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N-(*p*-Chlorophenyl)-3,3-diphenyl-4-(*β*-phenylstyryl)azetidin-2-one

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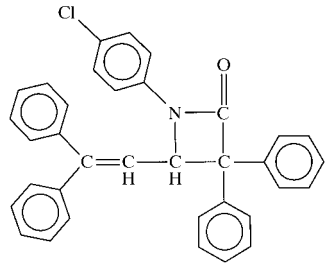
In the title compound, $C_{35}H_{26}ClNO$, the four-membered *β*-lactam ring is essentially planar, with a maximum deviation of 0.012 (1) Å for the N atom. The C—C bond lengths in the *β*-lactam ring are 1.591 (2) and 1.549 (2) Å. The two phenyl rings attached to the *β*-lactam ring are nearly perpendicular to each other [83.2 (1)°].

Comment

Since the structure and conformation of *β*-lactams play a key role in the biological activity of *β*-lactam antibiotics, it is worthwhile studying their activity when modified by substituents. The activity and selectivity of the 4-substituted 2-azetidinone ring can be decisively influenced by the subtituents attached to the *β*-lactam ring (Kumar *et al.*, 1993; Sharma *et al.*, 1994; Manhas *et al.*, 1988). Previously, some structural studies were made by changing the subtituents around the *β*-lactam ring (Ercan *et al.* 1996*a*,*b*; Kabak *et al.*, 1999*a*,*b*).

The four-membered *β*-lactam ring of (I) is nearly planar, with a slight deviation of the N1 atom [0.012 (1) Å]. The bond lengths on the lactam ring are comparable with those in monocyclic 3- or 4-substituted 2-azetidinones (Kabak *et al.*, 1999*a*,*b*, and references therein). Due to the different substituents attached to the *β*-lactam ring, a very significant elongation of the C8—C21 bond [1.591 (2) Å] is observed in this compound which is different from the previous works (Table 2). This may be due to the substituents at the C8 and C21 atoms. The diagonal contact distances deviate much from those observed in similar works (Table 2). The valence angles at the *β*-lactam ring deviate from 90° by 2–6°, producing a trapezoid rather than a rectangular shape for the ring.



(I)

The angle between two phenyl rings which are attached to the C8 atom shows that these two substituents are nearly perpendicular to each other [83.2 (1)°] and the corresponding torsion angle (C9—C8—C15—C16) is 69.2 (2)°. The other two phenyl groups in the phenylstyryl group, which are attached to the *β*-lactam ring *via* the C23 and C22 atoms to the C21 atom, are close to being perpendicular [88.8 (1)°].

There are no notable intermolecular interactions.

Experimental

A solution of diphenylacetyl chloride (0.002 mol, 1.92 ml) in dry benzene (20 ml) was added dropwise over 1 h at room temperature to a mixture of *β*-phenylcinnamaldehyde *N*-*p*-chlorophenylimine (0.001 mol, 0.242 g) and triethylamine (0.002 mol, 2.78 ml) in dry benzene. The mixture was stirred for 2 h at room temperature and the amine salt removed by filtration of the mixture. The filtrate was then washed with 5% HCl and water, and dried over sodium sulfate. The title compound was crystallized from ethanol.

Crystal data

$C_{35}H_{26}ClNO$
M_r = 512.02
Monoclinic, $P2_1/n$
a = 14.0672 (13) Å
b = 12.6920 (10) Å
c = 15.5238 (17) Å
β = 92.972 (9)°
V = 2767.9 (5) Å^3
Z = 4
D_x = 1.231 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 20.05–27.92°
μ = 0.166 mm^{-1}
T = 293 (2) K
Prism, white
0.85 × 0.55 × 0.35 mm

Data collection

Rigaku AFC-7*S* diffractometer
ω–2θ scans
Absorption correction: ψ scans (North *et al.*, 1968)
T_{min} = 0.866, T_{max} = 0.944
8362 measured reflections
8067 independent reflections
4115 reflections with >2$\sigma(I)$
R_{int} = 0.0305
θ_{max} = 30°
$h = 0 \rightarrow 19$
$k = 0 \rightarrow 17$
$l = -21 \rightarrow 21$
3 standard reflections every 150 reflections
intensity decay: 0.56%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.165
S = 1.031
8067 reflections
362 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0740P)^2 + 0.4079P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C3	1.7335 (19)	C7—C8	1.549 (2)
O1—C7	1.205 (2)	C8—C9	1.514 (2)
N1—C7	1.367 (2)	C8—C15	1.517 (2)
N1—C6	1.411 (2)	C8—C21	1.591 (2)
N1—C21	1.482 (2)		
C7—N1—C6	132.96 (14)	C6—N1—C21	131.50 (13)
C7—N1—C21	95.54 (13)	O1—C7—N1	131.52 (16)

Table 2
Bond lengths (Å) of the β-lactam ring compared with previous works.

Compd	O1—C7	N1—C7	N1—C21	C8—C21
(II)†	1.213 (4)	1.357 (4)	1.482 (4)	1.536 (5)
(III)	1.188	1.38 (1)	1.467	1.55 (2)
(IV)	1.186 (6)	1.362 (6)	1.469 (5)	1.571 (6)
(V)	1.193 (3)	1.370 (3)	1.474 (4)	1.568 (4)
(I)	1.205 (2)	1.367 (2)	1.482 (2)	1.591 (2)

Compd	C—C8	C7···C21	N1···C8
(II)	1.55 (1)	2.115	2.074
(III)	1.56 (1)	2.169	2.057
IV	1.56 (1)	2.127	2.068
(V)	1.56 (1)	2.121	2.082
(I)	1.57 (2)	2.111 (2)	2.117 (2)

† Notes: (II) 3,3-dichloro-4-(*p*-methoxyphenyl)-1-phenyl-2-azetidinone(Ercan *et al.*, 1996*a*); (III)3,3-dichloro-1-(*p*-chlorophenyl)-4-phenyl-2-azetidinone(Ercan *et al.*, 1996*b*); (IV) 3,3-dichloro-1,4-diphenyl-2-azetidinone(Kabak *et al.*, 1999*a*); (V)3,3-dichloro-4-(*p*-methoxyphenyl)-1-(*p*-chlorophenyl)-2-azetidinone(Kabak *et al.*, 1999*b*); (I)3,3–Diphenyl–N-*p*-chlorophenyl-4-(2-phenylstyryl)azetidin-2-one(this work).

H atoms were placed geometrically on the corresponding C atoms. Because of the large displacement parameters of the C10 and C11 atoms, the C9–C14 benzene ring was restrained during the refinement process.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1994); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997).

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