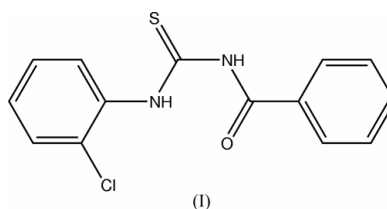


***N*-Benzoyl-*N'*-(2-chlorophenyl)thiourea****M. Sukeri M. Yusof and  
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43600 Bangi, Selangor, MalaysiaCorrespondence e-mail:  
bohari@pkrisc.cc.ukm.my**Key indicators**Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$   
 $R$  factor = 0.043  
 $wR$  factor = 0.113  
Data-to-parameter ratio = 17.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the molecule of the title compound,  $\text{C}_{14}\text{H}_{11}\text{ClN}_2\text{OS}$ , the dihedral angle between the *o*-chlorophenyl ring and the central carbonylthiourea fragment is  $29.36(8)^\circ$ . There is an intramolecular  $\text{N}-\text{H}\cdots\text{Cl}/\text{O}$  bifurcated hydrogen bond. The molecules are linked by  $\text{N}-\text{H}\cdots\text{S}$  hydrogen bonds, forming dimers which are arranged parallel to (100).

**Comment**

Recent studies have shown that thiourea derivatives are potential biologically active agents, such as antimicrobials and HIV inhibitors (Vankatachalam *et al.*, 2001). In the title compound, (I), the benzoyl and *o*-chlorophenyl groups lie *cis* and *trans*, respectively, to the S atom across the thiourea C—N bonds (Fig. 1 and Table 1). The central carbonylthiourea moiety (S1/C8/N1/N2/C9), phenyl (C1—C6) and *o*-chlorophenyl (C9—C14/Cl1) fragments are each planar. The maximum deviation is  $0.020(1)\text{ \AA}$  for N2. The central carbonylthiourea moiety makes dihedral angles with the phenyl and *o*-chlorophenyl fragments of  $11.96(9)$  and  $29.36(8)^\circ$ , respectively. The latter is larger than the angles of  $20.40(11)$  and  $7.52(9)^\circ$  in *N*-benzoyl-*N'*-(*p*-bromophenyl)thiourea (Yamin & Yusof, 2003*b*) and *N*-benzoyl-*N'*-phenylthiourea (Yamin & Yusof, 2003*a*), respectively. However, the phenyl group is inclined to the *o*-chlorophenyl fragment by  $38.67(10)^\circ$ , comparable with the angle in *N*-benzoyl-*N'*-(*p*-bromophenyl)thiourea [ $38.61(11)^\circ$ ].



There are three intramolecular hydrogen bonds (Fig. 1 and Table 2). As a result, pseudo-five- and six-membered rings are formed. In the crystal structure, the molecules are linked by an  $\text{N1}-\text{H1A}\cdots\text{S1}(-x, 1-y, -z)$  hydrogen bond to form dimers, which are arranged parallel to the *bc* plane (Fig. 2), which is in contrast to the polymeric hydrogen-bonded chains observed for *N*-benzoyl-*N'*-(*p*-bromophenyl)thiourea (Yamin & Yusof, 2003*b*).

**Experimental**

A solution of 2-chlorophenylaniline (2.56 g, 0.020 mol) in acetone (50 ml) was added dropwise to 50 ml of an acetone solution containing an equimolar amount of benzoyl isothiocyanate in a two-necked round-bottomed flask. The solution was refluxed for 2 h and

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then cooled in ice. The colourless precipitate was filtered off and washed with aqueous ethanol, then dried in a vacuum (yield 80%). Recrystallization from ethanol yielded crystals of (I) suitable for X-ray analysis.

Crystal data

C<sub>14</sub>H<sub>11</sub>ClN<sub>2</sub>OS  
*M<sub>r</sub>* = 290.76  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 8.1435 (8) Å  
*b* = 12.3788 (13) Å  
*c* = 13.2782 (14) Å  
 $\beta$  = 95.332 (2)°  
*V* = 1332.7 (2) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.449 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 2207 reflections  
 $\theta$  = 2.3–27.5°  
 $\mu$  = 0.44 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Block, colourless  
 0.39 × 0.35 × 0.34 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.849, *T<sub>max</sub>* = 0.866  
 7955 measured reflections

3039 independent reflections  
 2336 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.020  
 $\theta_{\text{max}}$  = 27.5°  
*h* = -10 → 10  
*k* = -15 → 16  
*l* = -17 → 12

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.043  
*wR* (*F*<sup>2</sup>) = 0.113  
*S* = 1.02  
 3039 reflections  
 172 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.3301P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

|             |              |               |           |
|-------------|--------------|---------------|-----------|
| S1—C8       | 1.6588 (19)  | N1—C8         | 1.390 (2) |
| O1—C7       | 1.218 (2)    | N2—C8         | 1.328 (2) |
| N1—C7       | 1.371 (2)    | N2—C9         | 1.413 (2) |
| C8—N1—C7—C6 | -171.04 (18) | C7—N1—C8—N2   | -8.9 (3)  |
| C1—C6—C7—N1 | 17.0 (3)     | N2—C9—C10—C11 | 3.6 (2)   |
| C9—N2—C8—N1 | -178.33 (17) |               |           |

Table 2

Hydrogen-bonding 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—H1A...S1 <sup>i</sup> | 0.86        | 2.73          | 3.4105 (17)           | 137                     |
| N2—H2A...C11             | 0.86        | 2.52          | 2.9165 (15)           | 109                     |
| N2—H2A...O1              | 0.86        | 1.94          | 2.654 (2)             | 139                     |
| C14—H14...S1             | 0.93        | 2.62          | 3.188 (2)             | 120                     |

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

After checking their presence in difference-density maps, all H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å, N—H = 0.86 Å, and with *U<sub>iso</sub>*(H) = 1.20 *U<sub>eq</sub>*(parent).

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve

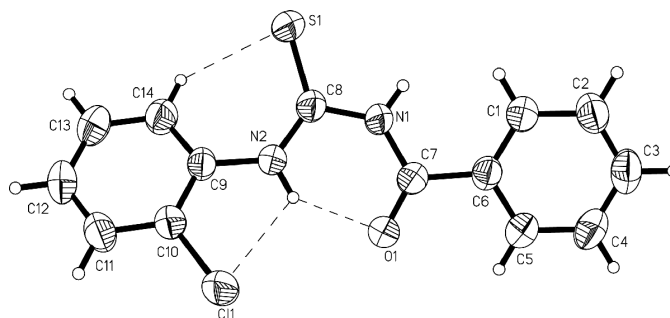


Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids. Dashed lines denote hydrogen bonds.

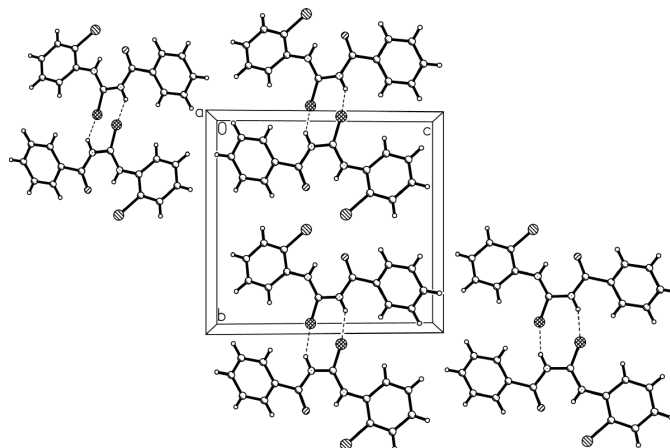


Figure 2

Packing diagram of (I), viewed down the *a* axis. Dashed lines denote the intermolecular N—H...S hydrogen bonds.

structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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