

Feng Wu,^{a*} Rong Wan,^a
Hong-Jing Fan,^b Rong Zhang^a
and Jin-Tang Wang^a^aDepartment of Applied Chemistry, College of Science, Nanjing University of Technology, No. 5 Ximofan Road, Nanjing 210009, People's Republic of China, and ^bDepartment of Analysis, Sinochem Corporation, No. 1 Bingjiang Road, Taicang 215433, People's Republic of ChinaCorrespondence e-mail:
wufeng197910@hotmail.com

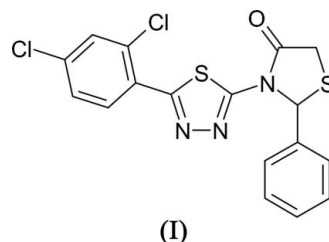
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.011$ Å
 R factor = 0.089
 wR factor = 0.216
Data-to-parameter ratio = 14.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

3-[5-(2,4-Dichlorophenyl)-1,3,4-thiadiazol-2-yl]-2-phenylthiazolidin-4-one

The title compound, $\text{C}_{17}\text{H}_{11}\text{Cl}_2\text{N}_3\text{OS}_2$, was synthesized by the reaction of benzylidene[5-(2,4-dichlorophenyl)-1,3,4-thiadiazol-2-yl]amine and mercaptoacetic acid. In the crystal structure, there are $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, resulting in a three-dimensional network. There is also a short intermolecular $\text{N}\cdots\text{Cl}$ interaction.Received 5 April 2006
Accepted 13 April 2006

Comment

Thiadiazole derivatives containing the thiazolidinone unit are of great interest because of their chemical and pharmaceutical properties. Some derivatives have fungicidal and herbicidal activities (Chen *et al.*, 2000; Kidwai *et al.*, 2000; Vicentini *et al.*, 1998), while others show insecticidal activities (Arun *et al.*, 1999; Wasfy *et al.*, 1996).We are focusing our synthetic and structural studies on thiadiazole derivatives and we have recently published the structure of 3-[5-(4-fluorophenyl)-[1,3,4]thiadiazol-2-yl]-2-phenylthiazolidin-4-one (Wan *et al.*, 2006). We report here the crystal structure of a close analogue, the title compound, (I), in which the 4-fluorophenyl substituent is replaced by 2,4-dichlorophenyl.In the molecular structure of (I) (Fig. 1), bond lengths and angles are normal (Allen *et al.*, 1987). Intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds result in a three-dimensional network (Fig. 2 and Table 1). There is also a short $\text{N}\cdots\text{Cl}$ interaction [$\text{N}1\cdots\text{Cl}1^i = 3.223$ (7) Å; symmetry code as in Table 1; Fig. 2].

Experimental

Benzylidene-[5-(2,4-dichlorophenyl)-[1,3,4]thiadiazol-2-yl]amine (5 mmol) and mercaptoacetic acid (5 mmol) were dissolved in toluene (50 ml). The resulting water was removed by distillation over a period of 5 h. The reaction mixture was left to cool to room temperature and filtered, and the solid was recrystallized from acetone to give pure compound (I) (m.p. 472–473 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution.

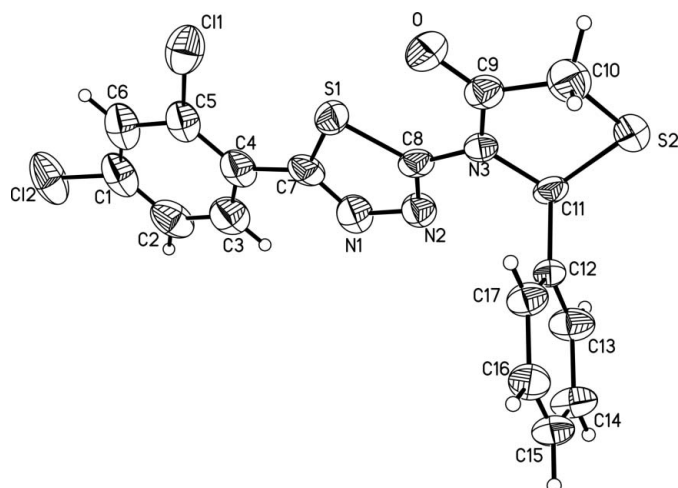


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

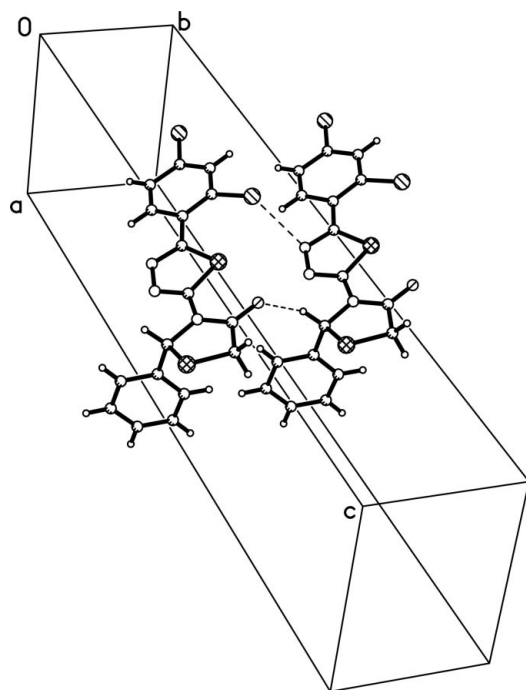


Figure 2
Part of the crystal structure of (I). Dashed lines indicate the intermolecular C—H...O hydrogen bond and the short N...Cl interaction.

Crystal data

$C_{17}H_{11}Cl_2N_3OS_2$
 $M_r = 408.31$
 Monoclinic, $P2_1/n$
 $a = 7.9700$ (16) Å
 $b = 6.1550$ (12) Å
 $c = 34.738$ (7) Å
 $\beta = 90.20$ (3)°
 $V = 1704.1$ (6) Å³

$Z = 4$
 $D_x = 1.592$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.64$ mm⁻¹
 $T = 293$ (2) K
 Block, colourless
 $0.30 \times 0.20 \times 0.20$ mm

Data collection

Enraf–Nonius CAD-4
 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.832$, $T_{\max} = 0.883$
 3336 measured reflections

3336 independent reflections
 2351 reflections with $I > 2\sigma(I)$
 $\theta_{\max} = 26.0^\circ$
 3 standard reflections
 every 200 reflections
 intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.089$
 $wR(F^2) = 0.216$
 $S = 1.19$
 3336 reflections
 227 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0285P)^2 + 11.9102P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.42$ e Å⁻³
 $\Delta\rho_{\min} = -0.41$ e Å⁻³
 Extinction correction: *SHELXL97*
 (Sheldrick, 1997)
 Extinction coefficient: 0.0016 (5)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C11-H11A\cdots O^i$	0.98	2.39	3.218 (9)	142

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

All H atoms were positioned geometrically, with C—H distances in the range 0.93–0.98 Å, and included in the refinement in a riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Arun, K. P., Nag, V. L. & Panda, C. S. (1999). *Indian J. Chem. Sect B*, **38**, 998–1001.
- Chen, H. S., Li, Z. M. & Han, Y. F. (2000). *J. Agric. Food. Chem.* **48**, 5312–5315.
- Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
- Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
- Kidwai, M., Negi, N. & Misra, P. J. (2000). *J. Indian Chem. Soc.* **77**, 46–48.
- North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Vicentini, C. B., Manfrini, M., Veronese, A. C. & Guarneri, M. (1998). *J. Heterocycl. Chem.* **35**, 29–36.
- Wasfy, A. A., Nassar, S. A. & Eissa, A. M. (1996). *Indian J. Chem. Sect B*, **35**, 1218–1220.
- Wan, R., Wu, F., Yin, J. & Wang, J.-T. (2006). *Acta Cryst.* **E62**, o746–o747.