component. The initial model was refined by least-squares techniques. A disordered component was observed for the terminal thienyl group. Occupancy of both parts refined to 0.55 and 0.45 and was fixed at these values for further refinement. Non-H atoms were refined with anisotropic displacement parameters. H atoms potentially involved in hydrogen bonds (*i.e.* on atoms O4 and O5) were located by Fourier difference while the others were calculated. The positions of all the H atoms except H4 and H5 were refined using the riding model method. *PLATON*94 (Spek, 1990) was used for geometric analysis of the structure. Most machine calculations were conducted on an IBM *RS*6000.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994). Cell refinement: *CAD*-4 *EXPRESS*. Data reduction: *NONIUS* (Baudoux & Evrard, 1993). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP* (Johnson, 1965). Software used to prepare material for publication: *PLATON*94 (Spek, 1990).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SX1017). Services for accessing these data are described at the back of the journal.

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2-Oxazolidinone

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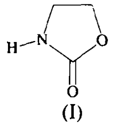
Abstract

Redetermination of the crystal structure of the title compound, $C_3H_5NO_2$, leads to a precise geometry for this molecule that is compared with the conformation of several aryl-substituted oxazolidinones. Molecular cohesion is stabilized by hydrogen bonds between the amine and carbonyl groups. The coplanar approach of the NH group can be rationalized in terms of the *ab initio* calculated molecular electrostatic potential generated by the C═O group.

Comment

As a part of our interest in the structural study of aryl oxazolidinones (Moureau *et al.*, 1992, 1994, 1995; Wouters *et al.*, 1993, 1994; Wouters, Evrard & Durant, 1994; Wouters, Perpete, Norberg, Evrard & Durant, 1994) we redetermined the structure of 2-oxazolidinone (R_1 = 0.039), (I), previously reported in the literature (R_1 = 0.132; Turley, 1972).



(I)

The molecular structure with the atom-numbering scheme is illustrated as an *ORTEP*II (Johnson, 1976) plot in Fig. 1. Bond distances and angles are close to those previously reported for the title compound but are determined with more precision. The N—C1 and N—C3 bonds [1.441 (2) and 1.326 (2) Å, respectively] are slightly shorter than corresponding bonds in γ-lactams [C*—NH—C═O: C_{sp^3}—N(3) = 1.457 and C_{sp^2}—N(3) = 1.331 Å according to Allen *et al.* (1987)]. The C3—O2 bond length [1.219 (2) Å] is slightly longer than a C═O double bond (C═O: 1.196 Å in esters and 1.201 Å in lactones; Allen *et al.*, 1987), while the C3—O1 bond [1.347 (2) Å] is significantly shorter than the corresponding C—O bond in γ-lactones (1.464 Å) underlying electronic delocalization from N to O1 *via* the C3—O2 group.

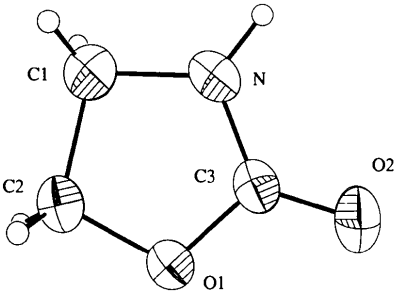


Fig. 1. The molecular structure and conformation of the title compound. Non-H atoms are represented by displacement ellipsoids at the 50% probability level. The atomic numbering scheme used in the paper is shown.

Structure comparison on a series of *N*-aryl-substituted oxazolidin-2-ones has been performed. Internal coordinates were retrieved from the Cambridge Structure Database (version 5.11). Statistical analysis of the distribution of bond lengths was performed using the *Vista* program (Allen & Kennard, 1993). In the following discussion, the mean value and the standard deviation are obtained from a set of 17 retrieved structures. Comparison of the geometry of the title compound with these *N*-aryl oxazolidin-2-ones shows that the introduction of an aromatic ring to the oxazolidinone cycle decreases the electronic delocalization in this entity. In particular, the N—C_{sp^2} bond (corresponding to N—C3 in the present structure) is statistically longer in aryl-substituted analogs [1.360 (13) Å]. The C3—O2 and C3—O1 bonds are also affected by the substitution of the oxazolidinone ring by an aromatic entity as their corresponding lengths are 1.206 (11) and 1.353 (10) Å.

The title molecule is overall planar (r.m.s. deviation from the best plane through all the atoms of molecule is 0.001 Å, with maximum deviations of −0.080 and 0.076 Å for C1 and C2, respectively).

Intermolecular hydrogen-bond interactions are indicated by the distance between the amine proton on N and the keto O2 atom of an adjacent molecule [N···O2^i 2.868 (2), H···O2^i 2.005 (17) Å and N—H···O2^i 170.2 (16)°; symmetry code: (i) $1-x$, $y-\frac{1}{2}$, $\frac{3}{4}-z$]. The hydrogen bonds create a chained structure in the y direction, while molecules in parallel planes are connected by dipole–dipole and van der Waals interactions. The coplanar approach of the NH group can be rationalized in terms of the *ab initio* calculated molecular electrostatic potential (MEP) generated by the C═O group (Ooms, Wouters & Durant, 1997). The preference for O2 *versus* O1 is explained by the deeper attractive potential well (−65 *versus* −55 kcal mol^{-1}) generated by this O atom. A coplanar approach is expected by the shape of the MEP (not shown), mainly in the plane of the molecule (Ooms, Wouters & Durant, 1997). This geometry is coherent with results from a crystal survey of three-dimensional hydrogen-bond geometries (Mills & Dean, 1996).

Experimental

The title compound was obtained from Fluka.

Crystal data

$C_3H_5NO_2$
$M_r = 87.08$
Monoclinic
$P2_1/c$
$a = 7.3180 (15)$ Å
$b = 5.6730 (11)$ Å
$c = 9.989 (2)$ Å
$\beta = 110.79 (3)°$
$V = 387.70 (13)$ Å^3
$Z = 4$
$D_x = 1.492$ Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation
$\lambda = 1.54178$ Å
Cell parameters from 25 reflections
$\theta = 40–45°$
$\mu = 1.087$ mm^{-1}
$T = 293 (2)$ K
Cube
0.40 × 0.40 × 0.40 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
1163 measured reflections
760 independent reflections
737 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.029$
$\theta_{\rm max} = 71.89°$
$h = -9 \rightarrow 9$
$k = -7 \rightarrow 0$
$l = -12 \rightarrow 0$
3 standard reflections
frequency: 60 min
intensity decay: 0.01%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.100$
$S = 1.120$
760 reflections
76 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.0456P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$

$\Delta\rho_{\rm max} = 0.191$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.265$ e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.55 (3)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
N	0.3559 (2)	−0.1725 (2)	0.5737 (1)	0.0469 (4)
O1	0.1609 (1)	0.0954 (2)	0.43782 (8)	0.0461 (4)
O2	0.3471 (2)	0.2011 (2)	0.6596 (1)	0.0608 (4)
C1	0.2481 (2)	−0.3047 (2)	0.4470 (1)	0.0512 (4)
C2	0.1400 (2)	−0.1082 (2)	0.3474 (1)	0.0464 (4)
C3	0.2960 (2)	0.0492 (2)	0.5675 (1)	0.0393 (4)

Table 2. *Selected geometric parameters (Å, °)*

N—C3	1.326 (2)	O1—C2	1.440 (2)
N—C1	1.441 (2)	O2—C3	1.219 (2)
O1—C3	1.347 (2)	C1—C2	1.516 (2)
C3—N—C1	112.6 (1)	O2—C3—N	128.9 (1)
C3—O1—C2	109.0 (1)	O2—C3—O1	120.8 (1)
N—C1—C2	100.9 (1)	N—C3—O1	110.3 (1)
O1—C2—C1	105.3 (1)		
C3—N—C1—C2	11.9 (2)	C1—N—C3—O1	−5.3 (2)
C3—O1—C2—C1	11.7 (1)	C2—O1—C3—O2	175.6 (1)
N—C1—C2—O1	−13.6 (1)	C2—O1—C3—N	−4.4 (1)
C1—N—C3—O2	174.6 (1)		

Non-H atoms were refined with anisotropic temperature factors. Positions and isotropic temperature factors were refined for H atoms. *PLATON*94 (Spek, 1990) was used for the geometry analysis of the structure. All computations were performed on IBM RS/6000 machines of the Namur Scientific Computing Facilities (SCF) centre.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1992). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Software used to prepare material for publication: *PLATON*94.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1055). Services for accessing these data are described at the back of the journal.

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1-(4-Chlorobenzoyloxy)-2-methoxy-4-(2-propenyl)benzene

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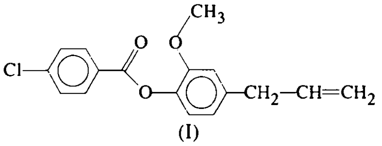
Abstract

In the title compound, 2-methoxy-4-(2-propenyl)phenyl 4-chlorobenzoate, $C_{17}H_{15}ClO_3$, the allyl group is observed to be in a disordered state. The two C atoms of the allyl group occupy two sets of sites in unequal proportions (68:32). The dihedral angle between the two aromatic rings is 71.64 (10)°.

Comment

The structure of the title compound, (I), was determined as part of our studies on the synthesis and characterization of this type of compound. An *ORTEP*II (Johnson, 1976) drawing of the molecular structure of (I) with the atomic labellling is shown in Fig. 1.



(I)

The phenyl rings and central carbonyl moiety in the molecule are similar to those described in the literature (Blake, Fallis, Parsons, Schröder & Bruce, 1996). The dihedral angle between the planes of the chlorophenyl and methoxyphenyl rings is 71.64 (10)°, and these two planes make angles of 10.3 (2) and 81.90 (9)°, respectively, with the plane of the central carbonyl moiety. The methoxy C14 atom deviates by 0.101 (6) Å