# organic compounds

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# N-[(5-Chlorothiophen-2-yl)methylene]-5-methylthiazol-2-amine

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Key indicators: single-crystal X-ray study; T = 298 K; mean  $\sigma$ (C–C) = 0.003 Å; R factor = 0.022; wR factor = 0.060; data-to-parameter ratio = 14.4.

The molecule of the title compound, a Schiff base,  $C_9H_7ClN_2S_2$ , is roughly planar, with the two rings twisted by only 8.8°. Molecules are interconnected by weak  $C-H \cdots S$ interactions leading to the formation of chains parallel to the c axis. Weak slipped  $\pi - \pi$  stacking between the thiophene rings may help in further stabilizing the packing (centroid-tocentroid distance = 3.947 Å, interplanar distance = 3.651 Å and offset angle =  $22.3^{\circ}$ ).

#### **Related literature**

For related literature, see: Alemi & Shaabani (2000); Alizadeh et al. (1999); Johnson et al. (1996); Kim & Shin (1999); Wang & Zheng (2007).



### **Experimental**

#### Crystal data

C<sub>9</sub>H<sub>7</sub>ClN<sub>2</sub>S<sub>2</sub>  $M_r = 242.74$ Monoclinic, P2 a = 3.9472 (4) Å b = 23.281 (2) Å c = 6.0379 (6) Å  $\beta = 104.214 \ (1)^{\circ}$ 

V = 537.87 (9) Å<sup>3</sup> Z = 2Mo  $K\alpha$  radiation  $\mu = 0.70 \text{ mm}^{-1}$ T = 298 (2) K  $0.31 \times 0.25 \times 0.19 \; \text{mm}$ 

#### Data collection

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Bruker APEX area-detector
                                            3269 measured reflections
  diffractometer
                                            1839 independent reflections
Absorption correction: multi-scan
                                            1766 reflections with I > 2\sigma(I)
  (SADABS; Sheldrick, 1996)
                                            R_{\rm int} = 0.027
  T_{\min} = 0.812, T_{\max} = 0.878
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# Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$	H-atom parameters constrained
$wR(F^2) = 0.060$	$\Delta \rho_{\rm max} = 0.18 \text{ e } \text{\AA}^{-3}$
S = 1.06	$\Delta \rho_{\rm min} = -0.12 \text{ e } \text{\AA}^{-3}$
1839 reflections	Absolute structure: Flack (1983),
128 parameters	with 836 Friedel pairs
1 restraint	Flack parameter: 0.04 (6)

# Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$C5-H5\cdots S2^i$	0.93	2.97	3.834 (2)	155
	1			

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

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2206).

#### References

- Alemi, A. A. & Shaabani, B. (2000). Acta Chim. Slov. 47, 363-369.
- Alizadeh, N., Ershad, S., Naeimi, H., Sharghi, H. & Shamsipur, M. (1999). Pol. J. Chem. 73, 915-925
- Bruker (1998). SMART (Version 5.0) and SHELXTL (Version 5.10). Bruker AXS Inc, Madison, Wisconsin, USA.
- Bruker (1999). SAINT. Version 6.0. Bruker AXS Inc., Madison, Wisconsin, USA.
- Flack, H. D. (1983). Acta Cryst. A39, 876-881.
- Johnson, C. P., Atwood, J. L., Steed, J. W., Bauer, C. B. & Rogers, R. D. (1996). Inorg. Chem. 35, 2602-2610.
- Kim, G. J. & Shin, J. W. (1999). Catal. Lett. 63, 83-89.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Wang, L.-G. & Zheng, Y.-F. (2007). Acta Cryst. E63, m390-m391.

supplementary materials

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# N-[(5-Chlorothiophen-2-yl)methylene]-5-methylthiazol-2-amine

# C.-N. Zhang and Y.-F. Zheng

## Comment

Schiff base ligands have significant importance in chemistry, especially in the development of Schiff base complexes, (Johnson *et al.*, 1996; Alizadeh *et al.*,1999; Wang & Zheng, 2007). Schiff bases that have solvent-dependent UV/vis spectra (solvatochromicity) can be suitable NLO (nonlinear optically active) materials (Alemi & Shaabani, 2000). They are also useful in the asymmetric oxidation of methyl phenyl sulfide and are enantioselective (Kim & Shin, 1999). In this paper, we report the synthesis and crystal structure of the title compound, (I).

The title compound is roughly planar with the two thiophene rings twisted by only (Fig. 1). The bond lengths and bond angles are usual for such compounds. The crystal packing is governed by weak C—H…S interactions (Table 1) forming chains parallel to the *c* axis and very weak slipped  $\pi$ – $\pi$  stacking between the thiophene rings with centroid to centroid distance of 3.947 Å and interplanar distance of 3.651 Å resulting in an offset angle of 22.3°.

# **Experimental**

Under nitrogen, a mixture of 5-chlorothiophene-2-carbaldehyde (1.67 g,10 mmol), Na<sub>2</sub>SO<sub>4</sub> (3.0 g) and 5-methylthiazol-2amine (1.58 g, 10 mmol) in absolute ethanol (20 ml) was refluxed for about 12 h to yield a yellow precipitate. The product was collected by vacuum filtration and washed with ethanol. The crude solid was redissolved in  $CH_2Cl_2$  (100 ml) and washed with water (2 x 15 ml) and brine (8 ml). After drying over Na<sub>2</sub>SO<sub>4</sub>, the solvent was removed under vacuum, and a yellow solid was isolated in 92% yield (3.1 g). Colourless single crystals of the Schiff base, (I), suitable for X-ray analysis were grown from  $CH_2Cl_2$  and absolute ethanol (4:1) by slow evaporation of the solvents at room temperature over a period of about one week.

## Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) or 0.98 Å (methyl) with  $U_{iso}(H) = xU_{eq}(C)$  where x = 1.2 for aromatic H and 1.5 for methyl H.

**Figures** 



Fig. 1. The molecular structure of (I), showing the atomic numbering scheme. Probability displacement ellipsoids are drawn at the 30% level.

# *N*-[(5-Chlorothiophen-2-yl)methylene]-5-methylthiazol-2-amine

Crystal data	
C9H7ClN2S2	$F_{000} = 248$
$M_r = 242.74$	$D_{\rm x} = 1.499 {\rm ~Mg} {\rm m}^{-3}$
Monoclinic, <i>P</i> 2 <sub>1</sub>	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 1839 reflections
a = 3.9472 (4) Å	$\theta = 3.5 - 25.2^{\circ}$
b = 23.281 (2)  Å	$\mu = 0.70 \text{ mm}^{-1}$
c = 6.0379 (6) Å	T = 298 (2)  K
$\beta = 104.214 \ (1)^{\circ}$	Block, colourless
$V = 537.87 (9) \text{ Å}^3$	$0.31\times0.25\times0.19~mm$
Z = 2	

## Data collection

Bruker APEX area-detector diffractometer	1839 independent reflections
Radiation source: fine-focus sealed tube	1766 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.027$
T = 298(2)  K	$\theta_{\text{max}} = 25.2^{\circ}$
$\phi$ and $\omega$ scans	$\theta_{\min} = 3.5^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -4 \rightarrow 4$
$T_{\min} = 0.812, \ T_{\max} = 0.878$	$k = -24 \rightarrow 27$
3269 measured reflections	$l = -7 \rightarrow 7$

# Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.022$	$w = 1/[\sigma^{2}(F_{o}^{2}) + (0.0362P)^{2} + 0.0225P]$ where $P = (F_{o}^{2} + 2F_{c}^{2})/3$
$wR(F^2) = 0.060$	$(\Delta/\sigma)_{\rm max} = 0.001$
<i>S</i> = 1.06	$\Delta \rho_{max} = 0.18 \text{ e } \text{\AA}^{-3}$
1839 reflections	$\Delta \rho_{min} = -0.12 \text{ e } \text{\AA}^{-3}$
128 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with 836 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.04 (6)

Secondary atom site location: difference Fourier map

# 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  $F^2 > 2 \operatorname{sigma}(F^2)$  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  $(A^2)$ 

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
C1	1.4257 (6)	0.94947 (11)	1.1100 (4)	0.0662 (6)
H1A	1.5326	0.9797	1.0429	0.099*
H1B	1.5992	0.9311	1.2282	0.099*
H1C	1.2463	0.9653	1.1742	0.099*
C2	1.2681 (5)	0.90636 (10)	0.9303 (4)	0.0501 (4)
C3	1.2361 (6)	0.90871 (10)	0.7032 (4)	0.0564 (5)
Н3	1.3129	0.9405	0.6359	0.068*
C4	1.0034 (5)	0.82366 (9)	0.7061 (3)	0.0469 (4)
C5	0.7404 (5)	0.75947 (9)	0.4337 (4)	0.0491 (4)
H5	0.7667	0.7873	0.3286	0.059*
C6	0.5772 (5)	0.70562 (9)	0.3507 (4)	0.0486 (5)
C7	0.4437 (7)	0.68890 (11)	0.1310 (4)	0.0634 (6)
H7	0.4465	0.7120	0.0059	0.076*
C8	0.3010 (6)	0.63335 (11)	0.1111 (4)	0.0657 (6)
H8	0.1995	0.6156	-0.0274	0.079*
C9	0.3287 (5)	0.60889 (9)	0.3165 (4)	0.0542 (5)
Cl1	0.18698 (18)	0.54193 (3)	0.36876 (14)	0.0784 (2)
N1	0.8487 (4)	0.77019 (7)	0.6444 (3)	0.0496 (4)
N2	1.0867 (5)	0.86277 (8)	0.5751 (3)	0.0559 (4)
S1	0.52770 (13)	0.65240 (2)	0.53993 (8)	0.05352 (14)
S2	1.10583 (13)	0.84148 (2)	0.99287 (8)	0.05410 (15)

Atomic displacement parameters  $(Å^2)$ 

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0655 (13)	0.0622 (16)	0.0671 (14)	-0.0105 (11)	0.0090 (11)	-0.0118 (11)
C2	0.0461 (9)	0.0458 (11)	0.0565 (11)	0.0005 (9)	0.0092 (8)	-0.0018 (9)
C3	0.0657 (12)	0.0436 (11)	0.0586 (12)	-0.0054 (10)	0.0127 (10)	0.0040 (9)
C4	0.0496 (10)	0.0436 (11)	0.0476 (10)	0.0025 (8)	0.0120 (8)	0.0017 (8)
C5	0.0520 (10)	0.0441 (11)	0.0520 (11)	0.0007 (8)	0.0139 (8)	0.0065 (8)
C6	0.0501 (10)	0.0447 (12)	0.0503 (11)	0.0024 (8)	0.0113 (8)	0.0041 (8)
C7	0.0821 (14)	0.0542 (14)	0.0505 (12)	-0.0005 (11)	0.0095 (11)	0.0023 (10)

# supplementary materials

CS         0.0784 (15)         0.0534 (15)         0.0534 (12) $-0.000 (10)$ 0.0001 (10) $-0.0081 (10)$ C9         0.0478 (10)         0.0433 (11)         0.0702 (13)         0.0128 (6) $-0.0084 (9)$ C11         0.0752 (4)         0.0445 (3)         0.1166 (5) $-0.0065 (3)$ 0.0253 (3)         0.0009 (3)           N1         0.0572 (4)         0.0445 (10)         0.0492 (9) $-0.0048 (8)$ 0.0114 (7)         0.0020 (7)           S1         0.0612 (3)         0.0480 (3)         0.0502 (3) $-0.0038 (2)$ 0.0114 (2) $0.0039 (2)$ S2         0.0625 (3)         0.0525 (3)         0.0464 (2) $-0.0038 (2)$ 0.0114 (2) $0.0024 (2)$ Geometric parameters (Å, ?)         C1-C2         1.496 (3)         C5-N1         1.264 (3)           C1-H1A         0.9600         C5-C6         1.442 (3)         C1-H1B         0.9600         C6-C7         1.358 (3)           C2-C3         1.347 (3)         C6-S1         1.729 (2)         C3-N2         1.366 (3)         C7-H17         0.9300           C3-H3         0.9300         C8-C9         1.345 (3)         C4-N2         1.396 (3)         C3-C11         1.712	CP	0.07((.15))	0.0574(15)	0.0549 (12)	0.0005 (10)	0.0001 (10)	0.0001 (10)
Cy         0.043 (11)         0.043 (11)         0.043 (11)         0.043 (11)         0.043 (11)         0.043 (11)         0.043 (11)         0.043 (11)         0.043 (11)         0.043 (11)         0.043 (11)         0.043 (11)         0.043 (11)         0.045 (11)         0.045 (11)         0.045 (11)         0.045 (11)         0.045 (11)         0.045 (11)         0.045 (11)         0.045 (11)         0.045 (11)         0.045 (11)         0.045 (11)         0.0009 (11)           N1         0.0533 (9)         0.0418 (10)         0.0522 (10)         -0.0006 (13)         0.0114 (17)         0.0021 (7)           S1         0.0612 (3)         0.0460 (3)         0.0550 (3)         -0.0033 (2)         0.0117 (2)         0.0039 (2)           S2         0.0625 (3)         0.0525 (3)         0.0464 (2)         -0.0038 (2)         0.0117 (2)         0.0034 (2)           C1C2         1.496 (3)         C5N1         1.264 (3)         C1H10         0.9600         C5C6         1.442 (3)           C1H1B         0.9600         C5H5         1.358 (3)         C2-C1         1.358 (3)<		0.0700(13)	0.0374(13)	0.0348(12) 0.0702(12)	-0.0003(10)	0.0001(10)	-0.0081(10)
Cli 0.0752 (4) 0.0445 (5) 0.1166 (5) -0.0005 (5) 0.0253 (5) 0.0009 (7) N1 0.0536 (9) 0.0418 (10) 0.0552 (10) -0.0004 (7) 0.0114 (7) 0.0020 (7) N2 0.0713 (11) 0.0466 (11) 0.0492 (9) -0.0048 (8) 0.0114 (7) 0.0020 (7) S1 0.0612 (3) 0.0480 (3) 0.0502 (3) -0.0033 (2) 0.0115 (2) 0.0039 (2) S2 0.0625 (3) 0.0525 (3) 0.0464 (2) -0.0058 (2) 0.0117 (2) 0.0024 (2) Geometric parameters ( $\hat{J}, {}^{0}$ ) C1-C2 1.496 (3) C5-N1 1.264 (3) C1-H1A 0.9600 C5-H5 0.9300 C1-H1C 0.9600 C6-C7 1.358 (3) C2-C3 1.347 (3) C6-S1 1.729 (2) C2-S2 1.719 (2) C7-C8 1.404 (4) C3-N2 1.366 (3) C7-H7 0.9300 C3-H3 0.9300 C8-C9 1.345 (3) C4-N1 1.396 (3) C9-C11 1.712 (2) C4-S2 1.300 (3) C8-H8 0.9300 C4-N1 1.396 (3) C9-C11 1.712 (2) C4-S2 1.729 (2) C9-S1 1.715 (2) C2-C1-H1B 109.5 C7-C6-C5 1.28.4 (2) H1A-C1-H1B 109.5 C7-C6-C5 1.28.4 (2) H1A-C1-H1B 109.5 C7-C6-C5 1.28.4 (2) H1A-C1-H1B 109.5 C7-C6-S1 111.11 (7) C2-C1-H1B 109.5 C7-C6-C5 1.28.4 (2) H1A-C1-H1B 109.5 C7-C6-S1 111.11 (7) C2-C1-H1B 109.5 C7-C6-C5 1.28.4 (2) H1A-C1-H1C 109.5 C6-C7-H7 1.23.2 C3-C2-C1 129.0 (2) C8-C7-H7 1.23.2 C3-C2-S2 117.6 (2) C7-C8-H8 1.24.1 C2-C3-H3 1.21.2 C8-C9-S1 1.13.16 (17) N2-C4-N1 1.28.43 (19) C11-C9-S1 1.13.16 (17) N2-C4-N1 1.28.43 (19) C11-C9-S1 1.13.16 (17) N2-C4-S2 1.14.16 (15) C5-N1-C4 1.17.54 (17) N1-C5-H5 1.18.9 C2-S2-C4 89.94 (10) Hydrogen-bond geometry ( $\hat{A}, {}^{0}$ ) D-H-A 2 0.93 2.97 3.3834 (2) 155	C9	0.04/8 (10)	0.0431(11)	0.0702(13)	0.0012 (8)	0.0118 (9)	-0.0034 (9)
N1       0.0353 (5)       0.0418 (10)       0.0522 (10) $-0.0044 (7)$ 0.0114 (7)       0.0020 (7)         S1       0.0612 (3)       0.0480 (3)       0.0522 (3) $-0.0033 (2)$ 0.0115 (2)       0.0021 (7)         S2       0.0625 (3)       0.0525 (3)       0.0464 (2) $-0.0038 (2)$ 0.0117 (2)       0.0024 (2)         Geometric parameters (Å, °)       C1—H1A       0.9600       C5—C6       1.442 (3)         C1—H1B       0.9600       C5—K1       1.759 (2)         C2—C3       1.347 (3)       C6—S1       1.729 (2)         C2—S2       1.719 (2)       C7—C8       1.404 (4)         C3—H3       0.9300       C8—C9       1.345 (3)         C4—N2       1.306 (3)       C9—S1       1.712 (2)         C4—N1       1.396 (3)       C9—S1       1.712 (2)         C4—N1       1.396 (3)       C9—S1       1.715 (2)         C2—C1—H1A       109.5       C6—C5—H5       118 9         C2—C1—H1B       109.5       C6—C5—S1       128.4 (2)         H1A—C1—H1B       109.5       C6—C7—K1       111.11 (17)         C2—C1—H1B       109.5       C6—C7=K1       118.9         C2—C1—H1B       109.5       C6—	CII	0.0752 (4)	0.0445 (3)	0.1166 (5)	-0.0065(3)	0.0253(3)	0.0009 (3)
N2         0.013 (11)         0.0462 (9)         -0.0038 (8)         0.013 (8)         0.0021 (7)           S1         0.0612 (3)         0.0480 (3)         0.0523 (3)         -0.0033 (2)         0.0115 (2)         0.0021 (2)           S2         0.0625 (3)         0.0525 (3)         0.0464 (2)         -0.0038 (2)         0.0117 (2)         0.0024 (2)           Geometric parameters (Å, ?)         C1—C2         1.496 (3)         C5—N1         1.264 (3)           C1—H1A         0.9600         C5—C6         1.442 (3)           C1—H1B         0.9600         C6—C7         1.358 (3)           C2—C3         1.347 (3)         C6—S1         1.729 (2)           C3—N2         1.366 (3)         C7—H7         0.9300           C3—N3         0.9300         C8—C9         1.345 (3)           C4—N2         1.300 (3)         C8—H8         0.9300           C4—N1         1.396 (3)         C9—C11         1.712 (2)           C4—N2         1.300 (3)         C6—C5         128 4(2)           H1A—C1—H1B         109.5         C7—C6—S1         111.11 (17)           C2—C1—H1B         109.5         C5—C6—S1         120.45 (16)           H1A~C1—H1E         109.5         C6—C7—H7 <t< td=""><td>NI</td><td>0.0539 (9)</td><td>0.0418 (10)</td><td>0.0522 (10)</td><td>-0.0004 (7)</td><td>0.0114 (7)</td><td>0.0020 (7)</td></t<>	NI	0.0539 (9)	0.0418 (10)	0.0522 (10)	-0.0004 (7)	0.0114 (7)	0.0020 (7)
S1 $0.0612 (3)$ $0.0480 (3)$ $0.052 (3)$ $0.0033 (2)$ $0.0115 (2)$ $0.0039 (2)$ S2 $0.0625 (3)$ $0.0525 (3)$ $0.0464 (2)$ $-0.0058 (2)$ $0.0117 (2)$ $0.0029 (2)$ Geometric parameters (Å, °)       C1—C2 $1.496 (3)$ C5—N1 $1.264 (3)$ C1—H1A $0.9600$ C5—C6 $1.442 (3)$ C1—H1B $0.9600$ C5—H5 $0.9300$ C2—C3 $1.347 (3)$ C6—S1 $1.729 (2)$ C2—C3 $1.347 (3)$ C6—S1 $1.729 (2)$ C3—N2 $1.366 (3)$ C7—H7 $0.9300$ C4—N2 $1.300 (3)$ C8—H8 $0.9300$ C4—N1 $1.396 (3)$ C9—C11 $1.715 (2)$ C2—C1—H1A $109.5$ C7—C6—S1 $118.9$ C2—C1—H1B $109.5$ C7—C6—S1 $111.11 (17)$ C2—C1—H1B $109.5$ C5—C6—C5 $128.4 (2)$ H1A—C1—H1B $109.5$ C6—C7—H7 $123.2$ C3—C2—C1 $129.0 (2)$ C8—C7 $111.8 (2)$ C1=C2—S2 $102.016 (6)$ C9—C8	N2	0.0/13 (11)	0.0466 (11)	0.0492 (9)	-0.0048 (8)	0.0134 (8)	0.0021 (7)
S2       0.0625 (3)       0.0525 (3)       0.0464 (2) $-0.0058 (2)$ 0.0117 (2)       0.0024 (2)         Geometric parameters (Å, ?)         CIC2       1.496 (3)       C5N1       1.264 (3)         CI-HIA       0.9600       C5C6       1.442 (3)         CIHIB       0.9600       C6C7       1.358 (3)         C2-C3       1.347 (3)       C6S1       1.729 (2)         C2S2       1.719 (2)       C7C8       1.404 (4)         C3H3       0.9300       C8C9       1.345 (3)         C4N2       1.306 (3)       C9-C11       1.712 (2)         C4-S2       1.709 (2)       C9-S1       1.715 (2)         C2-C1-HIA       109.5       C6-C5-H5       118.9         C2-C1-HIB       109.5       C7C6-C5       128.4 (2)         HIA-C1-HIB       109.5       C5C6-S1       113.5 (2)         HIA-C1-HIC       109.5       C6-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-C2       108.21 (16)       C9-C8-C7       113.5 (2)         HIA-C1-HIC       109.5       C6-C7-H7       123.2         C3-C2-C2       108.21 (16)       C9-C8	SI	0.0612 (3)	0.0480 (3)	0.0502 (3)	-0.0033(2)	0.0115 (2)	0.0039 (2)
Geometric parameters (Å, °)         C1C2       1.496 (3)       C5N1       1.264 (3)         C1H1A       0.9600       C5K5       0.9300         C1H1B       0.9600       C6C7       1.358 (3)         C2C3       1.347 (3)       C6-S1       1.729 (2)         C2S2       1.719 (2)       C7C8       1.404 (4)         C3N2       1.366 (3)       C7-H7       0.9300         C4N1       1.396 (3)       C9-C11       1.712 (2)         C4-N2       1.300 (3)       C8-H8       0.9300         C4-N1       1.396 (3)       C9-C11       1.712 (2)         C4-N2       1.300 (3)       C8-H8       0.9300         C4-N1       1.396 (3)       C9-C11       1.715 (2)         C2-C1-H1A       109.5       C7-C6-C5       128.4 (2)         H1A-C1-H1B       109.5       C7-C6-S1       111.11 (17)         C2-C1-H1B       109.5       C5-C6-S1       129.45 (16)         H1A-C1-H1C       109.5       C6-C7-H7       123.2         C3-C2-S2       108.21 (16)       C9-C8-H8       124.1         C2-C3-N2       117.6 (2)       C7-C8-H8       124.1         C2-C3-N2       117.6 (2) </td <td><b>S</b>2</td> <td>0.0625 (3)</td> <td>0.0525 (3)</td> <td>0.0464 (2)</td> <td>-0.0058 (2)</td> <td>0.0117 (2)</td> <td>0.0024 (2)</td>	<b>S</b> 2	0.0625 (3)	0.0525 (3)	0.0464 (2)	-0.0058 (2)	0.0117 (2)	0.0024 (2)
C1-C2       1 496 (3)       C5-N1       1 264 (3)         C1-H1A       0.9600       C5-C6       1.442 (3)         C1-H1B       0.9600       C6-C7       1.358 (3)         C2-C3       1.347 (3)       C6-S1       1.729 (2)         C2-S2       1.719 (2)       C7-C8       1.404 (4)         C3-H3       0.9300       C8-C9       1.345 (3)         C4-N2       1.306 (3)       C9       1.345 (3)         C4-N2       1.300 (3)       C8-H8       0.9300         C4-N1       1.396 (3)       C9-C11       1.712 (2)         C4-N2       1.200 (3)       C6-C5-H5       118.9         C2-C1-H1A       109.5       C6-C5-H5       118.9         C2-C1-H1B       109.5       C7-C6-C5       128.4 (2)         H1A-C1-H1B       109.5       C5-C6-S1       120.45 (16)         H1A-C1-H1C       109.5       C6-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-S2       108.21 (16)       C9-C8-C7       118.18 (2)         C1-C2-S2       108.21 (16)       C9-C8-H8       124.1         C2-C3-H3       121.2       C8-C9-S1       113.16 (17)         N2	Geometric paran	neters (Å, °)					
C1—H1A       0.9600       C5—C6       1.442 (3)         C1—H1B       0.9600       C5—H5       0.9300         C1—H1C       0.9600       C6—C7       1.358 (3)         C2—C3       1.347 (3)       C6—S1       1.729 (2)         C2—S2       1.719 (2)       C7—C8       1.404 (4)         C3—N2       1.366 (3)       C7—H7       0.9300         C4—N1       1.396 (3)       C9—C1       1.712 (2)         C4—N2       1.300 (3)       C8—C9       1.345 (3)         C4—N1       1.396 (3)       C9—C1       1.712 (2)         C4—S2       1.729 (2)       C9—S1       1.715 (2)         C2—C1—H1A       109.5       C6—C5—H5       118.9         C2—C1—H1B       109.5       C7—C6—C5       128.4 (2)         H1A—C1—H1B       109.5       C5—C6—S1       120.45 (16)         H1A—C1—H1C       109.5       C6—C7—H7       123.2         C3—C2—C1       129.0 (2)       C8—C7       111.8 (2)         C1—C2—S2       122.71 (17)       C9—C8—H8       124.1         C2—C3—N2       117.6 (2)       C7—C6—H8       124.1         C2—C3—N2       117.6 (2)       C7—C8—H8       124.1         C2—C3—N2<	C1—C2		1.496 (3)	С5—	-N1	1.2	64 (3)
C1—H1B       0.9600       C5—H5       0.9300         C1—H1C       0.9600       C6—C7       1.358 (3)         C2—C3       1.347 (3)       C6—S1       1.729 (2)         C2—S2       1.719 (2)       C7—C8       1.404 (4)         C3—N2       1.366 (3)       C7—H7       0.9300         C3—H3       0.9300       C8—C9       1.345 (3)         C4—N2       1.300 (3)       C8—H8       0.9300         C4—N1       1.396 (3)       C9—C11       1.712 (2)         C4—N1       1.396 (3)       C9—C11       1.715 (2)         C2—C1—H1A       109.5       C7—C6—C5       128.4 (2)         H1A—C1—H1B       109.5       C7—C6—S1       111.11 (17)         C2—C1—H1B       109.5       C6—C7—H7       123.2         C3—C2       1.90 (2)       C8—C7       113.5 (2)         H1B—C1—H1C       109.5       C6—C7—H7       123.2         C3—C2—C1       129 0 (2)       C8—C7       113.8 (2)         C1—C2—S2       108.21 (16)       C9—C8—C7       111.8 (2)         C1—C2—S2       108.21 (16)       C9—C8—C7       113.8 (6) (7)         N2—C4—N1       128.43 (19)       C1—C9—S1       120.00 (14)      N	C1—H1A		0.9600	С5—	-C6	1.442 (3)	
C1-H1C       0.9600       C6-C7       1.358 (3)         C2-C3       1.347 (3)       C6-S1       1.729 (2)         C2-S2       1.719 (2)       C7-C8       1.404 (4)         C3-H3       0.9300       C8-C9       1.345 (3)         C4-N2       1.366 (3)       C7-H7       0.9300         C4-N2       1.300 (3)       C8-C9       1.345 (3)         C4-N2       1.300 (3)       C8-H8       0.9300         C4-N1       1.396 (3)       C9-C11       1.715 (2)         C2-C1-H1A       109.5       C6-C5-H5       118.9         C2-C1-H1B       109.5       C7-C6-C5       128.4 (2)         H1A-C1-H1B       109.5       C7-C6-S1       111.11 (17)         C2-C1-H1C       109.5       C6-C7-C8       113.5 (2)         H1B-C1-H1C       109.5       C6-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-C1       129.0 (2)       C7-C8-H8       124.1         C2-C3	C1—H1B		0.9600	C5—	-H5	0.9	300
C2-C3       1.347 (3)       C6-S1       1.729 (2)         C2-S2       1.719 (2)       C7-C8       1.404 (4)         C3-N2       1.366 (3)       C7-H7       0.9300         C3-H3       0.9300       C8-C9       1.345 (3)         C4-N2       1.300 (3)       C8-H8       0.9300         C4-N1       1.396 (3)       C9-C11       1.712 (2)         C4-S2       1.729 (2)       C9-S1       1.715 (2)         C2-C1-H1A       109.5       C6-C5-H5       118.9         C2-C1-H1B       109.5       C7-C6-C5       128.4 (2)         H1A-C1-H1B       109.5       C7-C6-S1       111.11 (17)         C2-C1-H1C       109.5       C6-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-S2       108.21 (16)       C9-C8-C7       111.8 (2)         C1-C2-S2       122.77 (17)       C9-C8-H8       124.1         C2-C3-N13       121.2       C8-C9-S1       13.6 (17)         N2-C3-H3       121.2       C8-C9-S1       113.16 (17)         N2-C4-N1       128.43 (19)       C11-C9-S1       120.00 (14)         N2-C4-N1       128.43 (19)       C11-C9-S1       120.00 (14)	C1—H1C		0.9600	C6—	-C7	1.3	58 (3)
C2-82       1.719 (2)       C7-C8       1.404 (4)         C3-N2       1.366 (3)       C7-H7       0.9300         C3-H3       0.9300       C8-C9       1.345 (3)         C4-N2       1.300 (3)       C8-H8       0.9300         C4-N1       1.396 (3)       C9-C11       1.712 (2)         C4-S2       1.729 (2)       C9-S1       1.715 (2)         C2-C1-H1A       109.5       C6-C5-H5       118.9         C2-C1-H1B       109.5       C7-C6-C5       128.4 (2)         H1A-C1-H1B       109.5       C5-C6-S1       111.11 (17)         C2-C1-H1C       109.5       C6-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-S2       108.21 (16)       C9-C8-C7       111.8 (2)         C1-C2-S2       122.77 (17)       C9-C8-H8       124.1         C2-C3-H3       121.2       C8-C9-S1       113.16 (17)         N2-C4-N1       128.43 (19)       C11-C9-S1       120.00 (14)         N2-C4-S2       114.16 (15)       C5-N1-C4       117.54 (17)	C2—C3		1.347 (3)	C6—	-\$1	1.7	29 (2)
C3-N2       1.366 (3)       C7-H7       0.9300         C3-H3       0.9300       C8-C9       1.345 (3)         C4-N2       1.300 (3)       C8-H8       0.9300         C4-N1       1.396 (3)       C9-C11       1.712 (2)         C4-S2       1.729 (2)       C9-S1       1.715 (2)         C2-C1-H1A       109.5       C6-C5-H5       118.9         C2-C1-H1B       109.5       C7-C6-S1       111.11 (17)         C2-C1-H1B       109.5       C7-C6-S1       113.5 (2)         HA-C1-H1B       109.5       C5-C6-S1       113.5 (2)         H1A-C1-H1C       109.5       C6-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-S2       108.21 (16)       C9-C8-C7       111.8 (2)         C1-C2-S2       122.77 (17)       C9-C8-H8       124.1         C2-C3-H3       121.2       C8-C9-S1       113.16 (17)         N2-C4-N1       128.43 (19)       C1-C9-S1       113.16 (17)         N2-C4-N1       128.43 (19)       C1-C9-S1       113.16 (17)         N2-C4-N1       128.43 (19)       C1-C9-S1       113.16 (17)         N2-C4-N2       114.16 (15)       C5-N1-C4       11	C2—S2		1.719 (2)	С7—	-C8	1.4	04 (4)
C3-H3       0.9300       C8-C9       1.345 (3)         C4-N2       1.300 (3)       C8-H8       0.9300         C4-N1       1.396 (3)       C9-C11       1.712 (2)         C4-S2       1.729 (2)       C9-S1       1.715 (2)         C2-C1-H1A       109.5       C6-C5-H5       118.9         C2-C1-H1B       109.5       C7-C6-C5       128.4 (2)         H1A-C1-H1B       109.5       C7-C6-S1       111.11 (17)         C2-C1-H1C       109.5       C6-C7-C8       113.5 (2)         H1B-C1-H1C       109.5       C6-C7-C8       113.5 (2)         H1B-C1-H1C       109.5       C6-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-S2       108.21 (16)       C9-C8-C7       111.8 (2)         C1-C2-S2       122.77 (17)       C9-C8-H8       124.1         C2-C3-H3       121.2       C8-C9-S1       113.16 (17)         N2-C4-N1       128.43 (19)       C11-C9-S1       120.00 (14)         N2-C4-N1       128.43 (19)       C11-C9-S1       120.00 (14)         N2-C4-N1       128.43 (19)       C11-C9-S1       120.00 (14)         N1-C5-C6       122.24 (18)       C9-S1-C6	C3—N2		1.366 (3)	С7—	-H7	0.9300	
C4-N2       1.300 (3)       C8-H8       0.9300         C4-N1       1.396 (3)       C9-Cl1       1.712 (2)         C4-S2       1.729 (2)       C9-S1       1.715 (2)         C2-C1-H1A       109.5       C6-C5-H5       118.9         C2-C1-H1B       109.5       C7-C6-C5       128.4 (2)         H1A-C1-H1B       109.5       C7-C6-S1       111.11 (17)         C2-C1-H1C       109.5       C5-C6-S1       120.45 (16)         H1A-C1-H1C       109.5       C6-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-S2       108.21 (16)       C9-C8-C7       111.8 (2)         C1-C2-S2       122.77 (17)       C9-C8-H8       124.1         C2-C3-H3       121.2       C8-C9-C11       126.84 (18)         N2-C4-N1       128.43 (19)       C11-C9-S1       120.00 (14)         N2-C4-S2       117.41 (14)       C4-N2-C3       110.04 (18)         N1-C5-C6       122.24 (18)       C9-S1-C6       90.44 (11)         N1-C5-H5       118.9       C2-S2-C4       89.94 (10)	С3—Н3		0.9300	C8—	-C9	1.345 (3)	
C4-N1 $1.396$ (3)       C9-Cl1 $1.712$ (2)         C4-S2 $1.729$ (2)       C9-S1 $1.715$ (2)         C2-C1-H1A       109.5       C6-C5-H5       118.9         C2-C1-H1B       109.5       C7-C6-C5       128.4 (2)         H1A-C1-H1B       109.5       C7-C6-S1       111.11 (17)         C2-C1-H1C       109.5       C5-C6-S1       120.45 (16)         H1A-C1-H1C       109.5       C6-C7-C8       113.5 (2)         H1B-C1-H1C       109.5       C6-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-S2       108.21 (16)       C9-C8-C7       111.8 (2)         C1-C2-S2       122.77 (17)       C9-C8-H8       124.1         C2-C3-N2       117.6 (2)       C7-C8-H8       124.1         C2-C3-H3       121.2       C8-C9-C11       126.84 (18)         N2-C3-H3       121.2       C8-C9-S1       113.16 (17)         N2-C4-S2       114.16 (15)       C5-N1-C4       117.54 (17)         N1-C4-S2       117.41 (14)       C4-N2-C3       110.04 (18)         N1-C5-C6       122.24 (18)       C9-S1-C6       90.44 (11)         N1-C5-H5       118.9       C2	C4—N2		1.300 (3)	C8—	-H8	0.9300	
C4-S2 $1.729 (2)$ C9-S1 $1.715 (2)$ C2-C1-H1A       109.5       C6-C5-H5       118.9         C2-C1-H1B       109.5       C7-C6-C5       128.4 (2)         H1A-C1-H1B       109.5       C7-C6-S1       111.11 (17)         C2-C1-H1C       109.5       C5-C6-S1       120.45 (16)         H1A-C1-H1C       109.5       C6-C7-C8       113.5 (2)         H1B-C1-H1C       109.5       C6-C7-H7       123.2         C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-S2       108.21 (16)       C9-C8-C7       111.8 (2)         C1-C2-S2       122.77 (17)       C9-C8-H8       124.1         C2-C3-N2       117.6 (2)       C7-C8-H8       124.1         C2-C3-H3       121.2       C8-C9-C11       126.84 (18)         N2-C3-H3       121.2       C8-C9-S1       113.16 (17)         N2-C4-N1       128.43 (19)       C1-C9-S1       120.00 (14)         N2-C4-S2       114.16 (15)       C5-N1-C4       117.54 (17)         N1-C5-C6       122.24 (18)       C9-S1-C6       90.44 (11)         N1-C5-H5       118.9       C2-S2-C4       89.94 (10)	C4—N1		1.396 (3)	С9—	-Cl1	1.712 (2)	
C2C1H1A       109.5       C6C5H5       118.9         C2C1H1B       109.5       C7C6C5       128.4 (2)         H1AC1H1B       109.5       C7C6S1       111.11 (17)         C2C1H1C       109.5       C5C6S1       120.45 (16)         H1AC1H1C       109.5       C6C7C8       113.5 (2)         H1BC1H1C       109.5       C6C7H7       123.2         C3C2C1       129.0 (2)       C8C7H7       123.2         C3C2S2       108.21 (16)       C9C8C7       111.8 (2)         C1C2S2       122.77 (17)       C9C8H8       124.1         C2C3N2       117.6 (2)       C7C8H8       124.1         C2C3H3       121.2       C8C9C11       126.84 (18)         N2C4N1       128.43 (19)       C11C9S1       120.00 (14)         N2C4S2       114.16 (15)       C5N1C4       117.54 (17)         N1C5C6       122.24 (18)       C9S1C6       90.44 (11)         N1C5H5       118.9       C2S2C4       89.94 (10)	C4—S2		1.729 (2)	С9—	-S1	1.7	15 (2)
C2C1H1B109.5C7C6C5128.4 (2)H1AC1H1B109.5C7C6S1111.11 (17)C2C1H1C109.5C5C6S1120.45 (16)H1AC1H1C109.5C6C7C8113.5 (2)H1BC1H1C109.5C6C7H7123.2C3C2C1129.0 (2)C8C7H7123.2C3C2S2108.21 (16)C9C8C7111.8 (2)C1C2S2122.77 (17)C9C8H8124.1C2C3H3121.2C8C9C11126.84 (18)N2C4N1128.43 (19)C11C9S1120.00 (14)N2C4S2117.41 (14)C4N2C3110.04 (18)N1C5C6122.24 (18)C9S1C690.44 (11)N1C5H5118.9C2S2C489.94 (10)	C2—C1—H1A		109.5	С6—	-C5—H5	118	3.9
H1A—C1—H1B109.5C7—C6—S1111.11 (17)C2—C1—H1C109.5C5—C6—S1120.45 (16)H1A—C1—H1C109.5C6—C7—C8113.5 (2)H1B—C1—H1C109.5C6—C7—H7123.2C3—C2—C1129.0 (2)C8—C7—H7123.2C3—C2—S2108.21 (16)C9—C8—C7111.8 (2)C1—C2—S2122.77 (17)C9—C8—H8124.1C2—C3—N2117.6 (2)C7—C8—H8124.1C2—C3—H3121.2C8—C9—C11126.84 (18)N2—C4—N1128.43 (19)C11—C9—S1120.00 (14)N2—C4—S2114.16 (15)C5—N1—C4117.54 (17)N1—C5—C6122.24 (18)C9—S1—C690.44 (11)N1—C5—H5118.9C2—S2—C489.94 (10)Hydrogen-bond geometry (Å, °)D—HH···AD···AD—H···AC5—H5···S2 <sup>i</sup> 0.932.973.834 (2)155	C2-C1-H1B		109.5	С7—	-C6—C5	128	3.4 (2)
C2C1H1C109.5C5C6S1120.45 (16)H1AC1H1C109.5C6C7C8113.5 (2)H1BC1H1C109.5C6C7H7123.2C3C2C1129.0 (2)C8C7H7123.2C3C2S2108.21 (16)C9C8C7111.8 (2)C1C2S2122.77 (17)C9C8H8124.1C2C3H3121.2C8C9C11126.84 (18)N2C3H3121.2C8C9S1113.16 (17)N2C4N1128.43 (19)C11C9S1120.00 (14)N2C4S2114.16 (15)C5N1C4117.54 (17)N1C5C6122.24 (18)C9S1C690.44 (11)N1C5H5118.9C2S2C489.94 (10)Hydrogen-bond geometry (Å, °)DHH···AD···ADHH···AC5H5-··S2 <sup>1</sup> 0.932.973.834 (2)155	H1A—C1—H1B		109.5	С7—	-C6—S1	111	.11 (17)
H1A—C1—H1C109.5C6—C7—C8113.5 (2)H1B—C1—H1C109.5C6—C7—H7123.2C3—C2—C1129.0 (2)C8—C7—H7123.2C3—C2—S2108.21 (16)C9—C8—C7111.8 (2)C1—C2—S2122.77 (17)C9—C8—H8124.1C2—C3—H3121.2C8—C9—C11126.84 (18)N2—C4—N1128.43 (19)C11—C9—S1120.00 (14)N2—C4—S2117.41 (14)C4—N2—C3110.04 (18)N1—C5—C6122.24 (18)C9—S1—C690.44 (11)N1—C5—H5118.9C2—S2—C489.94 (10)	C2-C1-H1C		109.5	С5—	-C6—S1	120	0.45 (16)
H1B—C1—H1C109.5C6—C7—H7123.2C3—C2—C1129.0 (2)C8—C7—H7123.2C3—C2—S2108.21 (16)C9—C8—C7111.8 (2)C1—C2—S2122.77 (17)C9—C8—H8124.1C2—C3—N2117.6 (2)C7—C8—H8124.1C2—C3—H3121.2C8—C9—C11126.84 (18)N2—C4—N1128.43 (19)C11—C9—S1120.00 (14)N2—C4—S2114.16 (15)C5—N1—C4117.54 (17)N1—C4—S2117.41 (14)C4—N2—C3110.04 (18)N1—C5—C6122.24 (18)C9—S1—C690.44 (11)N1—C5—H5118.9C2—S2—C489.94 (10)	H1A—C1—H1C		109.5	С6—	-C7—C8	113	3.5 (2)
C3-C2-C1       129.0 (2)       C8-C7-H7       123.2         C3-C2-S2       108.21 (16)       C9-C8-C7       111.8 (2)         C1-C2-S2       122.77 (17)       C9-C8-H8       124.1         C2-C3-N2       117.6 (2)       C7-C8-H8       124.1         C2-C3-H3       121.2       C8-C9-C11       126.84 (18)         N2-C3-H3       121.2       C8-C9-S1       113.16 (17)         N2-C4-N1       128.43 (19)       C11-C9-S1       120.00 (14)         N2-C4-S2       114.16 (15)       C5-N1-C4       117.54 (17)         N1-C4-S2       117.41 (14)       C4-N2-C3       110.04 (18)         N1-C5-C6       122.24 (18)       C9-S1-C6       90.44 (11)         N1-C5-H5       118.9       C2-S2-C4       89.94 (10)	H1B—C1—H1C		109.5	С6—	-С7—Н7	123	3.2
C3-C2-S2108.21 (16)C9-C8-C7111.8 (2)C1-C2-S2122.77 (17)C9-C8-H8124.1C2-C3-N2117.6 (2)C7-C8-H8124.1C2-C3-H3121.2C8-C9-C11126.84 (18)N2-C3-H3121.2C8-C9-S1113.16 (17)N2-C4-N1128.43 (19)C11-C9-S1120.00 (14)N2-C4-S2114.16 (15)C5-N1-C4117.54 (17)N1-C4-S2117.41 (14)C4-N2-C3110.04 (18)N1-C5-C6122.24 (18)C9-S1-C690.44 (11)N1-C5-H5118.9C2-S2-C489.94 (10)	C3—C2—C1		129.0 (2)	C8—	-С7—Н7	123	3.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3—C2—S2		108.21 (16)	С9—	-C8—C7	111	.8 (2)
C2—C3—N2117.6 (2)C7—C8—H8124.1C2—C3—H3121.2C8—C9—Cl1126.84 (18)N2—C3—H3121.2C8—C9—S1113.16 (17)N2—C4—N1128.43 (19)Cl1—C9—S1120.00 (14)N2—C4—S2114.16 (15)C5—N1—C4117.54 (17)N1—C4—S2117.41 (14)C4—N2—C3110.04 (18)N1—C5—C6122.24 (18)C9—S1—C690.44 (11)N1—C5—H5118.9C2—S2—C489.94 (10)	C1—C2—S2		122.77 (17)	С9—	-С8—Н8	124	l.1
C2—C3—H3121.2C8—C9—C11126.84 (18)N2—C3—H3121.2C8—C9—S1113.16 (17)N2—C4—N1128.43 (19)C11—C9—S1120.00 (14)N2—C4—S2114.16 (15)C5—N1—C4117.54 (17)N1—C4—S2117.41 (14)C4—N2—C3110.04 (18)N1—C5—C6122.24 (18)C9—S1—C690.44 (11)N1—C5—H5118.9C2—S2—C489.94 (10)	C2-C3-N2		117.6 (2)	С7—	-С8—Н8	124	l.1
N2—C3—H3121.2C8—C9—S1113.16 (17)N2—C4—N1128.43 (19)C11—C9—S1120.00 (14)N2—C4—S2114.16 (15)C5—N1—C4117.54 (17)N1—C4—S2117.41 (14)C4—N2—C3110.04 (18)N1—C5—C6122.24 (18)C9—S1—C690.44 (11)N1—C5—H5118.9C2—S2—C489.94 (10)Hydrogen-bond geometry (Å, °)D—HH···AD—HD···AD—H···AC5—H5···S2 <sup>i</sup> 0.932.973.834 (2)155	С2—С3—Н3		121.2	C8—	-C9—Cl1	126	5.84 (18)
N2—C4—N1128.43 (19)Cl1—C9—S1120.00 (14)N2—C4—S2114.16 (15)C5—N1—C4117.54 (17)N1—C4—S2117.41 (14)C4—N2—C3110.04 (18)N1—C5—C6122.24 (18)C9—S1—C690.44 (11)N1—C5—H5118.9C2—S2—C489.94 (10)Hydrogen-bond geometry (Å, °)D—HH···AD—H···AD···AD—H···AC5—H5···S2 <sup>i</sup> 0.932.973.834 (2)155	N2—C3—H3		121.2	C8—	-C9—S1	113	5.16 (17)
N2—C4—S2114.16 (15)C5—N1—C4117.54 (17)N1—C4—S2117.41 (14)C4—N2—C3110.04 (18)N1—C5—C6122.24 (18)C9—S1—C690.44 (11)N1—C5—H5118.9C2—S2—C489.94 (10)Hydrogen-bond geometry (Å, °)D—HH···AD—H···AD—HH···AC5—H5···S2 <sup>i</sup> 0.932.973.834 (2)	N2-C4-N1		128.43 (19)	Cl1–	Cl1—C9—S1 120.00 (14)		0.00 (14)
N1—C4—S2       117.41 (14)       C4—N2—C3       110.04 (18)         N1—C5—C6       122.24 (18)       C9—S1—C6       90.44 (11)         N1—C5—H5       118.9       C2—S2—C4       89.94 (10)         Hydrogen-bond geometry (Å, °) $D$ —H       H···A $D$ ···A $D$ —H···A         C5—H5···S2 <sup>i</sup> 0.93       2.97       3.834 (2)       155	N2—C4—S2		114.16 (15)	C5—N1—C4 117.54 (1		7.54 (17)	
N1—C5—C6       122.24 (18)       C9—S1—C6       90.44 (11)         N1—C5—H5       118.9       C2—S2—C4 $89.94$ (10)         Hydrogen-bond geometry (Å, °) $D$ —H       H···A $D$ ···A $D$ —H···A         C5—H5···S2 <sup>i</sup> 0.93       2.97 $3.834$ (2)       155	N1—C4—S2		117.41 (14)	C4—	C4—N2—C3 110.04 (18)		0.04 (18)
N1—C5—H5       118.9       C2—S2—C4       89.94 (10)         Hydrogen-bond geometry (Å, °) $D$ —H       H···A $D$ ···A $D$ —H···A         C5—H5···S2 <sup>i</sup> 0.93       2.97       3.834 (2)       155	N1—C5—C6		122.24 (18)	C9—S1—C6		90.44 (11)	
Hydrogen-bond geometry (Å, °) $D$ —H       H···A $D$ ···A $D$ —H···A         C5—H5···S2 <sup>i</sup> 0.93       2.97       3.834 (2)       155	N1—C5—H5		118.9	C2—S2—C4 89.94 (10)		94 (10)	
D—H···A $D$ —H     H···A $D$ ···A $D$ —H···A       C5—H5···S2 <sup>i</sup> 0.93     2.97     3.834 (2)     155	Hydrogen-bond s	geometry (Å, °)					
C5—H5···S2 <sup>i</sup> 0.93 2.97 3.834 (2) 155	D—H…A			D—H	H…A	$D^{\dots}A$	D—H··· $A$
	C5—H5····S2 <sup>i</sup>			0.93	2.97	3.834 (2)	155

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



Fig. 1