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1-Benzoyl-3-(2,4,5-trichlorophenyl)thiourea

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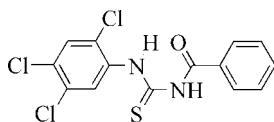
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.036; wR factor = 0.084; data-to-parameter ratio = 17.2.

The benzene and phenyl rings in the title compound, $\text{C}_{14}\text{H}_9\text{Cl}_3\text{N}_2\text{OS}$, form a dihedral angle of $40.98(6)^\circ$. The molecule exists in the thione form with typical thiourea $\text{C}-\text{S}$ [$1.666(2)$ Å] and $\text{C}-\text{O}$ [$1.227(3)$ Å] bond lengths as well as shortened $\text{C}-\text{N}$ bonds [$1.345(3)$ and $1.386(2)$ Å]. An intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond stabilizes the molecular conformation. In the crystal, pairs of $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds link the molecules into centrosymmetric dimers.

Related literature

For information on thiourea derivatives, see: Patil & Chedekel (1984); Baily *et al.* (1996); Namgun *et al.* (2001); Koch (2001); Wegner *et al.* (1986); Krishnamurthy *et al.* (1999); Murtaza *et al.* (2009a,b). For related structures, see: Khawar Rauf *et al.* (2009a,b). For bond-length data, see: Allen *et al.* (1987). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$\text{C}_{14}\text{H}_9\text{Cl}_3\text{N}_2\text{OS}$
 $M_r = 359.64$
 Monoclinic, $C2/c$
 $a = 33.111(8)$ Å
 $b = 3.8413(7)$ Å
 $c = 25.220(6)$ Å
 $\beta = 115.995(2)^\circ$

$V = 2883.1(11)$ Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.78$ mm⁻¹
 $T = 296$ K
 $0.20 \times 0.20 \times 0.20$ mm

Data collection

Rigaku/MSC Mercury CCD diffractometer

Absorption correction: multi-scan (REQAB; Rigaku, 1998)
 $T_{\min} = 0.800$, $T_{\max} = 1.000$

11264 measured reflections
 3264 independent reflections

2686 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.084$
 $S = 1.06$
 3264 reflections

190 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.42$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.39$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O1}$	0.86	1.89	2.586 (2)	137
$\text{N2}-\text{H2}\cdots\text{S1}^1$	0.86	2.83	3.6771 (19)	168

Symmetry code: (i) $-x + 1, y, -z + \frac{1}{2}$.

Data collection: *CrystalClear* (Molecular Structure Corporation and Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *TEXSAN* (Molecular Structure Corporation and Rigaku, 2004); software used to prepare material for publication: *Yadokari-XG_2009* (Kabuto *et al.*, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2439).

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supporting information

Acta Cryst. (2012). E68, o119 [doi:10.1107/S1600536811052780]

1-Benzoyl-3-(2,4,5-trichlorophenyl)thiourea

M. Khawar Rauf, Masahiro Ebihara, Amin Badshah and Imtiaz-ud-Din

S1. Comment

Thiourea derivatives are very useful building blocks for the synthesis of a wide range of aliphatic macromolecular and heterocyclic compounds. Thus, benzothiazoles have been prepared from arylthioureas in the presence of bromine (Patil & Chedekel, 1984), 2-aminothiazoles from the condensation of thiourea with α -halocarbonyl compounds (Baily *et al.*, 1996), and 2-Methyl-aminothiazolines from *N*-(2-hydroxyethyl)-*N'*-methylthioureas (Namgun *et al.*, 2001). *N*, *N*-dialkyl-*N*-aroylthioureas have been efficiently used for the extraction of Nickel, Palladium and Platinum metals (Koch, 2001). Aliphatic and acylthioureas are well known for their antimicrobial activities (Wegner *et al.*, 1986). Symmetrical and unsymmetrical thioureas have shown antifungal activity against the plant pathogens (Krishnamurthy *et al.*, 1999). We became interested in the synthesis of these thioureas as intermediates in the synthesis of novel guanidines (Murtaza *et al.*, 2009*a* ; 2009*b*) and heterocyclic compounds for the systematic study of bioactivity and Complexation behaviour. Hence, we present here the crystal structure of the title compound, (I), Fig. 1. Comparison with *N*-benzoyl-*N'*-phenylthioureas [Cambridge Structural Database (*Mogul* Version 1.7; Allen, 2002) and (Allen *et al.*, 1987)], show the molecule to exist in the thione form with typical thiourea C—S and C—O bonds, as well as shortened C—N bond lengths. Comparison with *N*-benzoyl-*N'*-phenylthioureas (Khawar Rauf *et al.*, 2009*a,b*) suggests the 2,4,5-trichloro substitution on phenyl ring implies no significant effect on these bond lengths. Compound (I) (Fig. 1) shows the typical Thiourea C=S and C=O double bonds as well as shortened C—N bond lengths. The thiocarbonyl and carbonyl groups are almost coplanar, as reflected by the torsion angles C1—N2—C2—O1 [-5.0 (3)] and N1—C1—N2—C2 [1.7 (3)]. This is associated with the expected typical thiourea intramolecular N—H \cdots O H-bond (Table 1), forming a six-membered ring commonly observed in this class of compounds (Khawar Rauf *et al.*, 2009*a,b*). The dihedral angles to the N1 C1 S1 N2 C2 O1 plane are 50.97 (4) $^\circ$ for the ring formed by C3 to C8 and 11.44 (7) $^\circ$ for the ring formed by C9 to C14. The crystal packing shows intramolecular N—H \cdots O and intermolecular N—H \cdots S H-bonds (Table 1, Fig. 2). The Cl atoms are not involved in any type of H-bonds.

S2. Experimental

Freshly prepared benzoylisothiocyanate (1.63 g, 10 mmol) was dissolved in acetone (50 ml) and stirred for 45 minutes. Afterwards neat 2,4,5-trichloroaniline (1.96 g, 10 mmol) was added and the resulting mixture was stirred for 1 h. The reaction mixture was then poured into acidified water and stirred well. The solid product was separated and washed with deionized water and purified by recrystallization from methanol/1,1-dichloromethane (1:1 *v/v*) to give fine crystals of the title compound (I), with an overall yield of 95%. Full spectroscopic and physical characterization will be reported elsewhere.

S3. Refinement

Hydrogen atoms were included in calculated positions and refined as riding on their parent atom with $N-H = 0.86 \text{ \AA}$ and $U_{iso}(H) = 1.2U(N_{eq})$, $C-H = 0.93 \text{ \AA}$ and $U_{iso}(H) = 1.2U(C_{eq})$.

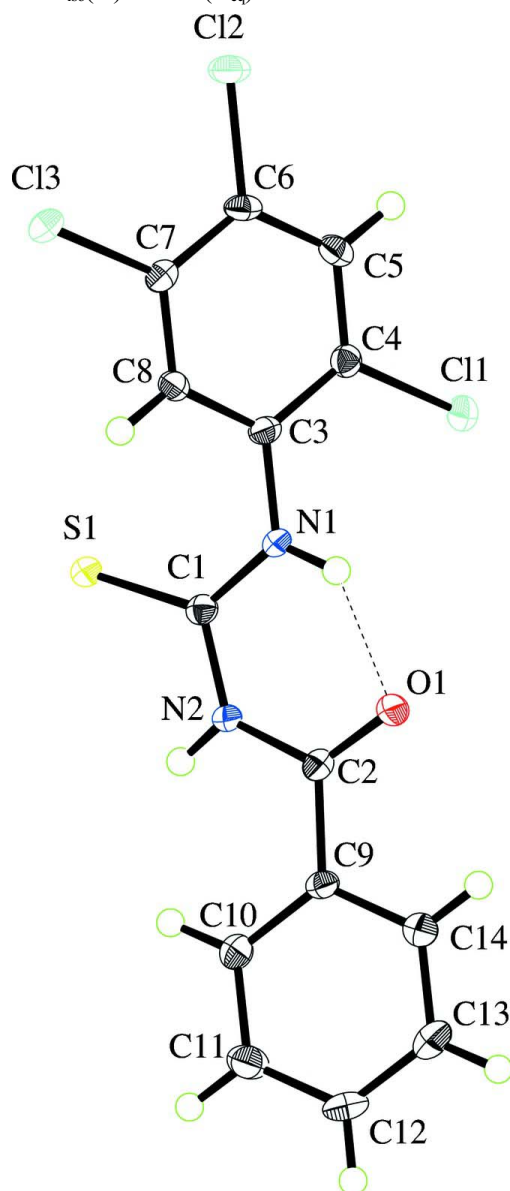
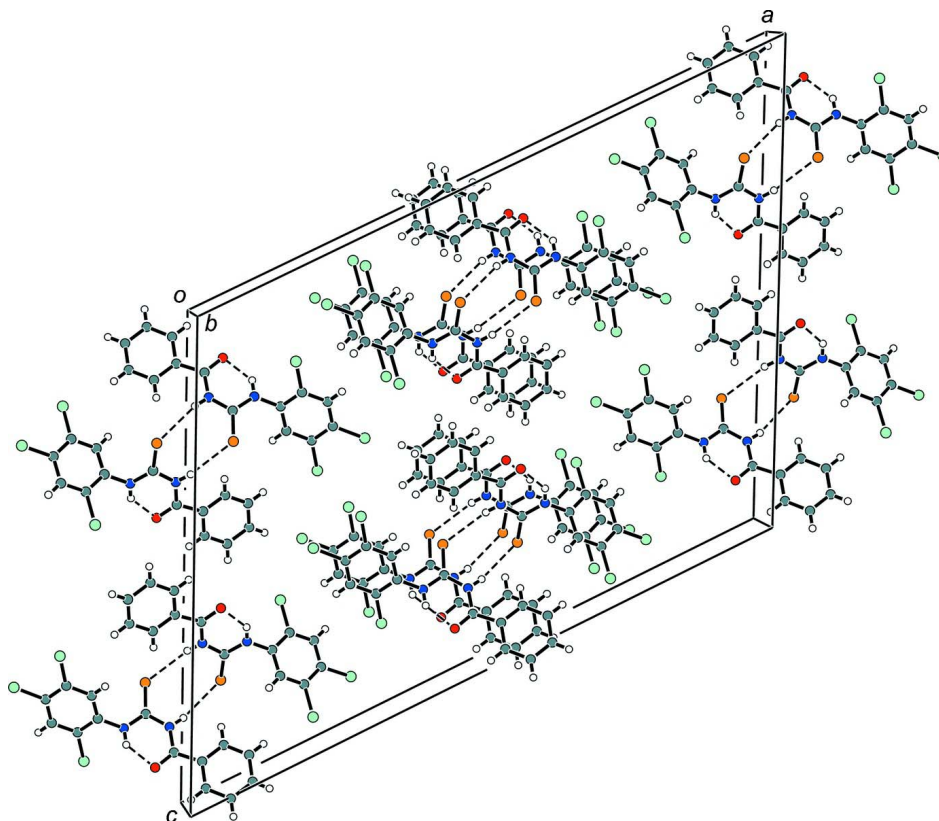


Figure 1

Molecular diagram of (I). Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds shown as dashed lines.

**Figure 2**

Packing diagram of (I) viewed along *b*-axis. Hydrogen bonds shown as dashed lines.

1-Benzoyl-3-(2,4,5-trichlorophenyl)thiourea

Crystal data

$C_{14}H_9Cl_3N_2OS$

$M_r = 359.64$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 33.111\ (8)\ \text{\AA}$

$b = 3.8413\ (7)\ \text{\AA}$

$c = 25.220\ (6)\ \text{\AA}$

$\beta = 115.995\ (2)^\circ$

$V = 2883.1\ (11)\ \text{\AA}^3$

$Z = 8$

$F(000) = 1456$

$D_x = 1.657\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71070\ \text{\AA}$

Cell parameters from 3588 reflections

$\theta = 3.4\text{--}27.5^\circ$

$\mu = 0.78\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Prism, colorless

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

Data collection

Rigaku/MSM Mercury CCD
diffractometer

Radiation source: Sealed Tube

Graphite Monochromator monochromator

Detector resolution: $14.6306\ \text{pixels mm}^{-1}$

dtprofit.ref scans

Absorption correction: multi-scan

(REQAB; Rigaku, 1998)

$T_{\min} = 0.800$, $T_{\max} = 1.000$

11264 measured reflections

3264 independent reflections

2686 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.2^\circ$

$h = -42 \rightarrow 31$

$k = -3 \rightarrow 4$

$l = -28 \rightarrow 32$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.084$
 $S = 1.06$
 3264 reflections
 190 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
 $w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.4746P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.39 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. ????

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.43321 (7)	0.2438 (4)	0.27137 (9)	0.0156 (4)
S1	0.435250 (18)	0.44890 (12)	0.21438 (2)	0.01721 (13)
N1	0.39554 (6)	0.1658 (4)	0.27661 (7)	0.0169 (4)
H1	0.3985	0.0785	0.3095	0.020*
N2	0.47294 (6)	0.1480 (4)	0.31893 (7)	0.0161 (4)
H2	0.4973	0.2018	0.3166	0.019*
C2	0.47806 (7)	-0.0243 (5)	0.36979 (9)	0.0183 (4)
O1	0.44567 (5)	-0.0919 (4)	0.37941 (7)	0.0262 (4)
C3	0.35153 (7)	0.2166 (5)	0.23204 (9)	0.0159 (4)
C4	0.31883 (7)	0.3736 (5)	0.24474 (9)	0.0169 (4)
C5	0.27552 (7)	0.4225 (4)	0.20171 (10)	0.0183 (5)
H5	0.2542	0.5274	0.2110	0.022*
C6	0.26409 (7)	0.3141 (5)	0.14447 (9)	0.0175 (4)
C7	0.29612 (7)	0.1512 (5)	0.13109 (9)	0.0170 (4)
C8	0.33904 (7)	0.0996 (4)	0.17480 (9)	0.0157 (4)
H8	0.3600	-0.0154	0.1658	0.019*
Cl1	0.332696 (18)	0.51597 (12)	0.31608 (2)	0.02171 (14)
Cl2	0.210441 (17)	0.39364 (12)	0.09054 (2)	0.02358 (14)
Cl3	0.283000 (19)	0.00640 (12)	0.06075 (2)	0.02230 (14)
C9	0.52450 (7)	-0.1244 (4)	0.41257 (9)	0.0160 (4)
C10	0.56177 (7)	-0.1060 (5)	0.40132 (10)	0.0202 (5)
H10	0.5589	-0.0209	0.3653	0.024*
C11	0.60327 (7)	-0.2139 (5)	0.44354 (10)	0.0262 (5)
H11	0.6282	-0.2027	0.4356	0.031*

C12	0.60807 (7)	-0.3382 (5)	0.49742 (10)	0.0236 (5)
H12	0.6361	-0.4100	0.5257	0.028*
C13	0.57106 (8)	-0.3556 (5)	0.50921 (10)	0.0278 (5)
H13	0.5741	-0.4375	0.5455	0.033*
C14	0.52959 (8)	-0.2506 (5)	0.46687 (10)	0.0250 (5)
H14	0.5047	-0.2644	0.4747	0.030*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0159 (11)	0.0153 (9)	0.0139 (11)	0.0006 (7)	0.0050 (9)	-0.0028 (7)
S1	0.0155 (3)	0.0206 (2)	0.0151 (3)	0.00181 (18)	0.0063 (2)	0.00292 (18)
N1	0.0143 (9)	0.0239 (8)	0.0117 (9)	0.0017 (6)	0.0048 (8)	0.0036 (7)
N2	0.0117 (9)	0.0228 (8)	0.0127 (9)	0.0001 (6)	0.0042 (8)	0.0017 (6)
C2	0.0181 (12)	0.0218 (10)	0.0136 (11)	0.0013 (8)	0.0058 (10)	0.0001 (8)
O1	0.0157 (9)	0.0441 (9)	0.0203 (9)	0.0027 (6)	0.0093 (8)	0.0103 (7)
C3	0.0135 (11)	0.0174 (9)	0.0143 (11)	-0.0006 (7)	0.0037 (9)	0.0029 (7)
C4	0.0176 (12)	0.0175 (9)	0.0162 (11)	-0.0011 (7)	0.0080 (10)	0.0005 (7)
C5	0.0143 (11)	0.0184 (9)	0.0237 (13)	0.0005 (7)	0.0096 (10)	0.0022 (8)
C6	0.0108 (11)	0.0175 (9)	0.0201 (12)	-0.0010 (7)	0.0031 (9)	0.0052 (8)
C7	0.0180 (11)	0.0170 (9)	0.0142 (11)	-0.0017 (7)	0.0054 (9)	0.0007 (7)
C8	0.0143 (11)	0.0161 (9)	0.0174 (11)	0.0009 (7)	0.0076 (9)	0.0011 (8)
C11	0.0205 (3)	0.0287 (3)	0.0170 (3)	0.00048 (19)	0.0092 (2)	-0.00330 (19)
C12	0.0140 (3)	0.0281 (3)	0.0231 (3)	0.00175 (19)	0.0030 (2)	0.0041 (2)
C13	0.0202 (3)	0.0295 (3)	0.0133 (3)	-0.00027 (19)	0.0038 (2)	-0.00146 (19)
C9	0.0144 (11)	0.0167 (9)	0.0138 (11)	0.0013 (7)	0.0033 (9)	-0.0008 (7)
C10	0.0217 (12)	0.0211 (10)	0.0182 (12)	0.0011 (8)	0.0091 (10)	0.0033 (8)
C11	0.0178 (12)	0.0298 (11)	0.0301 (14)	0.0022 (9)	0.0097 (11)	0.0056 (9)
C12	0.0176 (12)	0.0218 (10)	0.0213 (13)	0.0016 (8)	-0.0007 (10)	0.0033 (8)
C13	0.0291 (14)	0.0337 (12)	0.0168 (13)	0.0025 (9)	0.0066 (11)	0.0055 (9)
C14	0.0193 (13)	0.0349 (11)	0.0214 (13)	0.0032 (9)	0.0093 (11)	0.0054 (9)

Geometric parameters (Å, °)

C1—N1	1.345 (3)	C6—C12	1.727 (2)
C1—N2	1.386 (2)	C7—C8	1.379 (3)
C1—S1	1.666 (2)	C7—C13	1.723 (2)
N1—C3	1.410 (2)	C8—H8	0.9300
N1—H1	0.8600	C9—C10	1.384 (3)
N2—C2	1.386 (3)	C9—C14	1.391 (3)
N2—H2	0.8600	C10—C11	1.382 (3)
C2—O1	1.227 (3)	C10—H10	0.9300
C2—C9	1.491 (3)	C11—C12	1.382 (3)
C3—C8	1.391 (3)	C11—H11	0.9300
C3—C4	1.394 (3)	C12—C13	1.383 (3)
C4—C5	1.380 (3)	C12—H12	0.9300
C4—C11	1.739 (2)	C13—C14	1.379 (3)
C5—C6	1.386 (3)	C13—H13	0.9300

C5—H5	0.9300	C14—H14	0.9300
C6—C7	1.394 (3)		
N1—C1—N2	115.16 (18)	C8—C7—C6	119.9 (2)
N1—C1—S1	125.47 (16)	C8—C7—Cl3	118.89 (16)
N2—C1—S1	119.36 (15)	C6—C7—Cl3	121.24 (17)
C1—N1—C3	124.74 (18)	C7—C8—C3	121.12 (19)
C1—N1—H1	117.6	C7—C8—H8	119.4
C3—N1—H1	117.6	C3—C8—H8	119.4
C2—N2—C1	127.76 (18)	C10—C9—C14	119.02 (19)
C2—N2—H2	116.1	C10—C9—C2	124.6 (2)
C1—N2—H2	116.1	C14—C9—C2	116.36 (19)
O1—C2—N2	121.4 (2)	C11—C10—C9	120.1 (2)
O1—C2—C9	121.06 (19)	C11—C10—H10	119.9
N2—C2—C9	117.51 (18)	C9—C10—H10	119.9
C8—C3—C4	118.10 (19)	C12—C11—C10	120.5 (2)
C8—C3—N1	121.05 (18)	C12—C11—H11	119.7
C4—C3—N1	120.81 (19)	C10—C11—H11	119.7
C5—C4—C3	121.5 (2)	C11—C12—C13	119.8 (2)
C5—C4—Cl1	118.90 (16)	C11—C12—H12	120.1
C3—C4—Cl1	119.63 (16)	C13—C12—H12	120.1
C4—C5—C6	119.57 (19)	C14—C13—C12	119.6 (2)
C4—C5—H5	120.2	C14—C13—H13	120.2
C6—C5—H5	120.2	C12—C13—H13	120.2
C5—C6—C7	119.82 (19)	C13—C14—C9	120.9 (2)
C5—C6—Cl2	118.96 (16)	C13—C14—H14	119.5
C7—C6—Cl2	121.20 (17)	C9—C14—H14	119.5
N2—C1—N1—C3	-175.25 (16)	C5—C6—C7—Cl3	178.95 (14)
S1—C1—N1—C3	6.3 (3)	Cl2—C6—C7—Cl3	-2.6 (2)
N1—C1—N2—C2	1.7 (3)	C6—C7—C8—C3	-1.9 (3)
S1—C1—N2—C2	-179.68 (15)	Cl3—C7—C8—C3	178.94 (14)
C1—N2—C2—O1	-5.0 (3)	C4—C3—C8—C7	2.9 (3)
C1—N2—C2—C9	175.03 (17)	N1—C3—C8—C7	-179.55 (16)
C1—N1—C3—C8	49.5 (3)	O1—C2—C9—C10	169.75 (18)
C1—N1—C3—C4	-133.0 (2)	N2—C2—C9—C10	-10.3 (3)
C8—C3—C4—C5	-1.9 (3)	O1—C2—C9—C14	-9.0 (3)
N1—C3—C4—C5	-179.45 (17)	N2—C2—C9—C14	170.96 (17)
C8—C3—C4—Cl1	178.74 (14)	C14—C9—C10—C11	0.4 (3)
N1—C3—C4—Cl1	1.2 (2)	C2—C9—C10—C11	-178.33 (18)
C3—C4—C5—C6	-0.1 (3)	C9—C10—C11—C12	-0.5 (3)
Cl1—C4—C5—C6	179.25 (14)	C10—C11—C12—C13	0.1 (3)
C4—C5—C6—C7	1.2 (3)	C11—C12—C13—C14	0.4 (3)
C4—C5—C6—Cl2	-177.30 (14)	C12—C13—C14—C9	-0.6 (3)
C5—C6—C7—C8	-0.2 (3)	C10—C9—C14—C13	0.2 (3)
Cl2—C6—C7—C8	178.26 (14)	C2—C9—C14—C13	178.98 (19)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...O1	0.86	1.89	2.586 (2)	137
N2—H2...S1 ⁱ	0.86	2.83	3.6771 (19)	168

Symmetry code: (i) $-x+1, y, -z+1/2$.