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Methyl [6-(2-chlorobenzoyl)-2-oxo-2,3-dihydro-1,3-benzoxazol-3-yl]acetate

Abdullah Aydın,[a]* Yasemin Dündar,[b] Mehmet Akkurt,[c] Orhan Büyükgüngör[d] and M. Fethi Şahin[b]

[a]Department of Science Education, Faculty of Education, Kastamonu University, 37200 Kastamonu, Turkey, [b]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Gazi University, 06330 Ankara, Turkey, [c]Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, and [d]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey

Correspondence e-mail: aaydin@gazi.edu.tr

Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.092
Data-to-parameter ratio = 14.0

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

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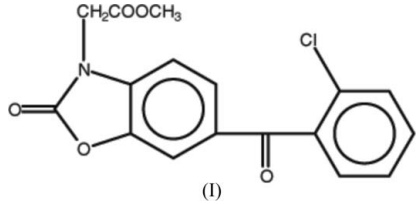
In the molecular structure of the title compound, $C_{17}H_{12}ClNO_5$, the 1,3-benzoxazole ring system makes a dihedral angle of 72.96 (7)° with the benzene ring of the 2-chlorobenzoyl group. In the crystal structure, two intramolecular C—H···O hydrogen bonds influence the molecular conformation.

Comment

It has been shown that (2-benzoxazolinon-3-yl)- or (2-benzothiazolinon-3-yl)acetamides and 6-acyl derivatives of these acetamides alleviate induced pain and suppress induced inflammation with no observed toxicity (Ünlü *et al.*, 2003). 2-Benzoxazolinone derivatives exhibit significant analgesic and anti-inflammatory activity (Şafak *et al.*, 1992). We report here the crystal structure of compound (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The bond lengths and bond angles in (I) are comparable to those observed in related structures (Işık *et al.*, 2004; Aydın *et al.*, 2006). In the molecular structure of (I), the 1,3-benzoxazole ring system (N1/O2/C8–C14) makes a dihedral angle of 72.96 (7)° with the benzene ring (C1–C6).

A quantum-chemical calculation was performed using the CNDO (Pople & Beveridge, 1970) approximation. A view of the calculated molecule is shown in Fig. 2. According to the theoretical CNDO and experimental X-ray results, the values of the geometric parameters of (I) are almost identical within experimental error. Indeed, this result may explain the absence of strong intermolecular interactions. The charges at atoms O1, O2, O3, O4, O5, C7, C14 and Cl6 are −0.295, −0.230, −0.416, −0.315, −0.234, 0.273, 0.512 and 0.395 e^-, respectively. The calculated dipole moment of (I) is 8.258 Debye. The HOMO and LUMO energy levels are −10.7178 and 2.2184 eV, respectively.

Two intramolecular C—H···O hydrogen bonds influence the molecular conformation (Table 1).

Experimental

A mixture of 6-(2-chlorobenzoyl)-2-benzoxazlinone (5 mmol), potassium carbonate (5.75 mmol) and methyl chloroacetate

(5.75 mmol) in 30 ml of acetone was heated to reflux and stirred for 4 h. Ice–water (100 g) was added to the cooled (273–283 K) reaction mixture. After stirring for 1 h, the precipitated solid product was collected by suction filtration, washed with water, dried and recrystallized from methanol–water (3:1, yield 86%, m.p. 381–382 K).

Crystal data

$C_{17}H_{12}ClNO_5$	V = 784.48 (10) Å^3
M_r = 345.73	Z = 2
Triclinic, $P\overline{1}$	D_x = 1.464 Mg m^{-3}
a = 7.0189 (5) Å	Mo $K\alpha$ radiation
b = 10.0329 (7) Å	μ = 0.27 mm^{-1}
c = 12.2791 (8) Å	T = 296 K
α = 112.968 (5)°	Prism, colourless
β = 95.782 (5)°	0.62 × 0.54 × 0.39 mm
γ = 95.013 (5)°	

Data collection

Stoe IPDS-2 diffractometer	16110 measured reflections
ω scans	3044 independent reflections
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)	2631 reflections with $I > 2\sigma(I)$
T_{min} = 0.850, T_{max} = 0.902	R_{int} = 0.054
	θ_{max} = 26.0°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 0.1526P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.092	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
S = 1.02	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
3044 reflections	
218 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15B···O3	0.97	2.55	2.9350 (19)	104
C17—H17A···O4	0.96	2.28	2.697 (2)	106

H atoms were positioned geometrically with C—H = 0.93 (aromatic), 0.96 (methyl), 0.97 Å (methylene) and constrained to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(methyl C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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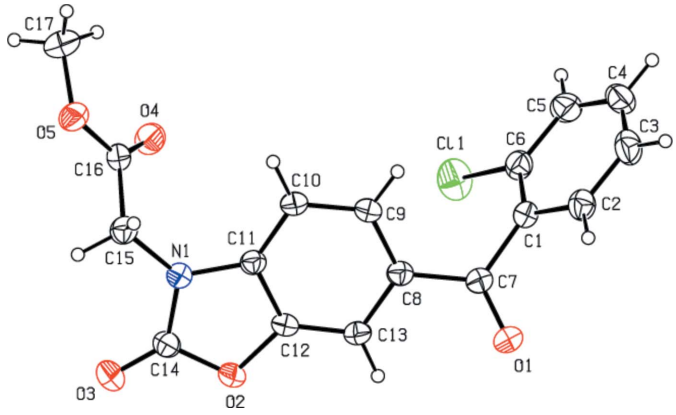

Figure 1
The molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.

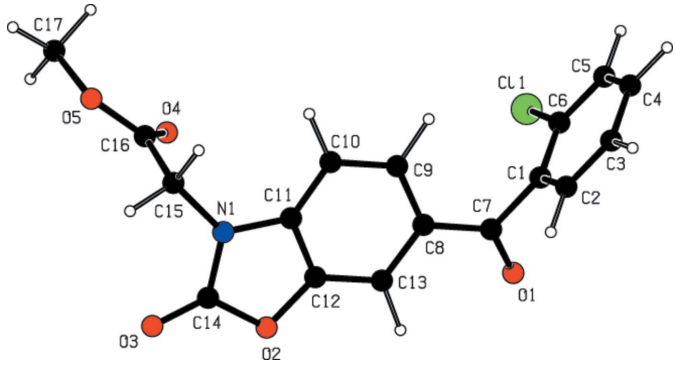

Figure 2
A view of the molecular structure of (I), calculated by the CNDO approximation.

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