Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(4-Chlorophenyl)-5-methyl-3*H*-1,3,4-oxadiazol-2-one

S. Thamotharan,[a]‡ V. Parthasarathi,[a]* P. Kalaivani,[a] Shanta G. Mallur,[b] Bharati Badami[b] and Kurt J. Schenk[c]

[a]Department of Physics, Bharathidasan University, Tiruchirappalli 620 024, India, [b]Post-Graduate Department of Studies in Chemistry, Karnatak University, Dharwad 580 003, India, and [c]Institut de Cristallographie, Université de Lausanne, BPS Dorigny, CH-1057 Lausanne, Switzerland

‡ Present address: Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560 012, India

Correspondence e-mail: vpsarati@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.058
wR factor = 0.168
Data-to-parameter ratio = 16.7

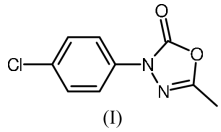
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 30 April 2004
Accepted 4 May 2004
Online 8 May 2004

The molecule of the title compound, $C_9H_7ClN_2O_2$, is planar. A weak intramolecular C—H···O interaction is observed in the solid state.

Comment

The title compound, (I), and its derivatives were obtained by a facile one-pot ring conversion of 3-arylsydnones in approximately 80% yield. The synthesis of a few related compounds which have been reported earlier have been obtained with difficulty in approximately 30% yield along with isomers from phenylhydrazine (Kametani *et al.*, 1970). Compound (I) and its derivatives can be used as synthetic precursors for other heterocycles. The title compound shows growth inhibition only against *P. pyocyanous* equal to that of the standard drug norfloxacin (Mallur & Badami, 2000). The present study was undertaken to determine the crystal and molecular structure of (I).



(I)

A view of the molecule is shown in Fig. 1. The bond lengths and angles in the oxadiazole moiety are comparable with those of related structures (Du *et al.*, 2004; Öztürk *et al.*, 2004). The dihedral angle between the mean planes of the benzene and oxadiazole rings is 3.63 (8)°. In the crystalline state, a weak intramolecular C—H···O interaction is observed between atoms C7 and O2 (Table 1), forming an *S*(6) motif (Bernstein *et al.*, 1995).

Experimental

3-(4-Chlorophenyl)sydnone (1 g) was suspended in acetic anhydride (5 ml) at 273 K and an ice-cold solution of bromine (0.5 ml) in acetic anhydride (5 ml) was added with stirring and cooling. 4-Bromo-

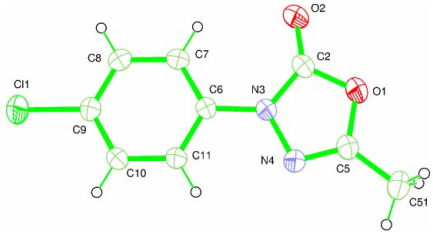


Figure 1
View of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

sydnone began to separate. The reaction mixture was then heated on a water bath for 30 min, gradually increasing the temperature to 323–333 K. Vigorous evolution of CO_2 was observed. The solution was then diluted with water and the resulting solid was filtered off and washed with water and crystallized from absolute ethanol (m.p. 372–373 K).

Crystal data

$C_9H_7ClN_2O_2$
M_r = 210.62
Orthorhombic, *Pnaa*
a = 6.8548 (14) Å
b = 12.042 (2) Å
c = 22.762 (5) Å
V = 1878.9 (7) Å^3
Z = 8
D_x = 1.489 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6328 reflections
θ = 3.5–27.9°
μ = 0.38 mm^{-1}
T = 293 (2) K
Prism, colourless
0.30 × 0.20 × 0.12 mm

Data collection

Stoe IPDS-I diffractometer
ω scans
Absorption correction: by integration (*X-RED*1.22 in *IPDS Software Package*; Stoe & Cie, 1997)
T_{min} = 0.850, T_{max} = 0.914
15537 measured reflections
2140 independent reflections
1841 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 28.0°
$h = -8 \rightarrow 8$
$k = -15 \rightarrow 15$
$l = -30 \rightarrow 29$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.168
S = 1.08
2140 reflections
128 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0844P)^2 + 0.5325P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
C—H···O interaction (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O2	0.93	2.38	2.994 (3)	124

The methyl H atoms were constrained to an ideal geometry (C—H = 0.96 Å), with U_{iso}(H) = 1.5U_{eq}(C). All remaining H atoms were placed in geometrically idealized positions (C—H = 0.93 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *IPDS Software Package* (Stoe & Cie, 1997); cell refinement: *IPDS Software Package*; data reduction: *IPDS Software Package*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Du, M., Zhao, X—J. & Guo, X—H. (2004). *Acta Cryst.* E**60**, o327–o328.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Kametani, T., Sota, K. & Shio, M. (1970). *J. Heterocycl. Chem.* **7**, 821–829.
Mallur, S. G. & Badami, B. V. (2000). *Il Farmaco*, **55**, 65–67.
Öztürk, S., Akkurt, M., Cansız, A., Çetin, A., Şekerci, M. & Heinemann, F. W. (2004). *Acta Cryst.* E**60**, o322–o323.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1997). *IPDS Software Package*. Version 2.89. Stoe & Cie GmbH, Darmstadt, Germany.