Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[3-(4-Chlorophenyl)isoxazol-5-yl]methanol

Li-Da Tang, Da-Tong Zhang, Fang-Gang Sun, Gui-Yun Duan and Jian-Wu Wang*

School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, People's Republic of China

Correspondence e-mail: yugp2005@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.120
Data-to-parameter ratio = 13.2

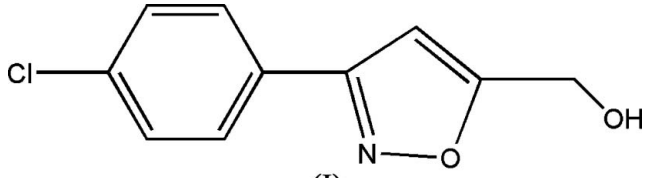
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 28 February 2006
Accepted 6 March 2006

In the title molecule, $C_{10}H_8ClNO_2$, the isoxazole ring shows normal values of bond lengths and angles. The mean planes of the benzene and isoxazole rings make a dihedral angle of 16.3 (2)°. Intermolecular O—H···N hydrogen bonds link the molecules into chains extended along the *b* axis. The crystal packing is further stablized by weak C—H···O interactions and van der Waals forces.

Comment

Isoxazoles play an important role in the synthesis of many complex natural products. They are often used as pharmacophores in medicinal chemistry (Aicher *et al.*, 1998). The title compound, (I), has been synthesized by the reaction of *p*-chlorobenzaldoxime with propargyl alcohol following the known preparative method in solution *via* 1,3-dipolar cycloaddition of alkynes with nitrile oxides (Moore & Norris, 1998). We present here the crystal structure of (I) (Fig. 1).



(I)

The bond lengths and angles of the isoxazole ring (Table 1) are normal and comparable to those reported for related structures (Kumar *et al.*, 1998; Xu *et al.*, 2004). The mean planes of the benzene and isoxazole rings make a dihedral angle of 16.3 (2)°. Intermolecular O—H···N hydrogen bond (Table 2) link the molecules into chains extended along the *b* axis. The crystal packing (Fig. 2) is further stablized by weak C—H···O interactions (Table 2) and van der Waals forces.

Experimental

To a solution of *p*-chlorobenzaldoxime (20.00 mmol) in anhydrous dichloromethane (30 ml) was added *N*-chlorosuccinimide (24.06 mmol). After stirring at room temperature for 1 h, propargyl alcohol (20.00 mmol) was added, followed by triethylamine (21.78 mmol). The reaction mixture was refluxed for 6 h; upon cooling it was washed with water and dried with anhydrous sodium carbonate. After concentrating, the residue was purified by column chromatography on silica gel (petroleum ether–ethyl acetate = 3:1) in 70% yield. Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of a mixture of hexane–dichloromethane (2:1 *v*/*v*) solution at room temperature over a period of one week.

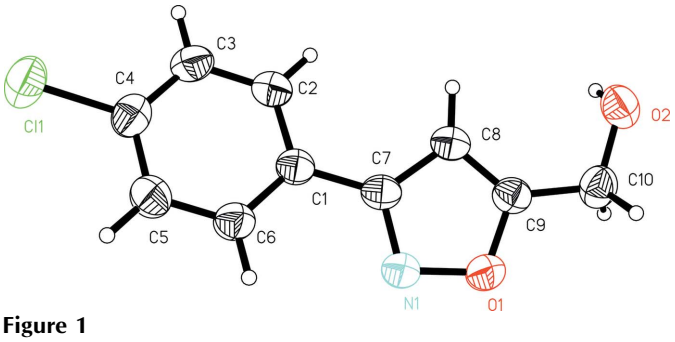


Figure 1
View of (I), with displacement ellipsoids drawn at the 40% probability level.

Crystal data

$C_{10}H_8ClNO_2$	D_x = 1.441 Mg m^{-3}
M_r = 209.62	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1048 reflections
a = 12.968 (3) Å	θ = 2.3–22.3°
b = 9.622 (2) Å	μ = 0.37 mm^{-1}
c = 7.8091 (17) Å	T = 291 (2) K
β = 97.450 (3)°	Block, colourless
V = 966.2 (4) Å^3	0.41 × 0.31 × 0.02 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	1705 independent reflections
φ and ω scans	1526 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.021
T_{min} = 0.865, T_{max} = 0.993	θ_{max} = 25.0°
4917 measured reflections	$h = -12 \rightarrow 15$
	$k = -11 \rightarrow 11$
	$l = -9 \rightarrow 8$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.3104P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.048	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.120	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
S = 1.15	$\Delta\rho_{min}$ = −0.22 e Å^{-3}
1705 reflections	Extinction correction: *SHELXL97*
129 parameters	Extinction coefficient: 0.024 (3)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cl1—C4	1.739 (3)	N1—C7	1.311 (3)
O1—C9	1.344 (3)	C7—C8	1.413 (3)
O1—N1	1.409 (2)		
C9—O1—N1	108.33 (16)	C7—N1—O1	105.74 (17)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1^{i}	0.82	2.00	2.822 (2)	178
C10—H10B···O2^{ii}	0.97	2.50	3.432 (3)	162

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

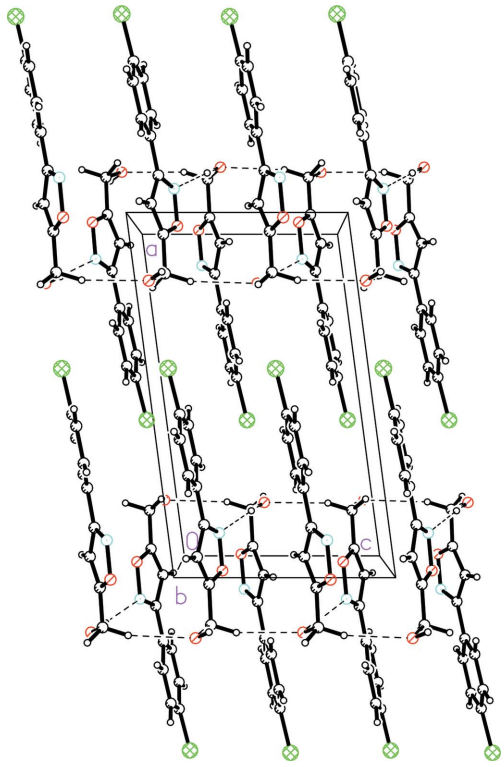


Figure 2
A packing diagram, viewed down the b axis. The dashed lines denote intermolecular hydrogen bonds.

All H atoms were placed in calculated positions, with O—H = 0.82 Å and C—H = 0.93 or 0.97 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2–1.5U_{eq} of the parent atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

References

Aicher, T. D., Balkan, B., Bell, B. A., Brand, L. T., Cheon, S. H., Deem, R. O., Fell, J. B., Fillers, W. S., Fraser, T. D., Gao, J., Knorr, D. C., Kahle, G. G., Leone, C. L., Nadelson, J., Simpson, R. & Smith, H. C. (1998). *J. Med. Chem.* **41**, 4556–4566.

Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (1999). *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Moore, M. & Norris, P. (1998). *Tetrahedron Lett.* **39**, 7027–7030.

Kumar, N., Roy, S., Parmarr, V. S. & Errington, W. (1998). *Acta Cryst.* C**54**, 1123–1125.

Sheldrick, D. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Xu, W.-M., Hu, X.-R., Gua, J.-M. & Huang, X. (2004). *Acta Cryst.* E**60**, o676–o677.