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## 3-[(*N*-Methylanilino)methyl]-5-(thiophen-2-yl)-1,3,4-oxadiazole-2(3*H*)-thione

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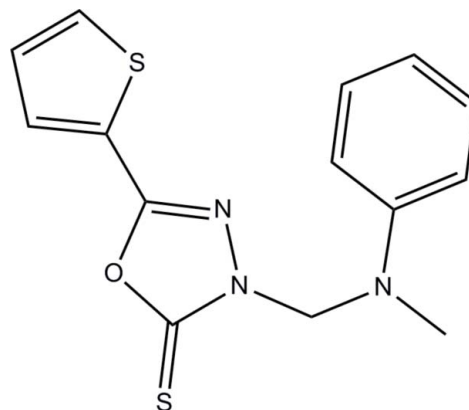
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å; disorder in main residue;  $R$  factor = 0.048;  $wR$  factor = 0.156; data-to-parameter ratio = 12.2.

In the title compound,  $\text{C}_{14}\text{H}_{13}\text{N}_3\text{OS}_2$ , the thiophene ring is disordered over two orientations by *ca* 180° about the C—C bond axis linking the ring to the rest of the molecule, with a site-occupancy ratio of 0.651 (5):0.349 (5). The central 1,3,4-oxadiazole-2(3*H*)-thione ring forms dihedral angles of 9.2 (5), 4.6 (11) and 47.70 (7)° with the major and minor parts of the disordered thiophene ring and the terminal phenyl ring, respectively. In the crystal, no significant intermolecular hydrogen bonds are observed. The crystal packing is stabilized by  $\pi$ – $\pi$  interactions [centroid–centroid distance = 3.589 (2) Å].

### Related literature

For the biological activity of 1,3,4-oxadiazole derivatives, see: Navarrete-Vázquez *et al.* (2007); Kadi *et al.* (2007); Padmavathi *et al.* (2009); El-Emam *et al.* (2004); Al-Deeb *et al.* (2006). For the synthesis of the title compound, see: Al-Omar (2010). For related 1,3,4-oxadiazole structures, see: Fun *et al.* (2011); El-Emam *et al.* (2012).



### Experimental

#### Crystal data

$\text{C}_{14}\text{H}_{13}\text{N}_3\text{OS}_2$   
 $M_r = 303.39$   
Monoclinic,  $P2_1/n$   
 $a = 11.9682$  (8) Å  
 $b = 7.4526$  (5) Å  
 $c = 17.0749$  (14) Å  
 $\beta = 108.072$  (6)°

$V = 1447.85$  (18) Å<sup>3</sup>  
 $Z = 4$   
Cu  $K\alpha$  radiation  
 $\mu = 3.32$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.92 \times 0.16 \times 0.09$  mm

#### Data collection

Bruker SMART APEXII CCD  
area-detector diffractometer  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 2009)  
 $T_{\min} = 0.150$ ,  $T_{\max} = 0.754$

10021 measured reflections  
2676 independent reflections  
1516 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.066$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.156$   
 $S = 0.97$   
2676 reflections

220 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.20$  e Å<sup>-3</sup>

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5107).

‡ Thomson Reuters ResearcherID: A-3561-2009.

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## supplementary materials

*Acta Cryst.* (2012). E68, o1345–o1346 [doi:10.1107/S1600536812014419]

**3-[(*N*-Methylanilino)methyl]-5-(thiophen-2-yl)-1,3,4-oxadiazole-2(3*H*)-thione**

**Ali A. El-Emam, Mohamed A. Al-Omar, Hazem A. Ghabbour, Hoong-Kun Fun and Tze Shyang Chia**

**Comment**

Considerable attention has been devoted to 1,3,4-oxadiazole derivatives which have long been known for their diverse chemotherapeutic properties as antiviral agents against the HIV-1 viruses (El-Emam *et al.*, 2004), antibacterial agents (Navarrete-Vázquez *et al.*, 2007; Padmavathi *et al.*, 2009) and anti-inflammatory agents (Kadi *et al.*, 2007; Al-Deeb *et al.*, 2006). The title compound (I) was synthesized among a series of 2-thienyl-1,3,4-oxadiazoles and related derivatives as potential antimicrobial agents (Al-Omar, 2010).

The molecular structure of the title compound is shown in Fig. 1. The thiophene ring is disordered by *ca.* 180° rotation about the C2—C3 bond axis with a site-occupancy ratio of 0.651 (5):0.349 (5). The central 1,3,4-oxadiazole-2(3*H*)-thione ring (N1/N2/C1/O1/C2/S2; maximum deviation = 0.0157 (12) Å at atom S2) forms dihedral angles of 9.23 (51), 4.6 (11) and 47.70 (7)° with the major and minor parts of the disordered thiophene ring [S1/C3—C6: maximum deviation = 0.024 (11) Å at atom C4 and S1A/C3/C4A—C6A: maximum deviation = 0.04 (3) Å at atom C6A] and the terminal phenyl ring (C9—C14), respectively.

In the crystal packing, no significant intermolecular hydrogen bondings are observed. The crystal packing is stabilized by a  $\pi$ – $\pi$  interaction with Cg2...Cg4 distance = 3.589 (2) Å (symmetry code: 3/2-*x*, -1/2+*y*, 3/2-*z*), where Cg2 and Cg4 are the centroids of O1/C1/C2/N1/N2 and C9—C14 rings, respectively.

**Experimental**

*N*-Methylaniline (214 mg, 2 mmol) and 37% formaldehyde solution (0.5 ml) were added to a solution of 5-(thiophen-2-yl)-1,3,4-oxadiazole-2-thiol (369 mg, 2 mmol) in ethanol (8 ml). The mixture was stirred at room temperature for 2 h and allowed to stand overnight. The precipitated crude product was filtered, washed with cold ethanol, dried, and crystallized from ethanol to yield 558 mg (92%) of the title compound (I) as colorless needle crystals. *M.p.*: 112–114 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500.13 MHz):  $\delta$  3.28 (s, 3H, CH<sub>3</sub>), 5.64 (d, 2H, NCH<sub>2</sub>N), 6.83–7.36 (m, 6H, Ar—H & Thiophene-H), 7.55 (d, 1H, Thiophene-H, *J* = 5.0 Hz), 7.70 (d, 1H, Thiophene-H, *J* = 5.0 Hz). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125.76 MHz):  $\delta$  39.54 (CH<sub>3</sub>), 66.80 (CH<sub>2</sub>), 113.72, 119.12, 123.65, 128.30, 129.36, 130.36, 131.07, 146.69 (Ar—C & Thiophene-C), 155.89 (Oxadiazole C-5), 176.32 (C=S).

**Refinement**

All H atoms were positioned geometrically (C—H = 0.93, 0.96 or 0.97 Å) and refined using a riding model with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5U_{\text{eq}}(\text{C})$ . A rotating group model was applied to the methyl group. Initially similarity and FLAT (only to the minor component) restraints were used. In the final refinement, these restraints were removed and the ratio of the refined site occupancies for the major and minor components of the disordered thiophene ring is 0.651 (5):0.349 (5).

## Computing details

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

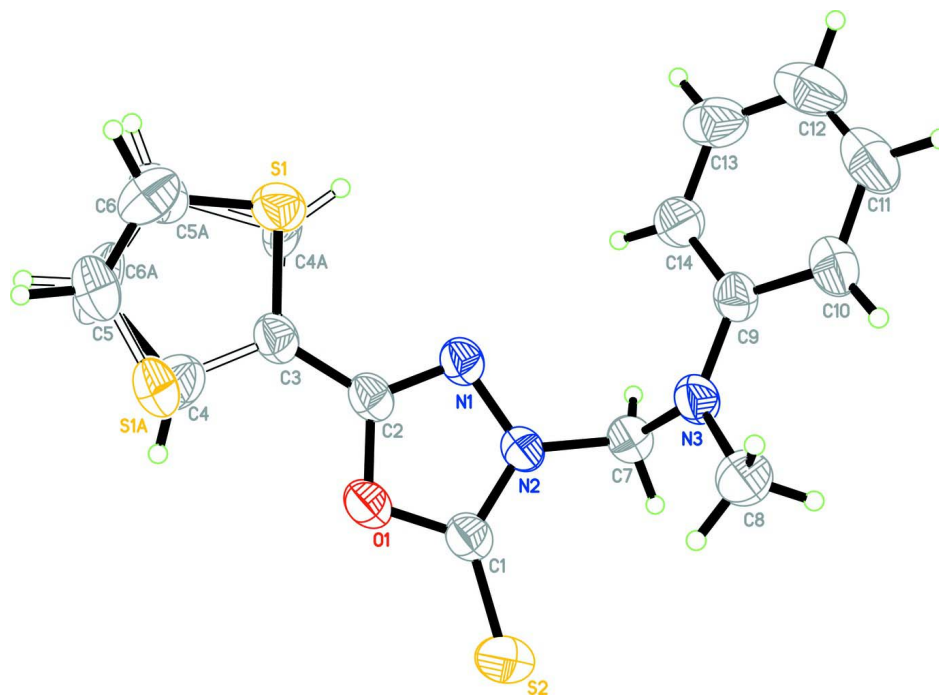


Figure 1

The molecular structure of the title compound with atom labels and 30% probability displacement ellipsoids. Atoms of the minor occupancy component are labelled with the suffix *A*.

3-[(*N*-Methylanilino)methyl]-5-(thiophen-2-yl)-1,3,4-oxadiazole- 2(3*H*)-thione*Crystal data*

$C_{14}H_{13}N_3OS_2$   
 $M_r = 303.39$   
 Monoclinic,  $P2_1/n$   
 Hall symbol:  $-P\ 2_1/n$   
 $a = 11.9682(8)\ \text{\AA}$   
 $b = 7.4526(5)\ \text{\AA}$   
 $c = 17.0749(14)\ \text{\AA}$   
 $\beta = 108.072(6)^\circ$   
 $V = 1447.85(18)\ \text{\AA}^3$   
 $Z = 4$

$F(000) = 632$   
 $D_x = 1.392\ \text{Mg m}^{-3}$   
 Cu  $K\alpha$  radiation,  $\lambda = 1.54178\ \text{\AA}$   
 Cell parameters from 587 reflections  
 $\theta = 4.0\text{--}45.3^\circ$   
 $\mu = 3.32\ \text{mm}^{-1}$   
 $T = 296\ \text{K}$   
 Needle, colorless  
 $0.92 \times 0.16 \times 0.09\ \text{mm}$

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2009)  
 $T_{\min} = 0.150$ ,  $T_{\max} = 0.754$   
 10021 measured reflections  
 2676 independent reflections  
 1516 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.066$   
 $\theta_{\text{max}} = 69.5^\circ$ ,  $\theta_{\text{min}} = 4.0^\circ$   
 $h = -14 \rightarrow 14$

$k = -8 \rightarrow 7$   
 $l = -20 \rightarrow 18$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.156$   
 $S = 0.97$   
 2676 reflections  
 220 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0811P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.16 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.20 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: *SHELXTL* (Sheldrick,  
 2008),  $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0019 (4)

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S2	0.86759 (10)	0.22270 (15)	1.02672 (6)	0.0941 (4)	
O1	0.6522 (2)	0.3191 (3)	0.93576 (13)	0.0697 (6)	
N1	0.6491 (2)	0.2726 (3)	0.80711 (15)	0.0627 (7)	
N2	0.7564 (2)	0.2228 (3)	0.86200 (15)	0.0628 (6)	
N3	0.8999 (2)	0.2802 (4)	0.79288 (16)	0.0707 (7)	
C1	0.7617 (3)	0.2516 (4)	0.94048 (19)	0.0672 (8)	
C2	0.5908 (3)	0.3288 (4)	0.85393 (19)	0.0620 (8)	
C3	0.4743 (3)	0.4013 (4)	0.8291 (2)	0.0651 (8)	
C4	0.413 (2)	0.451 (3)	0.8829 (15)	0.093 (8)	0.651 (5)
H4A	0.4370	0.4340	0.9396	0.111*	0.651 (5)
C5	0.2989 (18)	0.542 (3)	0.8296 (11)	0.083 (5)	0.651 (5)
H5A	0.2436	0.5951	0.8503	0.100*	0.651 (5)
C6	0.2904 (15)	0.533 (2)	0.7508 (13)	0.092 (5)	0.651 (5)
H6A	0.2254	0.5768	0.7096	0.110*	0.651 (5)
S1	0.4025 (5)	0.4400 (7)	0.7304 (4)	0.0799 (9)	0.651 (5)
S1A	0.4022 (12)	0.4715 (16)	0.8908 (8)	0.0785 (19)	0.349 (5)
C6A	0.293 (3)	0.522 (6)	0.825 (3)	0.125 (17)	0.349 (5)
H6AA	0.2263	0.5592	0.8375	0.150*	0.349 (5)
C5A	0.292 (3)	0.512 (4)	0.745 (2)	0.112 (13)	0.349 (5)
H5AA	0.2322	0.5508	0.6995	0.135*	0.349 (5)
C4A	0.416 (3)	0.420 (5)	0.745 (2)	0.090 (13)	0.349 (5)

H4AA	0.4405	0.3878	0.7008	0.108*	0.349 (5)
C7	0.8480 (3)	0.1488 (4)	0.83120 (19)	0.0694 (8)	
H7A	0.9088	0.0953	0.8767	0.083*	
H7B	0.8143	0.0545	0.7918	0.083*	
C8	0.9964 (3)	0.3838 (6)	0.8467 (2)	0.0919 (12)	
H8A	0.9945	0.5035	0.8255	0.138*	
H8B	1.0697	0.3280	0.8492	0.138*	
H8C	0.9887	0.3883	0.9010	0.138*	
C9	0.8762 (3)	0.2882 (4)	0.70804 (19)	0.0638 (8)	
C10	0.9562 (3)	0.3627 (4)	0.6735 (2)	0.0806 (10)	
H10A	1.0280	0.4050	0.7073	0.097*	
C11	0.9293 (5)	0.3740 (6)	0.5890 (3)	0.1074 (15)	
H11A	0.9838	0.4249	0.5669	0.129*	
C12	0.8256 (6)	0.3131 (7)	0.5371 (3)	0.1167 (17)	
H12A	0.8090	0.3218	0.4803	0.140*	
C13	0.7459 (4)	0.2383 (5)	0.5709 (3)	0.0997 (14)	
H13A	0.6744	0.1965	0.5363	0.120*	
C14	0.7697 (3)	0.2240 (4)	0.6550 (2)	0.0766 (9)	
H14A	0.7150	0.1717	0.6764	0.092*	

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S2	0.0998 (8)	0.1138 (8)	0.0625 (6)	0.0053 (5)	0.0162 (5)	-0.0036 (5)
O1	0.0771 (16)	0.0794 (14)	0.0594 (13)	-0.0076 (10)	0.0311 (12)	-0.0051 (9)
N1	0.0636 (17)	0.0670 (14)	0.0627 (15)	-0.0058 (12)	0.0270 (14)	-0.0015 (11)
N2	0.0631 (18)	0.0750 (15)	0.0545 (14)	-0.0025 (12)	0.0245 (14)	-0.0021 (11)
N3	0.0626 (17)	0.0918 (18)	0.0619 (16)	-0.0176 (12)	0.0255 (14)	-0.0119 (13)
C1	0.071 (2)	0.0719 (19)	0.0627 (19)	-0.0063 (14)	0.0268 (18)	-0.0024 (13)
C2	0.068 (2)	0.0644 (18)	0.0607 (18)	-0.0118 (14)	0.0297 (17)	-0.0054 (13)
C3	0.063 (2)	0.0739 (19)	0.065 (2)	-0.0117 (14)	0.030 (2)	-0.0079 (15)
C4	0.076 (11)	0.096 (9)	0.093 (13)	-0.001 (6)	0.010 (8)	-0.011 (6)
C5	0.092 (12)	0.080 (6)	0.099 (9)	-0.013 (5)	0.059 (9)	-0.012 (5)
C6	0.067 (9)	0.082 (6)	0.105 (11)	0.002 (5)	-0.002 (7)	0.002 (6)
S1	0.071 (2)	0.1025 (17)	0.0634 (11)	-0.0140 (14)	0.0171 (11)	-0.0039 (14)
S1A	0.082 (4)	0.087 (3)	0.082 (3)	-0.006 (3)	0.049 (3)	-0.006 (3)
C6A	0.044 (17)	0.13 (3)	0.20 (3)	0.002 (14)	0.03 (2)	-0.03 (2)
C5A	0.077 (18)	0.18 (3)	0.09 (2)	-0.040 (14)	0.050 (15)	0.024 (17)
C4A	0.044 (12)	0.130 (18)	0.11 (3)	0.011 (9)	0.041 (15)	0.031 (12)
C7	0.070 (2)	0.0747 (19)	0.067 (2)	0.0020 (15)	0.0258 (17)	0.0004 (15)
C8	0.077 (3)	0.115 (3)	0.080 (2)	-0.026 (2)	0.020 (2)	-0.016 (2)
C9	0.065 (2)	0.0672 (17)	0.0646 (19)	0.0082 (14)	0.0283 (17)	-0.0042 (13)
C10	0.088 (3)	0.078 (2)	0.090 (3)	0.0077 (17)	0.048 (2)	0.0057 (17)
C11	0.147 (4)	0.096 (3)	0.109 (4)	0.034 (3)	0.082 (3)	0.026 (3)
C12	0.175 (5)	0.110 (4)	0.072 (3)	0.050 (3)	0.049 (3)	0.013 (2)
C13	0.117 (4)	0.099 (3)	0.072 (2)	0.027 (2)	0.014 (3)	-0.010 (2)
C14	0.080 (2)	0.080 (2)	0.070 (2)	0.0079 (17)	0.024 (2)	-0.0098 (16)

Geometric parameters (Å, °)

S2—C1	1.632 (3)	C6A—C5A	1.35 (6)
O1—C2	1.364 (3)	C6A—H6AA	0.9300
O1—C1	1.382 (4)	C5A—C4A	1.63 (5)
N1—C2	1.283 (4)	C5A—H5AA	0.9300
N1—N2	1.385 (3)	C4A—H4AA	0.9300
N2—C1	1.339 (4)	C7—H7A	0.9700
N2—C7	1.464 (4)	C7—H7B	0.9700
N3—C9	1.388 (4)	C8—H8A	0.9600
N3—C7	1.423 (4)	C8—H8B	0.9600
N3—C8	1.455 (4)	C8—H8C	0.9600
C2—C3	1.432 (4)	C9—C10	1.386 (4)
C3—C4	1.388 (19)	C9—C14	1.400 (5)
C3—C4A	1.39 (3)	C10—C11	1.379 (5)
C3—S1A	1.641 (12)	C10—H10A	0.9300
C3—S1	1.663 (6)	C11—C12	1.360 (6)
C4—C5	1.55 (3)	C11—H11A	0.9300
C4—H4A	0.9300	C12—C13	1.377 (6)
C5—C6	1.32 (3)	C12—H12A	0.9300
C5—H5A	0.9300	C13—C14	1.378 (5)
C6—S1	1.641 (19)	C13—H13A	0.9300
C6—H6A	0.9300	C14—H14A	0.9300
S1A—C6A	1.49 (5)		
C2—O1—C1	106.2 (2)	C6A—C5A—C4A	107 (3)
C2—N1—N2	103.6 (2)	C6A—C5A—H5AA	126.3
C1—N2—N1	112.3 (3)	C4A—C5A—H5AA	126.3
C1—N2—C7	127.7 (3)	C3—C4A—C5A	102 (2)
N1—N2—C7	119.9 (2)	C3—C4A—H4AA	128.9
C9—N3—C7	122.2 (3)	C5A—C4A—H4AA	128.9
C9—N3—C8	120.1 (3)	N3—C7—N2	112.9 (3)
C7—N3—C8	116.7 (3)	N3—C7—H7A	109.0
N2—C1—O1	104.5 (3)	N2—C7—H7A	109.0
N2—C1—S2	131.6 (3)	N3—C7—H7B	109.0
O1—C1—S2	123.9 (2)	N2—C7—H7B	109.0
N1—C2—O1	113.4 (3)	H7A—C7—H7B	107.8
N1—C2—C3	127.3 (3)	N3—C8—H8A	109.5
O1—C2—C3	119.3 (3)	N3—C8—H8B	109.5
C4—C3—C4A	116.9 (19)	H8A—C8—H8B	109.5
C4—C3—C2	124.6 (12)	N3—C8—H8C	109.5
C4A—C3—C2	118.5 (15)	H8A—C8—H8C	109.5
C4A—C3—S1A	115.5 (15)	H8B—C8—H8C	109.5
C2—C3—S1A	126.0 (6)	C10—C9—N3	121.1 (3)
C4—C3—S1	114.3 (12)	C10—C9—C14	118.1 (3)
C2—C3—S1	121.0 (3)	N3—C9—C14	120.7 (3)
S1A—C3—S1	112.7 (6)	C11—C10—C9	120.1 (4)
C3—C4—C5	106.2 (16)	C11—C10—H10A	119.9
C3—C4—H4A	126.9	C9—C10—H10A	119.9
C5—C4—H4A	126.9	C12—C11—C10	122.1 (4)

C6—C5—C4	110.7 (15)	C12—C11—H11A	119.0
C6—C5—H5A	124.7	C10—C11—H11A	119.0
C4—C5—H5A	124.7	C11—C12—C13	118.2 (4)
C5—C6—S1	115.3 (13)	C11—C12—H12A	120.9
C5—C6—H6A	122.4	C13—C12—H12A	120.9
S1—C6—H6A	122.4	C12—C13—C14	121.4 (5)
C6—S1—C3	93.3 (8)	C12—C13—H13A	119.3
C6A—S1A—C3	96.2 (18)	C14—C13—H13A	119.3
C5A—C6A—S1A	118 (3)	C13—C14—C9	120.1 (4)
C5A—C6A—H6AA	120.8	C13—C14—H14A	120.0
S1A—C6A—H6AA	120.8	C9—C14—H14A	120.0
C2—N1—N2—C1	-0.7 (3)	C2—C3—S1—C6	-175.1 (6)
C2—N1—N2—C7	179.4 (2)	S1A—C3—S1—C6	-0.3 (8)
N1—N2—C1—O1	1.3 (3)	C4A—C3—S1A—C6A	3 (3)
C7—N2—C1—O1	-178.9 (3)	C2—C3—S1A—C6A	-179.0 (19)
N1—N2—C1—S2	-177.7 (2)	S1—C3—S1A—C6A	6 (2)
C7—N2—C1—S2	2.1 (5)	C3—S1A—C6A—C5A	-6 (4)
C2—O1—C1—N2	-1.3 (3)	S1A—C6A—C5A—C4A	7 (5)
C2—O1—C1—S2	177.8 (2)	C4—C3—C4A—C5A	4 (3)
N2—N1—C2—O1	-0.2 (3)	C2—C3—C4A—C5A	-177.8 (14)
N2—N1—C2—C3	178.2 (3)	S1A—C3—C4A—C5A	1 (3)
C1—O1—C2—N1	1.0 (3)	S1—C3—C4A—C5A	-52 (19)
C1—O1—C2—C3	-177.6 (3)	C6A—C5A—C4A—C3	-4 (4)
N1—C2—C3—C4	176.5 (11)	C9—N3—C7—N2	-106.3 (3)
O1—C2—C3—C4	-5.2 (11)	C8—N3—C7—N2	85.5 (4)
N1—C2—C3—C4A	-2.0 (17)	C1—N2—C7—N3	-107.6 (3)
O1—C2—C3—C4A	176.4 (17)	N1—N2—C7—N3	72.2 (3)
N1—C2—C3—S1A	179.8 (5)	C7—N3—C9—C10	-154.3 (3)
O1—C2—C3—S1A	-1.9 (6)	C8—N3—C9—C10	13.5 (4)
N1—C2—C3—S1	-6.1 (5)	C7—N3—C9—C14	26.8 (4)
O1—C2—C3—S1	172.2 (3)	C8—N3—C9—C14	-165.3 (3)
C4A—C3—C4—C5	-8 (2)	N3—C9—C10—C11	-178.1 (3)
C2—C3—C4—C5	173.5 (10)	C14—C9—C10—C11	0.8 (5)
S1A—C3—C4—C5	55 (29)	C9—C10—C11—C12	-0.3 (6)
S1—C3—C4—C5	-4.1 (17)	C10—C11—C12—C13	0.1 (6)
C3—C4—C5—C6	4 (2)	C11—C12—C13—C14	-0.3 (6)
C4—C5—C6—S1	-3 (2)	C12—C13—C14—C9	0.8 (5)
C5—C6—S1—C3	0.2 (15)	C10—C9—C14—C13	-1.0 (5)
C4—C3—S1—C6	2.6 (12)	N3—C9—C14—C13	177.9 (3)
C4A—C3—S1—C6	129 (20)		