The title compound, C_{12}H_{9}ClN_{2}O_{2}, was synthesized and characterized by ^1H NMR and IR spectroscopy and X-ray diffraction techniques. The chlorobenzoyl fragment in the structure is almost flat, whereas the carbonyl group is almost perpendicular to the pyrimidine ring plane.

Comment

We have previously described the crystal structures of a series of N-phenacyl-2-pyridones (Albov et al., 2004a,b, 2005). We report here the synthesis and crystal structure of theiraza-analog, (2). In contrast to well investigated reactions of pyridones with α-halogenoketones, analogous reactions for pyrimidones have been little studied. There are only a few examples, namely the reaction of (1) with the acetal of α-bromoacetaldehyde (Holy et al., 1984) or with chloroacetic acid derivatives (Gefenas & Vainilavichus, 2003) and phenacylation of the 5-chloro derivative of (1) (Benneche & Gandersen, 1988). In all of these cases, the products of N-alkylation were exclusively observed. Interestingly, in the study of the phenacylation of sterically hindered 4,6-dimethylpyrimidone, only the N-isomers have been isolated (Ivanov et al., 1983; Buchan et al., 1978). Usually these reactions are performed in aprotic bipolar solvents in the presence of bases, so that the alkylated species has been the pyrimidone anion.

We have found that reaction of (1) with p-chlorophenacyl bromide in the presence of K_{2}CO_{3} in acetone yields the title compound, (2). The ^1H NMR spectra were useless for distinguishing between O- and N-isomers. In the IR spectrum of (2), two C=O peaks were observed, one for the –N=O fragment of pyrimidone and another for the carbonyl group, thus clearly confirming selective N-alkylation (in the case of O-phenacylation no amide peak would be observed). The structure of the N-isomer was finally confirmed by X-ray crystallographic analysis.

In the pyrimidone ring of (2), the single and double bonds alternate (Table 1), though allowing some degree of conjugation. In the Cambridge Structural Database (CSD: Version 5.27; Allen, 2002), we found only one structure with the pyrimidone (2) fragment, namely the parent pyrimidone (1) (Furberg & Solbakk, 1970) with the same distribution of bond lengths. In the structure of (2), the dihedral angle between the

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1-(4-Chlorobenzoylmethyl)pyrimidin-2(1H)-one

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Key indicators

Single-crystal X-ray study

T = 293 K

Mean σ(C–C) = 0.004 Å

R factor = 0.054

wR factor = 0.161

Data-to-parameter ratio = 15.0

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

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The hydrochloride of (1) (26.5 g; 0.2 mol) was suspended in 500 ml of dry acetone. A solution of 0.1 mol of p-chlorophenyl bromide in 100 ml acetone and 0.4 mol K2CO3 was added with stirring. The reaction mixture was stirred for 2 d at room temperature, and then the solvent was evaporated under vacuum. The residue was washed with water and then with ethyl acetate. The product was isolated by suction and recrystallized from acetonitrile. (yield 95%, m.p. 497–499 K).1 1H NMR (DMSO-d6/TMS): δ J(Hz) 8.57 (m, 1H, H-6), 8.12–8.16 (m, 3H, 2H of p-CipH, H-4), 7.57 (m, 2H, p-CipH), 6.42 (m, 1H, H-5), 5.44 (s, 2H, NCH2). IR (nujol) ν̇ cṁ 1605, 1615. Analysis calculated for C12H9ClN2O2: C 57.96, H 3.65, N 11.27%; found: C 57.67, H 3.41, N 11.29%.

**Crystal data**

C12H9ClN2O2, Mw = 248.66

Monoclinic, P2₁/n

a = 10.2191 (10) Å

b = 10.8421 (14) Å

c = 11.3449 (15) Å

β = 115.065 (11)°

V = 1138.6 (3) Å³

**Data collection**

Enraf-Nonius CAD-4 diffractometer

ω scans

Absorption correction: none

2327 measured reflections

2327 independent reflections

**Refinement**

Refinement on F²

R[F² > 2σ(F²)] = 0.054

wR(F²) = 0.161

S = 1.14

2327 reflections

155 parameters

H-atom parameters constrained

Z = 4

D = 1.451 Mg m⁻³

Cu Kα radiation

μ = 2.91 mm⁻¹

T = 293 (2) K

Prism. colourless

0.2 × 0.2 × 0.2 mm

1842 reflections with I > 2σ(I)

I standard reflection intensity decay: 5%

All H atoms were refined using a riding model, with C–H = 0.93 Å and Uiso(H) = 1.2Ueq(C) for aromatic H atoms C–H = 0.97 Å and Uiso(H) = 1.5Ueq(C) for CH₃ H atoms, and C–H = 0.96 Å and Uiso(H) = 1.5Ueq(C) for CH₂ H atoms.

**Crystal data**

C₁₂H₉ClN₂O₂, Mw = 248.66

Monoclinic, P2₁/n

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b = 10.8421 (14) Å

c = 11.3449 (15) Å

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Cu Kα radiation

μ = 2.91 mm⁻¹

T = 293 (2) K

Prism. colourless

0.2 × 0.2 × 0.2 mm

1842 reflections with I > 2σ(I)

I standard reflection frequency: 120 min

intensity decay: 5%

All H atoms were refined using a riding model, with C–H = 0.93 Å and Uiso(H) = 1.2Ueq(C) for aromatic H atoms C–H = 0.97 Å and Uiso(H) = 1.5Ueq(C) for CH₃ H atoms, and C–H = 0.96 Å and Uiso(H) = 1.5Ueq(C) for CH₂ H atoms.

**References**


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