

Wei-Lin Ding, Yong-Mei Shen,  
Zhi-Tao Xing, Pin-Liang Wang  
and Hai-Bo Wang\*Department of Applied Chemistry, College of  
Science, Nanjing University of Technology,  
Xinmofan Road No. 5 Nanjing, Nanjing  
210009, People's Republic of ChinaCorrespondence e-mail:  
wanghaibo@njut.edu.cn

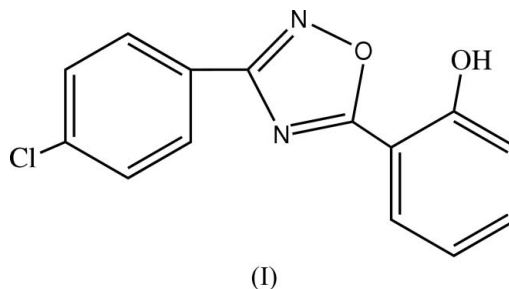
## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.009\text{ \AA}$   
 $R$  factor = 0.053  
 $wR$  factor = 0.140  
Data-to-parameter ratio = 7.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## 2-[3-(4-Chlorophenyl)-1,2,4-oxadiazol-5-yl]phenol

In the approximately planar molecule of the title compound,  $\text{C}_{14}\text{H}_9\text{ClN}_2\text{O}_2$ , an intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond helps to establish the molecular conformation.Received 7 November 2006  
Accepted 7 November 2006

## Comment

1,2,4-Oxadiazole derivatives possess biological properties, such as intrinsic analgesic (Terashita *et al.*, 2002) and anticoronaviral (Romero, 2001) effects. As part of our studies in this area, we report here the synthesis and crystal structure of the title compound, (I) (Fig. 1).The molecule is approximately planar: the dihedral angles between the central  $\text{N1}/\text{O2}/\text{C7}/\text{N2}/\text{C8}$  ring and the benzene rings are  $4.60$  ( $19$ ) and  $7.0$  ( $18$ ) $^\circ$  for the  $\text{C1}-\text{C6}$  and  $\text{C9}-\text{C14}$  rings, respectively. An intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond (Table 1) helps to establish the molecular conformation of (I).

## Experimental

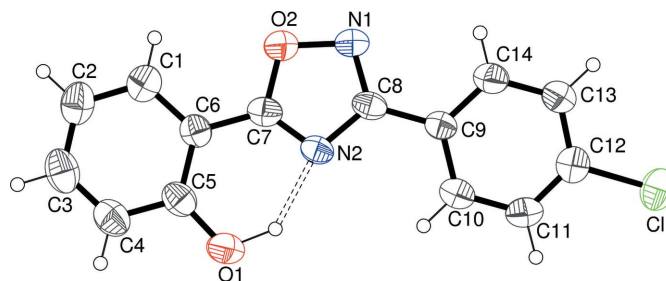
4-Chlorobenzoic acid amidoxime (50 mmol) and methyl salicylate (100 mmol) were dissolved in 150 ml anhydrous ethanol mixed with 2.3 g of sodium and heated three times for 25 min (with a 5 min break each time) in a 400 W microwave. The reaction mixture was concentrated by evaporation *in vacuo* to about one-third of its

Figure 1

A view of the molecular structure of (I), showing 40% displacement ellipsoids (arbitrary spheres for the H atoms). A dashed line indicates the hydrogen bond.

volume and the residue was mixed with water. Whilst cooling, the pH was adjusted to 8–9 with 2 M hydrochloric acid, and the resulting precipitate was suction filtered and washed with water. In order to remove all traces of water, the mixture was dissolved in dichloromethane, dried with sodium sulfate and concentrated by evaporation. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

#### Crystal data

$C_{14}H_9ClN_2O_2$   
 $M_r = 272.68$   
 Monoclinic,  $P2_1$   
 $a = 6.3900$  (13) Å  
 $b = 5.0380$  (10) Å  
 $c = 19.255$  (4) Å  
 $\beta = 97.98$  (3)°  
 $V = 613.9$  (2) Å<sup>3</sup>  
 $Z = 2$   
 $D_x = 1.475$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.31$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, colourless  
 $0.30 \times 0.20 \times 0.10$  mm

#### Data collection

Enraf–Nonius CAD-4  
 diffractometer  
 $\omega/2\theta$  scans  
 Absorption correction:  $\psi$  scan  
 (North *et al.*, 1968)  
 $T_{\min} = 0.913$ ,  $T_{\max} = 0.970$   
 1466 measured reflections  
 1343 independent reflections  
 904 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.046$   
 $\theta_{\max} = 26.0^\circ$   
 3 standard reflections  
 every 200 reflections  
 intensity decay: none

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.053$   
 $wR(F^2) = 0.140$   
 $S = 1.05$   
 1343 reflections  
 175 parameters  
 H atoms treated by a mixture of  
 independent and constrained  
 refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0624P)^2 + 0.1265P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.21$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.23$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983)  
 Flack parameter: 0.1 (2)

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1–H $\cdots$ N2	1.06 (7)	1.78 (6)	2.680 (6)	139 (5)

The O-bound H atom was located in a difference map and its position was freely refined with the constraint  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ . The C-bound H atoms were positioned geometrically (C–H = 0.93–0.96 Å) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

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: *PLATON* (Spek, 2003).

#### References

- Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.  
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
 Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.  
 North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.  
 Romero, J. R. (2001). *Exp. Opin. Invest. Drugs*, **10**, 369–379.  
 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.  
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.  
 Terashita, Z., Naruo, K. & Morimoto, S. (2002). PCT Int. Appl. WO, 02060439.