Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

3-Chlorobenzoxazolo[3,2-*b*]isoquinolin-6-one

Anwar Usman,[a] Lei Wang,[b] Hoong-Kun Fun,[a]* Ke-Qing Ling[b] and Jian-Hua Xu[b]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]Department of Chemistry, Nanjing University, Nanjing 210093, People's Republic of China

Correspondence e-mail: hkfun@usm.my

Received 20 November 2002
Accepted 10 December 2002
Online 19 December 2002

Key indicators

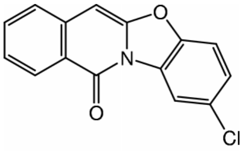
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.063
wR factor = 0.150
Data-to-parameter ratio = 13.8

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

The title molecule, $C_{15}H_8ClNO_2$, is essentially planar. The molecular packing in the crystal is stabilized by weak intermolecular C—H$\cdots\pi$ interactions and van der Waals forces.

Comment

We have recently investigated the photocycloaddition reactions with electron-deficient alkenes (Ling *et al.*, 1999) and photoinduced oxygenation reactions of a new class of polycyclic heterocycles, namely 11*H*-benzoxazolo[3,2-*b*]isoquinolin-11-ones, which are benzannelated 5*H*-oxazolo[3,2-*a*]pyridine derivatives. The title compound, (I), one of the derivatives, was isolated from the reaction mixture of the reaction of homophthalic acid with 2-amino-4-chlorophenol. An X-ray crystal structure determination of (I) was undertaken in order to elucidate the conformation, and the results are presented here.



(I)

The bond lengths and angles in (I) are in good agreement with those observed for a closely related structure (Ravishankar *et al.*, 2001). The molecule is essentially planar, with a maximum deviation of 0.043 (3) Å for atom C11. The dihedral angle between the planes of the isoquinoline and benzoxazole moieties is 1.46 (8)°. The coplanarity extends the π-conjugation between these two aromatic substituents. The crystal packing is stabilized by weak intermolecular C—H$\cdots\pi$ interactions, involving both aromatic rings of the isoquinoline moieties of glide-related molecules.

Experimental

The title compound was prepared by refluxing homophthalic anhydride (25 mmol) and 2-amino-4-chlorophenol (25 mmol) in acetic acid for 6 h. The solid product was collected by filtration. Single crystals suitable for crystallographic analysis were obtained by slow evaporation of an acetone–petroleum ether (1:20 *v*/*v*) solution.

Crystal data

$C_{15}H_8ClNO_2$
M_r = 269.67
Monoclinic, $P2_1/c$
a = 23.831 (2) Å
b = 5.9716 (6) Å
c = 8.1549 (8) Å
β = 95.195 (2)°
V = 1155.7 (2) Å^3
Z = 4

D_x = 1.550 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2228 reflections
θ = 2.6–28.3°
μ = 0.33 mm^{-1}
T = 293 (2) K
Block, colorless
0.40 × 0.24 × 0.24 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.881$, $T_{\max} = 0.926$
7010 measured reflections
2823 independent reflections
1976 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
$\theta_{\max} = 28.3°$
$h = -31 \rightarrow 23$
$k = -7 \rightarrow 7$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.150$
$S = 1.08$
2823 reflections
204 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 0.7591P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.26$ e Å^{-3}
$\Delta\rho_{\min} = -0.40$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C3	1.742 (3)	C1—N1	1.400 (3)
O1—C7	1.367 (3)	C7—C8	1.334 (4)
O1—C6	1.381 (3)	C7—N1	1.384 (3)
O2—C15	1.216 (3)	C15—N1	1.401 (3)
C6—O1—C7—C8	−178.5 (2)	O1—C7—C8—C9	179.8 (2)

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

Cg(*A*) and *Cg*(*B*) denote the centroids of the pyridine and benzene rings of the isoquinoline moiety.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···$Cg(B)^{\rm i}$	0.92 (3)	2.79 (3)	3.532 (4)	139 (2)
C13—H13···$Cg(A)^{\rm ii}$	0.96 (3)	2.75 (3)	3.476 (4)	133 (2)

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

All H atoms were located from a difference Fourier map and were refined isotropically. The C—H distances are in the range 0.89 (3)–0.96 (3) Å.

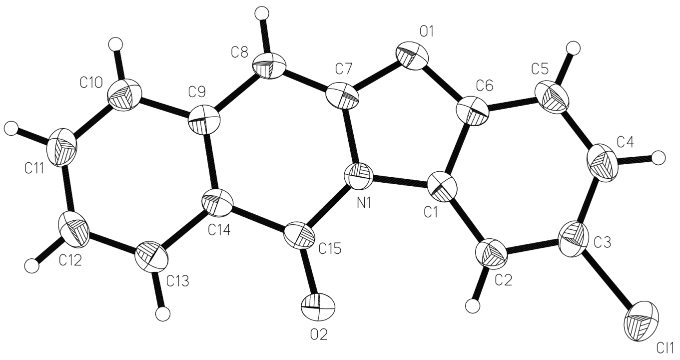


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government and Universiti Sains Malaysia for research grant R&D No. 305/PFIZIK/610961. AU thanks Universiti Sains Malaysia for a Visiting Postdoctoral Fellowship.

References

Ling, K. Q., Cai, H., He, J. H. & Xu, J.-H. (1999). *Tetrahedron*, **55**, 1707–1716.
Ravishankar, T., Chinnakali, K., Senthilvelan, A., Fun, H.-K., Ramakrishnan, V. T., Chandrapromma, S., Razak, I. A. & Usman, A. (2001). *Acta Cryst.* E**57**, o1209–o1210.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

o60 Anwar Usman *et al.* • $C_{15}H_8ClNO_2$ *Acta Cryst.* (2003). E**59**, o59–o60