Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

6-Chloro-3-hydroxy-3-(2-oxopropyl)indolin-2-one

Xiao-Ning Xing,[a] Liang Li,[a] Xiao-Yu Zhu[b] and Jia-Rong Chen[a]*

[a]Key Laboratory of Pesticides & Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China, and [b]Department of Chemistry, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

Correspondence e-mail: jiarongchen2003@yahoo.com.cn.

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.038
wR factor = 0.102
Data-to-parameter ratio = 16.3

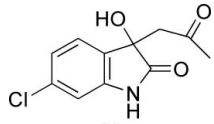
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 29 March 2007
Accepted 25 April 2007

In the crystal structure of the title compound, $C_{11}H_{10}ClNO_3$, an indole derivative, weak intermolecular hydrogen bonds cause the formation of a three-dimensional network.

Comment

Indole derivatives have many applications, oxindole being a common structural unit in various natural products and biologically active compounds. In particular, 3-substituted 3-hydroxyoxindole represents a prominent structural feature in such biological natural products (Tang *et al.*, 2001). We report here the crystal structure of one such oxindole derivative, the title compound, (I).



(I)

In the crystal structure of (I), bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The indole ring systems (N1/C1–C8) are close to planar, with a maximum deviation of 0.052 (2) Å for atom C8. Weak intermolecular hydrogen bonds (Table 1) cause the formation of a three-dimensional network (Fig. 2). N1—H1*A*···O2^{ii} and O1—H1···O2^{i} hydrogen bonds generate edge-fused centrosymmetric $R_2^2(9)$ ring motifs linked by C11—H11*C*···O3^{iii} intermolecular hydrogen bonds and this hydrogen bond generates $C_2^2(10)$ chains (Fig. 2) (Etter, 1990).

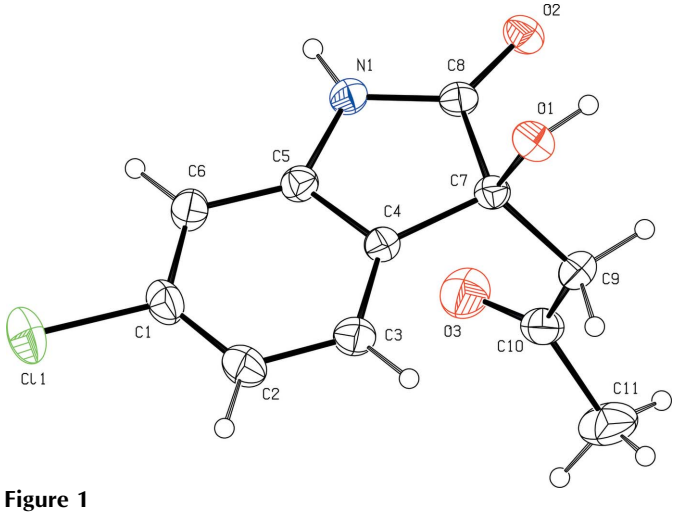


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

Experimental

The title compound was synthesized according to a reported procedure (Chen *et al.*, 2006). Crystals suitable for data collection were obtained by slow evaporation of an *i*-PrOH solution at 283 K.

Crystal data

$C_{11}H_{10}ClNO_3$
M_r = 239.03
Orthorhombic, $P2_12_12_1$
a = 6.5958 (6) Å
b = 7.8459 (8) Å
c = 21.202 (2) Å
V = 1097.19 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 298 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
6687 measured reflections
2391 independent reflections
2277 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.102
S = 1.05
2391 reflections
147 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983), 978 Friedel pairs
Flack parameter: 0.03 (8)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.96	2.7510 (18)	162
N1—H1A···O2^{ii}	0.85	2.19	2.9776 (19)	154
C11—H11C···O3^{iii}	0.96	2.58	3.235 (3)	126

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

O-bound H atoms and the N-bound H atom were located in a difference Fourier map and refined freely with fixed isotropic displacement parameters. All other H atoms were positioned geometrically, with C—H = 0.93, 0.97 or 0.96 Å for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

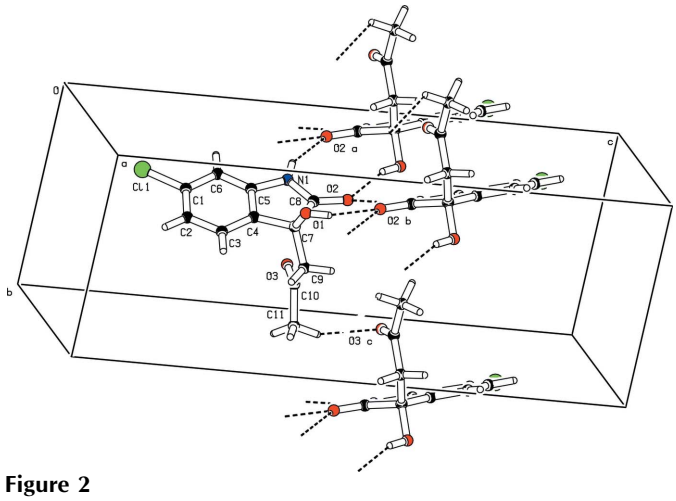


Figure 2
A partial packing diagram for (I). Hydrogen bonds are shown as dashed lines. [Symmetry codes: (*a*) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (*b*) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (*c*) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$.]

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

The authors are grateful to the Central China Normal University and Professor Xiao Wenjing.

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.
Bruker (2001). *SMART* (Version 5.628), *SAINT* (Version 6.45) and *SHELXTL* (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, J. R., Li, X. Y., Xing, X. N. & Xiao, W. J. (2006). *J. Org. Chem.* **71**, 8198–8202.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Tang, Y. Q., Sattler, I., Thiericke, R., Grabley, S. & Feng, X. Z. (2001). *Eur. J. Org. Chem.* pp. 261–267.