15)
C5—N2—C2—N1	176.60 (18)	C15—N4—C12—N3	179.76 (18)
C4—N2—C2—N1	9.7 (2)	C14—N4—C12—N3	-4.7 (2)
C5—N2—C2—S1	-2.0 (3)	C15—N4—C12—S2	-1.8 (3)
C4—N2—C2—S1	-168.90 (15)	C14—N4—C12—S2	173.74 (15)
C2—N1—C3—C4	-14.2 (2)	C12—N3—C13—C14	16.1 (2)
C1—N1—C3—C4	172.68 (19)	C11—N3—C13—C14	176.06 (17)
C2—N2—C4—C3	-17.8 (2)	C12—N4—C14—C13	14.1 (2)
C5—N2—C4—C3	173.97 (16)	C15—N4—C14—C13	-169.94 (17)
N1—C3—C4—N2	18.21 (19)	N3—C13—C14—N4	-17.1 (2)
C2—N2—C5—C6	-148.43 (19)	C12—N4—C15—C16	140.89 (19)
C4—N2—C5—C6	17.4 (3)	C14—N4—C15—C16	-34.3 (3)
C2—N2—C5—C10	35.6 (3)	C12—N4—C15—C20	-42.8 (3)
C4—N2—C5—C10	-158.57 (17)	C14—N4—C15—C20	141.95 (18)
C10—C5—C6—C7	-0.9 (3)	C20—C15—C16—C17	-0.4 (3)
N2—C5—C6—C7	-176.94 (18)	N4—C15—C16—C17	175.99 (18)
C5—C6—C7—C8	-0.5 (3)	C15—C16—C17—C18	0.3 (3)
C6—C7—C8—C9	1.0 (3)	C16—C17—C18—C19	0.1 (3)
C7—C8—C9—C10	-0.1 (3)	C17—C18—C19—C20	-0.4 (3)
C8—C9—C10—C5	-1.3 (3)	C18—C19—C20—C15	0.3 (3)
C6—C5—C10—C9	1.8 (3)	C16—C15—C20—C19	0.0 (3)
N2—C5—C10—C9	177.65 (17)	N4—C15—C20—C19	-176.19 (17)

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

Cg1 and Cg2 are the centroids of the C5—C10 and C15—C20 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C11—H11C $\cdots$ Cg1 <sup>i</sup>	0.98	2.96	3.759 (2)	140
C19—H19 $\cdots$ Cg1 <sup>ii</sup>	0.95	2.85	3.612 (2)	138
C6—H6 $\cdots$ Cg2 <sup>iii</sup>	0.95	2.89	3.719 (2)	147
C17—H17 $\cdots$ Cg2 <sup>iv</sup>	0.95	2.76	3.577 (2)	144

Symmetry codes: (i)  $x-1/2, -y+3/2, -z+1$ ; (ii)  $-x+3/2, -y+2, z-1/2$ ; (iii)  $-x+5/2, -y+2, z+1/2$ ; (iv)  $x+1/2, -y+3/2, -z$ .