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1-(Thiophen-2-yl)-N-(4-[(E)-[(thiophen-2-yl)methyl]iminomethyl]benzylidene)-methanamine

 Haleden Chiririwa,^{a*} John R. Moss,^a Denver Hendricks^b and Reinout Meijboom^c

^aDepartment of Chemistry, University of Cape Town, Private Bag, Rondebosch, 7707, South Africa, ^bDivision of Medical Biochemistry, Faculty of Health Sciences, Private Bag X3, Observatory 7935, South Africa, and ^cResearch Centre for Synthesis and Catalysis, Department of Chemistry, University of Johannesburg, PO Box 524 Auckland Park, Johannesburg, 2006, South Africa
Correspondence e-mail: harrychiririwa@yahoo.com

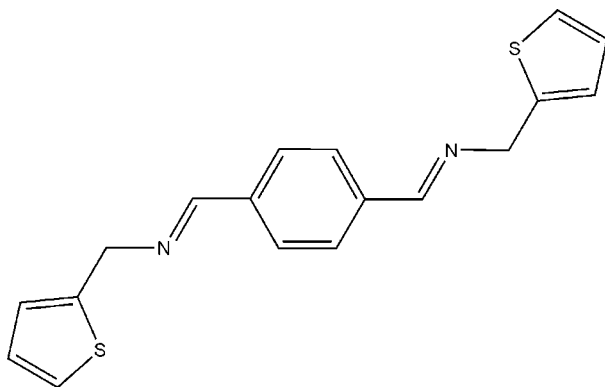
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; disorder in main residue; R factor = 0.045; wR factor = 0.125; data-to-parameter ratio = 15.9.

The title compound $\text{C}_{18}\text{H}_{16}\text{N}_2\text{S}_2$, crystallizes with two independent half-molecules in the asymmetric unit, in one of which the thiophene rings are disordered in a 0.67:0.33 ratio. Each independent molecule lies across a crystallographic centre of symmetry. The dihedral angle between central (half) benzene ring and the thiophene ring is 11.82° .

Related literature

For similar thiophenyldimine-based bridging ligands, see: Chakraborty *et al.* (1999); Haga & Koizumi (1985); Chiririwa *et al.* (2011a,b).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{16}\text{N}_2\text{S}_2$	$\gamma = 72.394$ (2) $^\circ$
$M_r = 324.45$	$V = 803.22$ (6) Å ³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 8.8517$ (3) Å	Mo $K\alpha$ radiation
$b = 10.3937$ (5) Å	$\mu = 0.33$ mm ⁻¹
$c = 10.5763$ (4) Å	$T = 173$ K
$\alpha = 63.836$ (2) $^\circ$	$0.22 \times 0.20 \times 0.13$ mm
$\beta = 69.023$ (2) $^\circ$	

Data collection

Nonius KappaCCD diffractometer	34407 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2007)	3282 independent reflections
$T_{\min} = 0.931$, $T_{\max} = 0.959$	2478 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.052$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$	9 restraints
$wR(F^2) = 0.125$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.34$ e Å ⁻³
3282 reflections	$\Delta\rho_{\text{min}} = -0.48$ e Å ⁻³
206 parameters	

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT-Plus (Bruker, 2007); data reduction: SAINT-Plus and XPREP (Bruker, 2007); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg & Putz, 2005), ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

Mintek and Project AuTEK are acknowledged for funding this project.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GO2071).

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1-(Thiophen-2-yl)-N-(4-{(E)-[(thiophen-2-yl)methyl]iminomethyl}benzylidene)methanamine

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S1. Comment

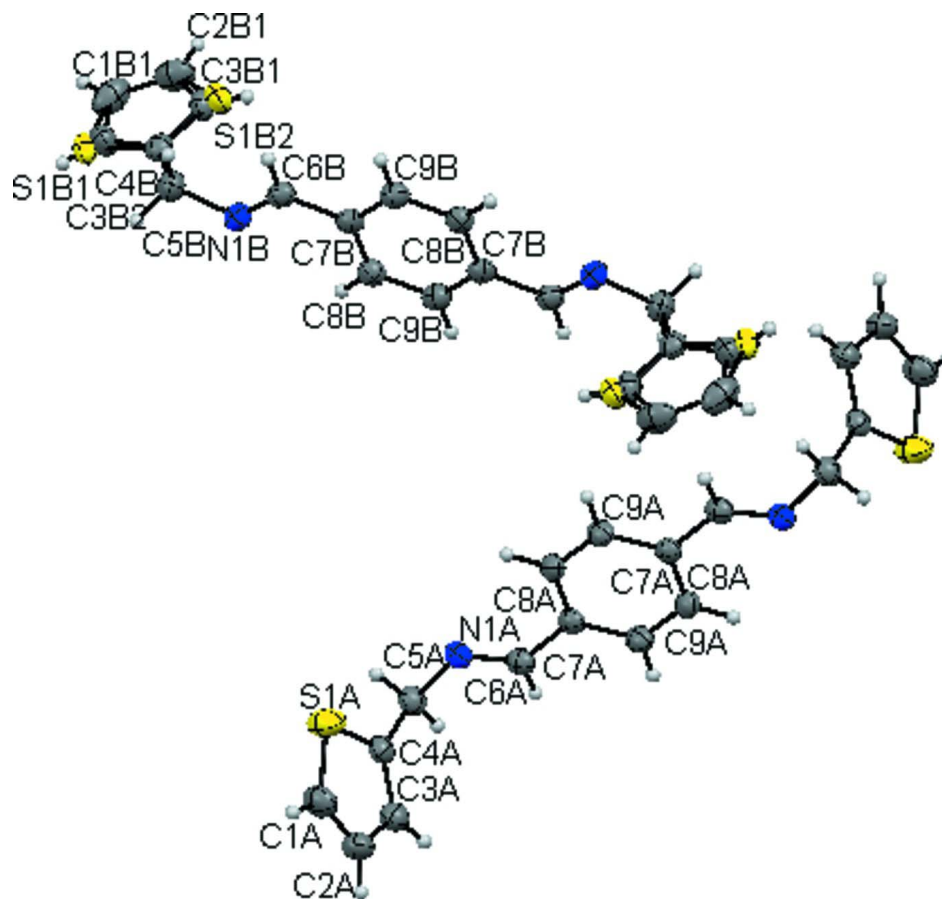
The title compound belongs to a class of tetradentate ligands. To the best of our knowledge, this is the second example of a neutral thiophenyldimine-based bridging ligand, the first of which was reported earlier by our group (Chiririwa *et al.*, 2011a) and (Chiririwa *et al.*, 2011b). This compound is expected to chelate in a tetradentate manner with both nitrogen atoms coordinating along with the two thiophenyl sulphur atoms. Chakraborty *et al.* reported coordination of similar ligands to ruthenium (Chakraborty *et al.* 1999) whilst Haga and Kiozumi reported their coordination to molybdenum, (Haga & Koizumi, 1985). The bond lengths N1A—C6A = 1.265 (3) and N1B—C6B = 1.266 (3) Å are consistent with C=N double bonding.

S2. Experimental

A solution of benzene 1,4-dicarboxaldehyde (0.50 g, 3.73 mmol) in methanol (10 ml) was added dropwise to a stirred solution of 2-thiophenylmethylamine (1.20 g, 7.42 mmol) in methanol (10 ml). The mixture stirred at room temperature for *ca* 16 h. The precipitate was filtered off and washed with diethylether and dried under vacuum for 4 h affording a white powder in 85% yield. Crystals suitable for X-ray determination were obtained by recrystallization from CH₂Cl₂–hexane mixture at room temperature.: Calc. for C₁₈H₁₆N₂S₂: C, 66.63%; H, 4.97%; N, 8.63%; S, 19.77 Found: C, 66.59%; H, 4.62%; N, 8.72%; S, 19.65 1H NMR: (400 MHz) ?H 8.38 (t, 2H, J = 1.3 Hz) 7.82 (s, 2H) 7.25 (m, 4H) 7.00 (d, 4H, J = 3.4 Hz) 5.00 (d, 4H, J = 1.3 Hz). IR (KBr): 1612 cm⁻¹ (C=N, imine)

S3. Refinement

The methine and aromatic H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with with C—H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic, C—H = 0.99 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH₂ C—H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH. Disorder refinement models were applied to the thiophenes of one independent molecule in the asymmetric unit. Geometrical (*FLAT*) restraints were applied to keep the ring C1B1-C2B2-C3B1-C3B2-S1B1-S1B2 planar. Bond distance (*DFIX*) and 1,3 distance similarity restraints (*SADI*) were applied to obtain reasonable geometries. Ellipsoid displacement (*SIMU* and *DELU*) restraints were also applied to the disordered moieties. Free variables were connected to the disordered component to add to unity.

**Figure 1**

The structure of the (1,4-phenylenebis(methan-1-yl-1-ylidene)) bis(1-(thiophen-2-yl)methanamine) showing 40% probability displacement ellipsoids. Hydrogen atoms were omitted for clarity.

1-(Thiophen-2-yl)-N-(4-((E)-[(thiophen-2-yl)methyl]iminomethyl)benzylidene)methanamine

Crystal data

$C_{18}H_{16}N_2S_2$

$M_r = 324.45$

Triclinic, $P\bar{1}$

Hall symbol: -p 1

$a = 8.8517(3) \text{ \AA}$

$b = 10.3937(5) \text{ \AA}$

$c = 10.5763(4) \text{ \AA}$

$\alpha = 63.836(2)^\circ$

$\beta = 69.023(2)^\circ$

$\gamma = 72.394(2)^\circ$

$V = 803.22(6) \text{ \AA}^3$

$Z = 2$

$F(000) = 340$

$D_x = 1.341 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 34407 reflections

$\theta = 2.9\text{--}26.4^\circ$

$\mu = 0.33 \text{ mm}^{-1}$

$T = 173 \text{ K}$

Plate, colourless

$0.22 \times 0.20 \times 0.13 \text{ mm}$

Data collection

Nonius KappaCCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$1.2^\circ \varphi$ scans and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2007)

$T_{\min} = 0.931$, $T_{\max} = 0.959$

34407 measured reflections

3282 independent reflections

2478 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$
 $\theta_{\text{max}} = 26.4^\circ$, $\theta_{\text{min}} = 2.9^\circ$

$h = 0 \rightarrow 11$
 $k = -11 \rightarrow 13$
 $l = -11 \rightarrow 13$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.125$
 $S = 1.06$
 3282 reflections
 206 parameters
 9 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
 $w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.4946P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.34 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.48 \text{ e } \text{\AA}^{-3}$

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.

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S1A	0.69140 (9)	-0.07229 (9)	0.71753 (8)	0.0551 (3)	
N1A	0.8877 (2)	0.1968 (2)	0.4771 (2)	0.0338 (5)	
C1A	0.4849 (3)	-0.0628 (3)	0.7957 (3)	0.0479 (7)	
H1A	0.4372	-0.1242	0.8918	0.058*	
C2A	0.3981 (3)	0.0419 (3)	0.7047 (3)	0.0431 (6)	
H2A	0.2815	0.0627	0.7295	0.052*	
C3A	0.4989 (3)	0.1187 (3)	0.5671 (3)	0.0383 (6)	
H3A	0.4571	0.1966	0.4905	0.046*	
C4A	0.6632 (3)	0.0676 (3)	0.5574 (3)	0.0322 (5)	
C5A	0.8063 (3)	0.1240 (3)	0.4339 (3)	0.0352 (6)	
H5A1	0.8850	0.0425	0.4092	0.042*	
H5A2	0.7678	0.1938	0.3465	0.042*	
C6A	0.8751 (3)	0.3337 (3)	0.4146 (3)	0.0312 (5)	
H6A	0.8204	0.3833	0.3389	0.037*	
C7A	0.9431 (3)	0.4184 (2)	0.4562 (2)	0.0284 (5)	
C8A	1.0455 (3)	0.3496 (3)	0.5499 (3)	0.0327 (5)	
H8A	1.0777	0.2468	0.5838	0.039*	
C9A	0.8997 (3)	0.5696 (3)	0.4064 (3)	0.0334 (5)	
H9A	0.8313	0.6177	0.3413	0.040*	
N1B	0.1122 (2)	0.6222 (2)	1.0089 (2)	0.0352 (5)	
C4B	0.3208 (3)	0.4419 (2)	0.9269 (3)	0.0335 (5)	
C5B	0.1887 (3)	0.4689 (3)	1.0535 (3)	0.0366 (6)	

H5B1	0.1048	0.4074	1.0881	0.044*	
H5B2	0.2367	0.4426	1.1349	0.044*	
C6B	0.1358 (3)	0.6967 (3)	1.0657 (3)	0.0324 (5)	
H6B	0.2009	0.6504	1.1335	0.039*	
C7B	0.0661 (3)	0.8528 (3)	1.0305 (3)	0.0316 (5)	
C8B	-0.0294 (3)	0.9267 (3)	0.9307 (3)	0.0327 (5)	
H8B	-0.0496	0.8767	0.8833	0.039*	
C9B	0.0946 (3)	0.9276 (3)	1.0991 (3)	0.0332 (5)	
H9B	0.1595	0.8779	1.1670	0.040*	
S1B1	0.34911 (15)	0.29538 (12)	0.88477 (13)	0.0351 (3)	0.67
C1B1	0.5072 (4)	0.3432 (3)	0.7441 (3)	0.0555 (8)	
H1B1	0.5647	0.2863	0.6858	0.067*	
C2B1	0.5492 (3)	0.4673 (3)	0.7172 (3)	0.0534 (8)	
H2B1	0.6371	0.5103	0.6402	0.064*	
C3B1	0.4387 (8)	0.5249 (7)	0.8248 (6)	0.0351 (3)	0.67
H3B1	0.4460	0.6137	0.8260	0.042*	0.67
S1B2	0.4503 (4)	0.5553 (3)	0.8214 (4)	0.0443 (7)	0.33
C3B2	0.3679 (13)	0.3308 (11)	0.8727 (12)	0.0443 (7)	0.33
H3B2	0.3115	0.2505	0.9179	0.053*	0.33

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0367 (4)	0.0570 (5)	0.0504 (5)	-0.0094 (3)	-0.0160 (3)	0.0026 (4)
N1A	0.0311 (11)	0.0349 (11)	0.0371 (11)	-0.0090 (9)	-0.0081 (9)	-0.0134 (9)
C1A	0.0417 (15)	0.0519 (17)	0.0424 (16)	-0.0179 (13)	-0.0059 (12)	-0.0085 (13)
C2A	0.0320 (13)	0.0457 (15)	0.0534 (17)	-0.0068 (11)	-0.0105 (12)	-0.0204 (13)
C3A	0.0357 (13)	0.0390 (14)	0.0441 (15)	-0.0068 (11)	-0.0132 (11)	-0.0167 (12)
C4A	0.0354 (13)	0.0311 (12)	0.0367 (13)	-0.0079 (10)	-0.0115 (10)	-0.0155 (10)
C5A	0.0368 (13)	0.0357 (13)	0.0384 (14)	-0.0084 (11)	-0.0099 (11)	-0.0171 (11)
C6A	0.0295 (12)	0.0350 (13)	0.0275 (12)	-0.0078 (10)	-0.0066 (9)	-0.0097 (10)
C7A	0.0260 (11)	0.0302 (12)	0.0252 (11)	-0.0086 (9)	-0.0034 (9)	-0.0073 (9)
C8A	0.0319 (12)	0.0281 (12)	0.0344 (13)	-0.0068 (10)	-0.0098 (10)	-0.0064 (10)
C9A	0.0324 (12)	0.0332 (13)	0.0317 (13)	-0.0070 (10)	-0.0135 (10)	-0.0049 (10)
N1B	0.0316 (11)	0.0335 (11)	0.0402 (12)	-0.0020 (9)	-0.0094 (9)	-0.0160 (9)
C4B	0.0346 (13)	0.0326 (13)	0.0354 (13)	-0.0008 (10)	-0.0162 (10)	-0.0123 (10)
C5B	0.0391 (14)	0.0308 (12)	0.0384 (14)	-0.0037 (10)	-0.0112 (11)	-0.0125 (11)
C6B	0.0275 (12)	0.0340 (13)	0.0324 (13)	-0.0038 (10)	-0.0063 (10)	-0.0118 (10)
C7B	0.0252 (11)	0.0348 (13)	0.0322 (13)	-0.0048 (10)	-0.0033 (9)	-0.0137 (10)
C8B	0.0313 (12)	0.0356 (13)	0.0330 (13)	-0.0078 (10)	-0.0049 (10)	-0.0158 (10)
C9B	0.0287 (12)	0.0367 (13)	0.0328 (13)	-0.0047 (10)	-0.0079 (10)	-0.0126 (10)
S1B1	0.0441 (6)	0.0294 (6)	0.0375 (5)	-0.0095 (4)	-0.0131 (4)	-0.0136 (5)
C1B1	0.0624 (19)	0.0591 (19)	0.0555 (19)	0.0135 (15)	-0.0272 (16)	-0.0368 (16)
C2B1	0.0373 (15)	0.067 (2)	0.0419 (16)	-0.0066 (14)	-0.0023 (12)	-0.0158 (14)
C3B1	0.0441 (6)	0.0294 (6)	0.0375 (5)	-0.0095 (4)	-0.0131 (4)	-0.0136 (5)
S1B2	0.0408 (12)	0.0379 (16)	0.0556 (13)	-0.0146 (10)	-0.0074 (10)	-0.0177 (11)
C3B2	0.0408 (12)	0.0379 (16)	0.0556 (13)	-0.0146 (10)	-0.0074 (10)	-0.0177 (11)

Geometric parameters (Å, °)

S1A—C1A	1.708 (3)	C4B—C3B2	1.399 (5)
S1A—C4A	1.719 (3)	C4B—C5B	1.500 (3)
N1A—C6A	1.265 (3)	C4B—S1B2	1.640 (3)
N1A—C5A	1.473 (3)	C4B—S1B1	1.694 (2)
C1A—C2A	1.342 (4)	C5B—H5B1	0.9900
C1A—H1A	0.9500	C5B—H5B2	0.9900
C2A—C3A	1.424 (4)	C6B—C7B	1.476 (3)
C2A—H2A	0.9500	C6B—H6B	0.9500
C3A—C4A	1.372 (3)	C7B—C9B	1.394 (3)
C3A—H3A	0.9500	C7B—C8B	1.396 (3)
C4A—C5A	1.498 (3)	C8B—C9B ⁱⁱ	1.381 (3)
C5A—H5A1	0.9900	C8B—H8B	0.9500
C5A—H5A2	0.9900	C9B—C8B ⁱⁱ	1.381 (3)
C6A—C7A	1.478 (3)	C9B—H9B	0.9500
C6A—H6A	0.9500	S1B1—C1B1	1.642 (3)
C7A—C8A	1.394 (3)	C1B1—C2B1	1.332 (3)
C7A—C9A	1.394 (3)	C1B1—C3B2	1.459 (5)
C8A—C9A ⁱ	1.380 (3)	C1B1—H1B1	0.9500
C8A—H8A	0.9500	C2B1—C3B1	1.435 (5)
C9A—C8A ⁱ	1.380 (3)	C2B1—S1B2	1.591 (3)
C9A—H9A	0.9500	C2B1—H2B1	0.9500
N1B—C6B	1.266 (3)	C3B1—H3B1	0.9500
N1B—C5B	1.461 (3)	C3B2—H3B2	0.9500
C4B—C3B1	1.384 (5)		
C1A—S1A—C4A	92.37 (13)	C5B—C4B—S1B1	123.56 (17)
C6A—N1A—C5A	117.3 (2)	S1B2—C4B—S1B1	115.94 (16)
C2A—C1A—S1A	111.7 (2)	N1B—C5B—C4B	109.8 (2)
C2A—C1A—H1A	124.1	N1B—C5B—H5B1	109.7
S1A—C1A—H1A	124.1	C4B—C5B—H5B1	109.7
C1A—C2A—C3A	113.0 (2)	N1B—C5B—H5B2	109.7
C1A—C2A—H2A	123.5	C4B—C5B—H5B2	109.7
C3A—C2A—H2A	123.5	H5B1—C5B—H5B2	108.2
C4A—C3A—C2A	112.4 (2)	N1B—C6B—C7B	122.5 (2)
C4A—C3A—H3A	123.8	N1B—C6B—H6B	118.8
C2A—C3A—H3A	123.8	C7B—C6B—H6B	118.8
C3A—C4A—C5A	128.2 (2)	C9B—C7B—C8B	119.3 (2)
C3A—C4A—S1A	110.46 (19)	C9B—C7B—C6B	119.5 (2)
C5A—C4A—S1A	121.24 (18)	C8B—C7B—C6B	121.2 (2)
N1A—C5A—C4A	109.30 (19)	C9B ⁱⁱ —C8B—C7B	120.0 (2)
N1A—C5A—H5A1	109.8	C9B ⁱⁱ —C8B—H8B	120.0
C4A—C5A—H5A1	109.8	C7B—C8B—H8B	120.0
N1A—C5A—H5A2	109.8	C8B ⁱⁱ —C9B—C7B	120.7 (2)
C4A—C5A—H5A2	109.8	C8B ⁱⁱ —C9B—H9B	119.7
H5A1—C5A—H5A2	108.3	C7B—C9B—H9B	119.7
N1A—C6A—C7A	121.8 (2)	C1B1—S1B1—C4B	94.00 (13)

N1A—C6A—H6A	119.1	C2B1—C1B1—C3B2	102.2 (3)
C7A—C6A—H6A	119.1	C2B1—C1B1—S1B1	115.4 (2)
C8A—C7A—C9A	118.8 (2)	C2B1—C1B1—H1B1	122.3
C8A—C7A—C6A	121.2 (2)	C3B2—C1B1—H1B1	135.5
C9A—C7A—C6A	120.0 (2)	S1B1—C1B1—H1B1	122.3
C9A ⁱ —C8A—C7A	120.2 (2)	C1B1—C2B1—C3B1	108.1 (3)
C9A ⁱ —C8A—H8A	119.9	C1B1—C2B1—S1B2	119.7 (2)
C7A—C8A—H8A	119.9	C1B1—C2B1—H2B1	126.0
C8A ⁱ —C9A—C7A	121.1 (2)	C3B1—C2B1—H2B1	126.0
C8A ⁱ —C9A—H9A	119.5	S1B2—C2B1—H2B1	114.3
C7A—C9A—H9A	119.5	C4B—C3B1—C2B1	115.3 (4)
C6B—N1B—C5B	116.7 (2)	C4B—C3B1—H3B1	122.3
C3B1—C4B—C3B2	97.2 (4)	C2B1—C3B1—H3B1	122.3
C3B1—C4B—C5B	129.2 (3)	C2B1—S1B2—C4B	94.97 (16)
C3B2—C4B—C5B	133.6 (3)	C4B—C3B2—C1B1	117.2 (5)
C3B2—C4B—S1B2	105.9 (3)	C4B—C3B2—H3B2	121.4
C5B—C4B—S1B2	120.50 (18)	C1B1—C3B2—H3B2	121.4
C3B1—C4B—S1B1	107.2 (3)		
C4A—S1A—C1A—C2A	-0.1 (2)	C3B1—C4B—S1B1—C1B1	0.7 (4)
S1A—C1A—C2A—C3A	-0.2 (3)	C3B2—C4B—S1B1—C1B1	-2 (4)
C1A—C2A—C3A—C4A	0.5 (3)	C5B—C4B—S1B1—C1B1	-179.4 (2)
C2A—C3A—C4A—C5A	-177.0 (2)	S1B2—C4B—S1B1—C1B1	-0.5 (2)
C2A—C3A—C4A—S1A	-0.6 (3)	C4B—S1B1—C1B1—C2B1	-0.5 (3)
C1A—S1A—C4A—C3A	0.4 (2)	C4B—S1B1—C1B1—C3B2	2 (3)
C1A—S1A—C4A—C5A	177.1 (2)	C3B2—C1B1—C2B1—C3B1	-0.3 (9)
C6A—N1A—C5A—C4A	-110.5 (2)	S1B1—C1B1—C2B1—C3B1	0.2 (5)
C3A—C4A—C5A—N1A	108.5 (3)	C3B2—C1B1—C2B1—S1B2	0.9 (7)
S1A—C4A—C5A—N1A	-67.7 (2)	S1B1—C1B1—C2B1—S1B2	1.5 (4)
C5A—N1A—C6A—C7A	176.1 (2)	C3B2—C4B—C3B1—C2B1	-0.2 (8)
N1A—C6A—C7A—C8A	10.0 (3)	C5B—C4B—C3B1—C2B1	179.4 (3)
N1A—C6A—C7A—C9A	-167.3 (2)	S1B2—C4B—C3B1—C2B1	172 (4)
C9A—C7A—C8A—C9A ⁱ	0.9 (4)	S1B1—C4B—C3B1—C2B1	-0.7 (7)
C6A—C7A—C8A—C9A ⁱ	-176.4 (2)	C1B1—C2B1—C3B1—C4B	0.4 (7)
C8A—C7A—C9A—C8A ⁱ	-0.9 (4)	S1B2—C2B1—C3B1—C4B	-174 (3)
C6A—C7A—C9A—C8A ⁱ	176.4 (2)	C1B1—C2B1—S1B2—C4B	-1.5 (4)
C6B—N1B—C5B—C4B	-112.6 (2)	C3B1—C2B1—S1B2—C4B	4 (2)
C3B1—C4B—C5B—N1B	42.8 (6)	C3B1—C4B—S1B2—C2B1	-6 (3)
C3B2—C4B—C5B—N1B	-137.8 (9)	C3B2—C4B—S1B2—C2B1	1.4 (8)
S1B2—C4B—C5B—N1B	44.0 (3)	C5B—C4B—S1B2—C2B1	-179.9 (2)
S1B1—C4B—C5B—N1B	-137.1 (2)	S1B1—C4B—S1B2—C2B1	1.1 (3)
C5B—N1B—C6B—C7B	179.9 (2)	C3B1—C4B—C3B2—C1B1	-0.1 (11)
N1B—C6B—C7B—C9B	178.8 (2)	C5B—C4B—C3B2—C1B1	-179.6 (5)
N1B—C6B—C7B—C8B	-0.5 (4)	S1B2—C4B—C3B2—C1B1	-1.2 (13)
C9B—C7B—C8B—C9B ⁱⁱ	0.0 (4)	S1B1—C4B—C3B2—C1B1	177 (5)
C6B—C7B—C8B—C9B ⁱⁱ	179.3 (2)	C2B1—C1B1—C3B2—C4B	0.3 (12)

C8B—C7B—C9B—C8B ⁱⁱ	0.0 (4)	S1B1—C1B1—C3B2—C4B	-178 (4)
C6B—C7B—C9B—C8B ⁱⁱ	-179.3 (2)		

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