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Methyl 2-(2-chlorobenzamido)benzoate

Bishwa Nath Yadav, Shambhu Prasad and Satya Murti Prasad*

Department of Physics, Ranchi University, Ranchi 834008, India

Correspondence e-mail: prasadsm50@hotmail.com

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Key indicators

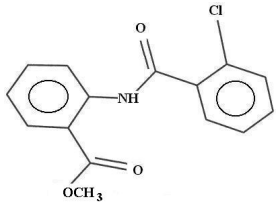
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.065
wR factor = 0.174
Data-to-parameter ratio = 13.3

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

In the title molecule, $C_{15}H_{12}ClNO_3$, the planar chlorophenyl moiety forms a dihedral angle of 60.70 (7)° with the mean plane through the rest of the non-H atoms in the molecule. The carbonyl O atoms are involved in intramolecular N—H···O and C—H···O hydrogen bonds. In the solid state, the molecules exist as centrosymmetric C—H···O hydrogen-bonded dimers.

Comment

As part of our project to study the crystal structures of benzoxinone derivatives, we have previously reported the structure of 2-(2-nitrophenyl)-4,5-benz-1,3-oxazin-6-one (Yadav *et al.*, 2002). We report here the structure of the title compound, (I), which is the hydrolysis product of a benzoxinone.



(I)

A displacement ellipsoid plot of (I) is shown in Fig. 1. The chlorophenyl moiety is planar, with the Cl atom deviating by a maximum of 0.028 (2) Å, and it forms a dihedral angle of 60.70 (7)° with the mean plane through the rest of the non-H atoms (C1–C9/N1/O1–O3), in which the maximum deviation is 0.194 (3) Å for atom O3. The carbomethoxy group (C7/C8/

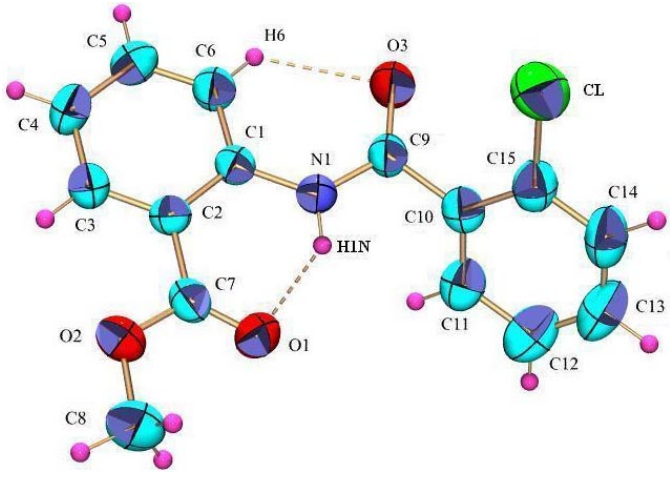


Figure 1
An *ORTEP*-3 plot (Farrugia, 1997) of the molecule, with 50% probability displacement ellipsoids for non-H atoms. Hydrogen bonds are shown as dashed lines.

O1/O2) is twisted out of the plane of the attached benzene ring by 5.6 (3)°. The carbonyl O atoms, O1 and O3, are involved in intramolecular N—H···O and C—H···O hydrogen bonds, respectively (Table 2). In the crystal, the molecules exist as centrosymmetric C13—H13···O1($-x$, $-y$, $1-z$) hydrogen-bonded dimers. Selected intermolecular short contacts observed in the structure are listed in Table 3.

Experimental

The title compound, (I), was prepared by the hydrolysis of 2-(2-chlorophenyl)-4,5-benz-1,3-oxazin-6-one with methanol, which in turn was prepared by the reaction of anthranilic acid with 2-chlorobenzoyl chloride in the presence of pyridine (Kumar *et al.*, 1977).

Crystal data

$C_{15}H_{12}ClNO_3$
M_r = 289.71
Monoclinic, $P2_1/n$
a = 10.072 (1) Å
b = 12.371 (2) Å
c = 11.275 (1) Å
β = 99.62 (2)°
V = 1385.1 (3) Å^3
Z = 4
D_x = 1.389 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10.1–15.4°
μ = 0.28 mm^{-1}
T = 293 (2) K
Rectangular plate, colourless
0.38 × 0.26 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.868, T_{max} = 0.998
2571 measured reflections
2425 independent reflections
1236 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 25.0°
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 14$
$l = -13 \rightarrow 13$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.174
S = 1.03
2425 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0851P)^2 + 0.2726P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C9	1.354 (4)	C2—C3	1.375 (5)
N1—C1	1.386 (4)	C2—C7	1.483 (5)
O1—C7	1.202 (4)	C3—C4	1.385 (5)
O2—C7	1.333 (4)	C4—C5	1.371 (5)
O2—C8	1.461 (5)	C5—C6	1.368 (5)
O3—C9	1.213 (4)	C9—C10	1.509 (5)
C1—C6	1.405 (5)	Cl—C15	1.735 (4)
C1—C2	1.419 (5)		
C9—N1—C1	130.4 (3)	O2—C7—C2	112.5 (3)
C7—O2—C8	115.4 (3)	O3—C9—N1	125.0 (3)
O1—C7—C2	126.3 (3)	N1—C9—C10	112.9 (3)
C9—N1—C1—C6	9.9 (6)	O3—C9—C10—C15	51.3 (5)
C1—C2—C7—O1	−6.7 (6)	N1—C9—C10—C11	53.0 (5)
C3—C2—C7—O2	−4.5 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1	0.86	1.93	2.639 (4)	139
C6—H6···O3	0.93	2.32	2.912 (5)	121
C13—H13···O1^{i}	0.93	2.51	3.300 (6)	143

Symmetry code: (i) $-x, -y, 1-z$.

Table 3
Contact distances (Å).

Cl···N1^{ii}	3.494 (3)	O3···C8^{ii}	3.385 (5)
Cl···C1^{ii}	3.463 (4)	O3···C12^{vii}	3.595 (7)
Cl···C8^{iii}	3.392 (5)	O3···C13^{vii}	3.537 (7)
N1···C3^{iv}	3.517 (4)	C1···C2^{iv}	3.537 (5)
O1···C4^{v}	3.598 (5)	C1···C3^{iv}	3.534 (5)
O2···C6^{iv}	3.567 (4)	C5···C7^{iv}	3.574 (5)
O2···C12^{vi}	3.525 (6)	C6···C7^{iv}	3.567 (5)

Symmetry codes: (ii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$; (iii) $1+x, y, z$; (iv) $-x, 1-y, 1-z$; (v) $-\frac{1}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$; (vi) $-\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (vii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$.

After checking their presence in a difference map, all the H atoms were fixed geometrically and treated as riding on their parent C or N atoms, with C—H = 0.93 and 0.96 Å, and N—H = 0.86 Å.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); 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.

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