Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(2,4-Dichlorophenoxyacetyl)-*N*′-(2,4,6-trichlorophenyl)thiourea

Qian-Jin Li, Chun-Long Yang* and Xue-Qun Xie

College of Science, Nanjing Agricultural University, Nanjing 210095, People's Republic of China

Correspondence e-mail: chunlongyang@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.057
wR factor = 0.145
Data-to-parameter ratio = 16.0

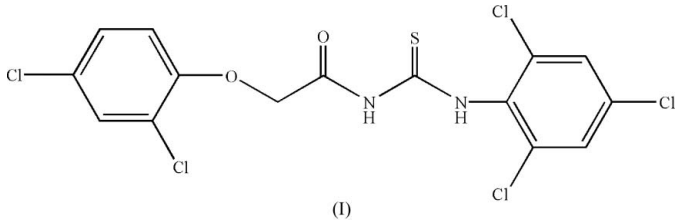
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 4 December 2006
Accepted 13 December 2006

In the title molecule, $C_{15}H_9Cl_5N_2O_2S$, all bond lengths and angles are normal. Weak intermolecular C—H···S hydrogen bonds link the molecules into spiral chains running along the *c* axis. The crystal packing exhibits a short Cl···Cl distance of 3.364 (3) Å, which suggests the existence of intermolecular Cl···Cl interactions.

Comment

We have previously reported the structure of *N*-(2,4-dichlorophenoxyacetyl)-*N*′-(4-nitrophenyl)thiourea, (II) (Li, Yang, Xie & Luo, 2006). In continuation of our study of aroylthiourea compounds, we report here the crystal structure of the title compound, (I).



(I)

In (I) (Fig. 1), all bond lengths and angles agree with those observed in related compounds (Li, Yang, Xie & Luo, 2006; Li, Yang & Xie, 2006). The mean planes C1–C6/Cl1/Cl2 (*A*), C7–C9/O1/O2/N1/N2/S1 (*B*) and C10–C15/Cl3–Cl5 (*C*) make the following dihedral angles: *A*/*B* = 12.15 (16)° [1.10 (10)° in (II)], *A*/*C* = 81.58 (14)° [9.96 (13)° in (II)] and *B*/*C* = 80.70 (13)° [8.86 (12)° in (II)]. The intramolecular N—H···O hydrogen bonds (Table 1) influence the molecular conformation.

The weak intermolecular C—H···S hydrogen bonds (Table 1) link the molecules into spiral chains running along the *c* axis (Fig. 2). The relatively short distance Cl3···Cl5^{iii} [symmetry code: (iii) 1 + *x*, *y*, *z*] of 3.364 (3) Å [C15—Cl3···Cl5^{iii} = 158.1 (3)°] suggests the existence of intermolecular Cl···Cl interactions (Matsumoto *et al.*, 2002).

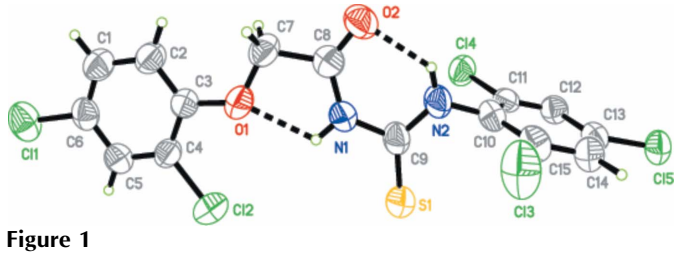


Figure 1
The molecular structure of (I), showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. Dashed lines indicate the intramolecular hydrogen bonds.

Experimental

The title compound was prepared according to the literature method of Zhang & Lin (1992). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a solution in *N*,*N*-dimethylformamide at 293 K.

Crystal data

$C_{15}H_9Cl_5N_2O_2S$
M_r = 458.55
Tetragonal, $P4_3$
a = 7.9580 (11) Å
c = 29.249 (6) Å
V = 1852.3 (5) Å^3
Z = 4
D_x = 1.644 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.91 mm^{-1}
T = 293 (2) K
Prism, colourless
0.40 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.713, T_{max} = 0.839
3624 measured reflections
3624 independent reflections
2336 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.145
S = 0.99
3624 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), 1771 Friedel pairs
Flack parameter: −0.01 (12)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.86	2.05	2.516 (7)	113
N2—H2A···O2	0.86	1.99	2.675 (7)	136
C1—H1B···O2^{i}	0.93	2.57	3.326 (9)	139
C5—H5A···S1^{ii}	0.93	2.87	3.716 (7)	152

Symmetry codes: (i) $y, -x+2, z+\frac{1}{4}$; (ii) $y+1, -x+1, z+\frac{1}{4}$.

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å; N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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*.

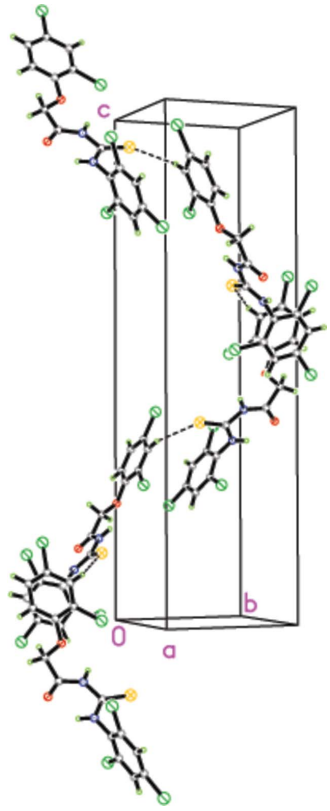


Figure 2
A portion of the crystal packing showing the spiral hydrogen-bonded (dashed lines) chain in (I).

We are grateful to H.-Q. Wang for the data collection.

References

Bruker (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Li, Q.-J., Yang, C.-L. & Xie, X.-Q. (2006). *Acta Cryst.* E**62**, o4104–o4105.
Li, Q.-J., Yang, C.-L., Xie, X.-Q. & Luo, J.-X. (2006). *Acta Cryst.* E**62**, o4102–o4103.
Matsumoto, A., Tanaka, T., Tsubouchi, T., Tashiro, K., Saragai, S. & Nakamoto, S. (2002). *J. Am. Chem. Soc.* **124**, 8891–8902.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, Z. Y. & Lin, H. X. (1992). *Chem. J. Chin. Univ.* **13**, 936–937.