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SYNTHESIS, CRYSTAL AND MOLECULAR STRUCTURE OF 2-(3-CHLOROPROPYL)-6-METHYL-4-PHENYLQUINAZOLINE 3-OXIDE

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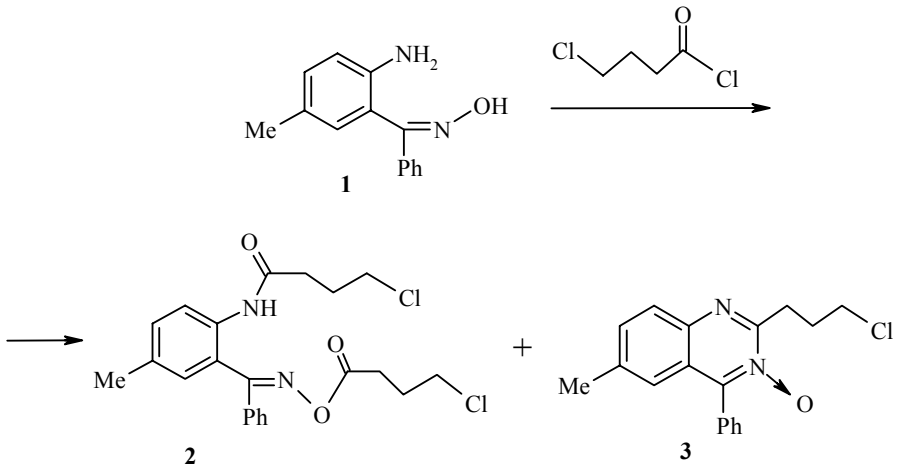
The acylation of the syn isomer of the oxime of 2-amino-5-methylbenzophenone with 4-chlorobutyryl chloride gives a mixture of the anti isomer of the 4-chlorobutyryloximine of 2-(4-chlorobutyryl)amino-5-methylbenzophenone and 2-(3-chloropropyl)-6-methyl-4-phenylquinazoline 3-oxide. The crystal and molecular structure of this oxide was established by X-ray diffraction structural analysis. The molecule is planar. The electron impact fragmentation of 2-(3-chloropropyl)-6-methyl-4-phenylquinazoline 3-oxide was discussed.

Keywords: quinazoline, mass spectrometry, X-ray diffraction structural analysis.

The acylation of oximes of 2-aminobenzophenones with different agents such as chloroacetyl chloride and 3-chloropropionyl chloride holds interest since the acyl derivatives, as shown in our previous work [1-3], are valuable intermediates for the synthesis of 16- and 18-membered dibenzodioxatetraazamacroheterocycles. In our attempt to obtain intermediates for the synthesis of 20-membered macroheterocycles, we studied the acylation of the *syn* isomer of the oxime of 2-amino-5-methylbenzophenone (**1**) using 4-chlorobutyryl chloride and found that, in the absence of base and in the presence of excess acylating agent, 2-(3-chloropropyl)-6-methyl-4-phenylquinazoline 3-oxide (**3**) was found in addition to the *anti* isomer of the 4-chlorobutyryloximine of 2-(4-chlorobutyryl)amino-5-methylbenzophenone (**2**).



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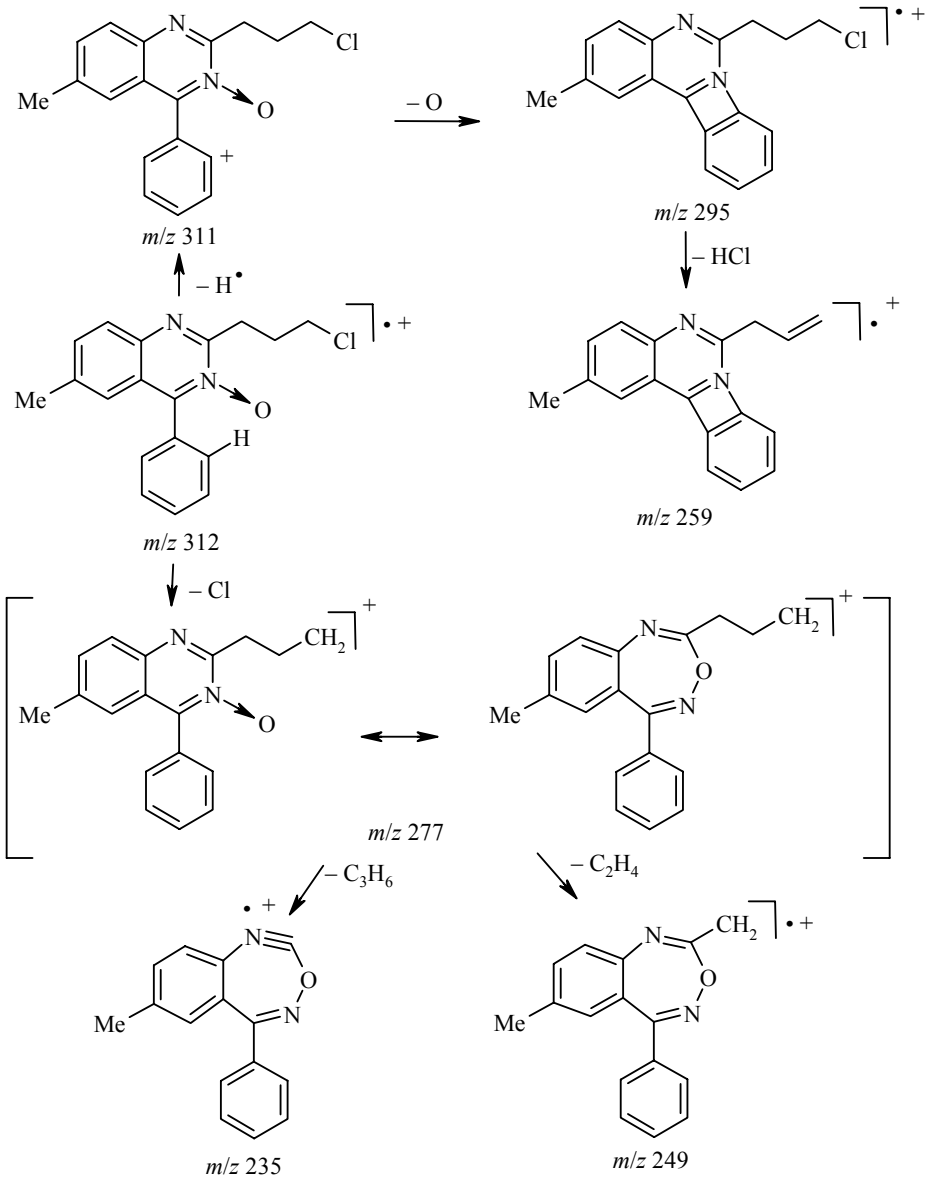
The mechanism for the formation of quinazoline **3** in the present work was not studied in detail. This transformation is probably analogous to the acylation described in the literature for the oximes of 2-aminobenzophenones by chloroacetyl chloride to give 2-chloromethyl-4-phenylquinazoline 3-oxides [4].

The mass spectrometry of quinazolines has been examined by a number of workers [5-10]. In previous work [5], we showed that the initial pathways for the decomposition of the molecular ions of quinazoline 3-oxides are accompanied by the elimination of the methyl substituent or oxygen atom, followed only then by opening of the heteroaryl ring. The molecular ion peaks in the mass spectra of these compounds are rather strong. In contrast, the molecular ion of **3** is unstable relative to electron impact (the intensity of the M^+ peak is only 1.5%). The fragmentation of **3**, represented by the scheme given below, probably proceeds through two alternative pathways.

The scheme below shows that one of the fragmentation pathways results from elimination of a hydrogen atom from the *ortho* position of the phenyl substituent* (ion 311, 1.6%). Strong peaks for the $[M-H]^+$ ions



* Here and henceforward, the *m/z* (I_{rel}, %) values are given for the ion peaks.

attributed to a similar mechanism were observed for 4-phenylquinazolin-2-ones [6]. The subsequent loss of the oxygen atom leads to an ion, which probably has azetidine structure (ion 295, 84.4%), followed only then by the fragmentation of the substituent at $C_{(2)}$ accompanied by the elimination of an HCl molecule. The alternative fragmentation pathway does not lead to loss of the oxygen atom, but rather to decomposition of the 3-chloropropyl substituent. The elimination of the chlorine atom leads to the formation of ion 277, whose peak has maximum intensity in the mass spectrum. The finding that the oxygen atom is not lost suggests that this atom is involved in the expansion of the quinazoline ring. Changing the means of ionization does not lead to change in the nature of the fragmentation. The FAB mass spectrum shows a strong peak for the $[M+H]^+$ ions with maximum intensity as well as fragmentation ions 295 (27.2%) and 277 (20.0%).

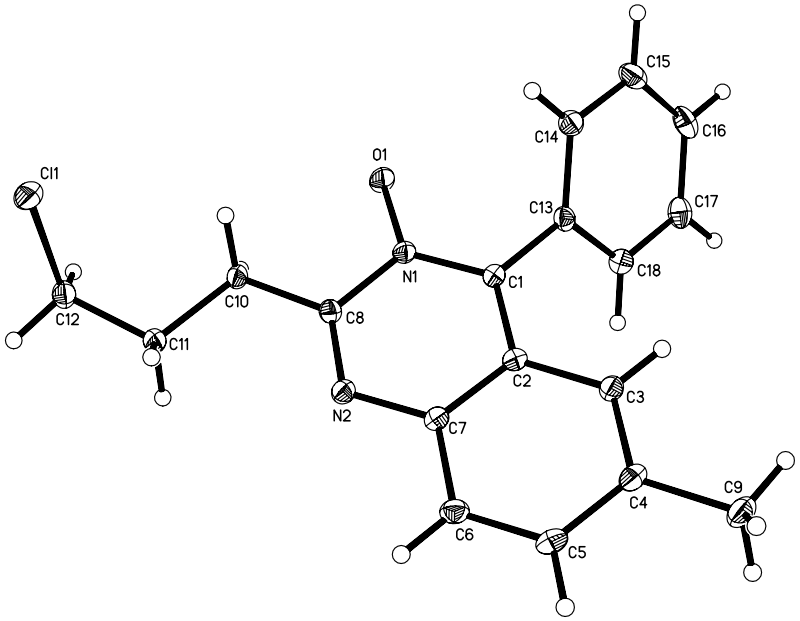


Fig. 1. Molecular structure of compound **3**.

In previous work [3], we showed that bands at 3390-3400 cm^{-1} corresponding to the NH bond of the free amide group are characteristic for the IR spectra of *syn* isomers of acyl derivatives of oximes, while these bands are lacking in the IR spectra of the corresponding *anti* isomers. The absence of a band in the IR spectrum of **2** in the region characteristic for the *syn* isomers suggests that the diacyl derivative of oxime **2** is an *anti* isomer. The isomerization of **2** during the acylation may be attributed to the acidic reaction medium (by analogy to the isomerization of the *syn* isomers of oximes of 2-aminobenzophenones upon their acylation by 3-chloropropionyl chloride in the absence of base [3]).

TABLE 1. Some Bond Lengths (*l*) in the Structure of Compound **3**

Bond	*l*, Å	Bond	*l*, Å	Bond	*l*, Å
$Cl_{(1)}$–$C_{(12)}$	1.8118(12)	$C_{(14)}$–$C_{(15)}$	1.3880(15)	$C_{(7)}$–$C_{(6)}$	1.4132(14)
$O_{(1)}$–$N_{(1)}$	1.2970(11)	$C_{(14)}$–$C_{(13)}$	1.3992(14)	$C_{(6)}$–$C_{(5)}$	1.3737(15)
$N_{(1)}$–$C_{(1)}$	1.3500(13)	$C_{(10)}$–$C_{(8)}$	1.4906(14)	$C_{(18)}$–$C_{(17)}$	1.3908(15)
$N_{(1)}$–$C_{(8)}$	1.4168(13)	$C_{(2)}$–$C_{(7)}$	1.4135(14)	$C_{(16)}$–$C_{(17)}$	1.3890(16)
$N_{(2)}$–$C_{(8)}$	1.2983(13)	$C_{(2)}$–$C_{(3)}$	1.4179(14)	$C_{(16)}$–$C_{(15)}$	1.3935(17)
$N_{(2)}$–$C_{(7)}$	1.3755(13)	$C_{(2)}$–$C_{(1)}$	1.4214(14)	$C_{(3)}$–$C_{(4)}$	1.3784(14)
$C_{(11)}$–$C_{(12)}$	1.5173(14)	$C_{(13)}$–$C_{(18)}$	1.3973(15)	$C_{(4)}$–$C_{(5)}$	1.4171(15)
$C_{(11)}$–$C_{(10)}$	1.5220(14)	$C_{(13)}$–$C_{(1)}$	1.4821(14)	$C_{(4)}$–$C_{(9)}$	1.5049(15)

We have already studied the structure of several quinazoline 3-oxides [11]. The X-ray diffraction structural data show that the phenyl substituent in **3** (Fig. 1) forms a dihedral angle of 57.6° with the planar quinazoline system; $C_{(10)}$ and $C_{(11)}$ are also in this plane. The geometrical parameters of this molecule have standard values with the exception of the parameters involving $N_{(1)}$. The bond lengths are given in Table 1, while the valence angles and torsion angles are given in Table 2. Comparison of these data with the literature

TABLE 2. Valence Angles (ω) and Torsion Angles (φ) in the Structure of Compound **3**

Angle	ω, deg	Angle	φ, deg
$O_{(1)}$–$N_{(1)}$–$C_{(1)}$	122.24(9)	$C_{(12)}$–$C_{(11)}$–$C_{(10)}$–$C_{(8)}$	173.50(9)
$O_{(1)}$–$N_{(1)}$–$C_{(8)}$	117.13(8)	$C_{(15)}$–$C_{(14)}$–$C_{(13)}$–$C_{(18)}$	1.04(15)
$C_{(1)}$–$N_{(1)}$–$C_{(8)}$	120.60(9)	$C_{(15)}$–$C_{(14)}$–$C_{(13)}$–$C_{(1)}$	-176.95(10)
$C_{(8)}$–$N_{(2)}$–$C_{(7)}$	118.72(9)	$C_{(7)}$–$N_{(2)}$–$C_{(8)}$–$N_{(1)}$	1.42(15)
$C_{(12)}$–$C_{(11)}$–$C_{(10)}$	110.72(8)	$C_{(7)}$–$N_{(2)}$–$C_{(8)}$–$C_{(10)}$	-179.25(9)
$C_{(15)}$–$C_{(14)}$–$C_{(13)}$	120.00(10)	$O_{(1)}$–$N_{(1)}$–$C_{(8)}$–$N_{(2)}$	179.37(9)
$C_{(8)}$–$C_{(10)}$–$C_{(11)}$	114.67(8)	$C_{(1)}$–$N_{(1)}$–$C_{(8)}$–$N_{(2)}$	1.57(15)
$C_{(7)}$–$C_{(2)}$–$C_{(3)}$	119.21(9)	$O_{(1)}$–$N_{(1)}$–$C_{(8)}$–$C_{(10)}$	-0.02(13)
$C_{(7)}$–$C_{(2)}$–$C_{(1)}$	118.15(9)	$C_{(1)}$–$N_{(1)}$–$C_{(8)}$–$C_{(10)}$	-177.82(9)
$C_{(3)}$–$C_{(2)}$–$C_{(1)}$	122.64(9)	$C_{(11)}$–$C_{(10)}$–$C_{(8)}$–$N_{(2)}$	-0.67(14)
$C_{(18)}$–$C_{(13)}$–$C_{(14)}$	119.56(10)	$C_{(11)}$–$C_{(10)}$–$C_{(8)}$–$N_{(1)}$	178.71(8)
$C_{(18)}$–$C_{(13)}$–$C_{(1)}$	118.29(9)	$O_{(1)}$–$N_{(1)}$–$C_{(1)}$–$C_{(2)}$	177.68(9)
$C_{(14)}$–$C_{(13)}$–$C_{(1)}$	122.12(9)	$C_{(8)}$–$N_{(1)}$–$C_{(1)}$–$C_{(2)}$	-4.63(14)
$N_{(2)}$–$C_{(8)}$–$N_{(1)}$	122.71(9)	$O_{(1)}$–$N_{(1)}$–$C_{(1)}$–$C_{(13)}$	-5.52(14)
$N_{(2)}$–$C_{(8)}$–$C_{(10)}$	123.43(9)	$C_{(8)}$–$N_{(1)}$–$C_{(1)}$–$C_{(13)}$	172.17(9)
$N_{(1)}$–$C_{(8)}$–$C_{(10)}$	113.86(8)	$C_{(7)}$–$C_{(2)}$–$C_{(1)}$–$N_{(1)}$	4.77(14)
$N_{(1)}$–$C_{(1)}$–$C_{(2)}$	118.03(9)	$C_{(3)}$–$C_{(2)}$–$C_{(1)}$–$N_{(1)}$	-174.32(9)
$N_{(1)}$–$C_{(1)}$–$C_{(13)}$	117.94(9)	$C_{(7)}$–$C_{(2)}$–$C_{(1)}$-$C_{(13)}$	-171.83(9)
$C_{(2)}$–$C_{(1)}$–$C_{(13)}$	123.94(9)	$C_{(3)}$–$C_{(2)}$–$C_{(1)}$–$C_{(13)}$	9.08(16)
$N_{(2)}$–$C_{(7)}$–$C_{(6)}$	118.98(9)	$C_{(18)}$–$C_{(13)}$–$C_{(1)}$–$N_{(1)}$	-122.01(11)
$N_{(2)}$–$C_{(7)}$–$C_{(2)}$	121.62(9)	$C_{(14)}$–$C_{(13)}$–$C_{(1)}$–$N_{(1)}$	56.00(13)
$C_{(6)}$–$C_{(7)}$–$C_{(2)}$	119.40(9)	$C_{(18)}$–$C_{(13)}$–$C_{(1)}$–$C_{(2)}$	54.59(14)
$C_{(5)}$–$C_{(6)}$–$C_{(7)}$	119.93(10)	$C_{(14)}$–$C_{(13)}$–$C_{(1)}$–$C_{(2)}$	-127.40(11)
$C_{(17)}$–$C_{(18)}$–$C_{(13)}$	120.08(10)	$C_{(8)}$–$N_{(2)}$–$C_{(7)}$–$C_{(6)}$	179.33(9)
$C_{(11)}$–$C_{(12)}$–$Cl_{(1)}$	110.97(8)	$C_{(8)}$–$N_{(2)}$–$C_{(7)}$–$C_{(2)}$	-1.14(15)
$C_{(17)}$–$C_{(16)}$–$C_{(15)}$	119.86(10)	$C_{(3)}$–$C_{(2)}$–$C_{(7)}$–$N_{(2)}$	177.16(9)
$C_{(16)}$–$C_{(17)}$–$C_{(18)}$	120.20(10)	$C_{(1)}$–$C_{(2)}$–$C_{(7)}$–$N_{(2)}$	-1.96(15)
$C_{(14)}$–$C_{(15)}$–$C_{(16)}$	120.26(10)	$C_{(3)}$–$C_{(2)}$–$C_{(7)}$–$C_{(6)}$	-3.30(15)
$C_{(4)}$–$C_{(3)}$–$C_{(2)}$	121.05(10)	$C_{(1)}$–$C_{(2)}$–$C_{(7)}$–$C_{(6)}$	177.57(9)
$C_{(3)}$–$C_{(4)}$–$C_{(5)}$	118.82(10)	$N_{(2)}$–$C_{(7)}$–$C_{(6)}$–$C_{(5)}$	-178.59(9)
$C_{(3)}$–$C_{(4)}$–$C_{(9)}$	121.47(10)	$C_{(2)}$–$C_{(7)}$–$C_{(6)}$–$C_{(5)}$	1.86(15)
$C_{(5)}$–$C_{(4)}$–$C_{(9)}$	119.71(10)	$C_{(14)}$–$C_{(13)}$–$C_{(18)}$–$C_{(17)}$	-0.93(15)
$C_{(6)}$–$C_{(5)}$–$C_{(4)}$	121.50(10)	$C_{(1)}$–$C_{(13)}$–$C_{(18)}$–$C_{(17)}$	177.14(9)
		$C_{(10)}$–$C_{(11)}$–$C_{(12)}$–$Cl_{(1)}$	-71.14(10)
		$C_{(15)}$–$C_{(16)}$–$C_{(17)}$–$C_{(18)}$	1.56(17)
		$C_{(13)}$–$C_{(18)}$–$C_{(17)}$–$C_{(16)}$	-0.37(16)
		$C_{(13)}$–$C_{(14)}$–$C_{(15)}$–$C_{(16)}$	0.14(16)
		$C_{(17)}$–$C_{(16)}$–$C_{(15)}$–$C_{(14)}$	-1.44(17)
		$C_{(7)}$–$C_{(2)}$–$C_{(3)}$–$C_{(4)}$	1.97(15)
		$C_{(1)}$–$C_{(2)}$–$C_{(3)}$–$C_{(4)}$	-178.95(9)
		$C_{(2)}$–$C_{(3)}$–$C_{(4)}$–$C_{(5)}$	0.81(15)
		$C_{(2)}$–$C_{(3)}$–$C_{(4)}$–$C_{(9)}$	-179.92(9)
		$C_{(7)}$–$C_{(6)}$–$C_{(5)}$–$C_{(4)}$	0.97(16)
		$C_{(3)}$–$C_{(4)}$–$C_{(5)}$–$C_{(6)}$	-2.32(16)
		$C_{(9)}$-$C_{(4)}$-$C_{(5)}$-$C_{(6)}$	178.40(10)

data for 6-isopropyl-2,4-diphenylquinazoline [12] and a macrocycle containing quinazoline fragments [13] suggests that the presence of the N-oxide atom $O_{(1)}$ leads to extension of the $N_{(1)}$–$C_{(1)}$ and $N_{(1)}$–$C_{(8)}$ bonds, expansion of the $C_{(1)}$–$N_{(1)}$–$C_{(8)}$ bond angle, and contraction of the $N_{(1)}$–$C_{(8)}$–$N_{(2)}$ bond angle in comparison with the previously described molecules [12, 13].

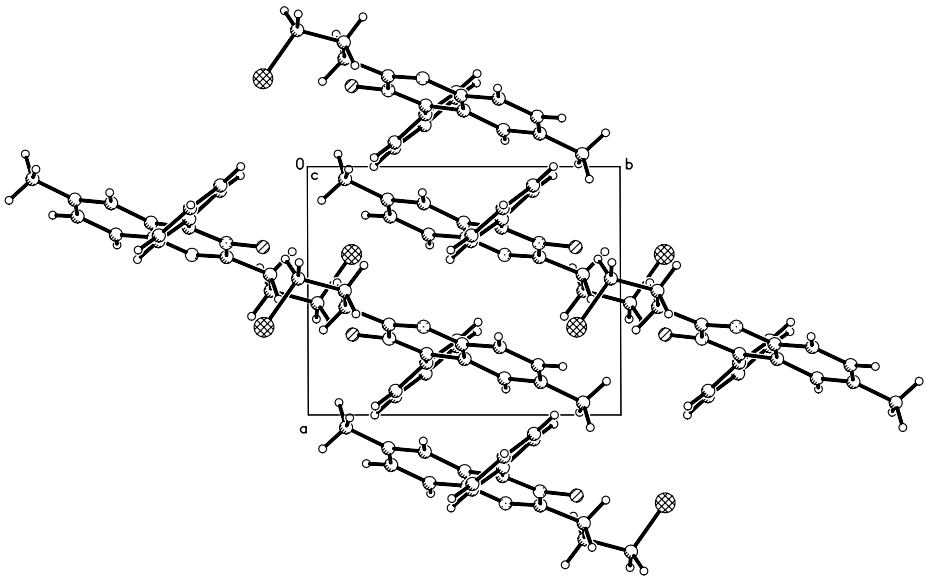


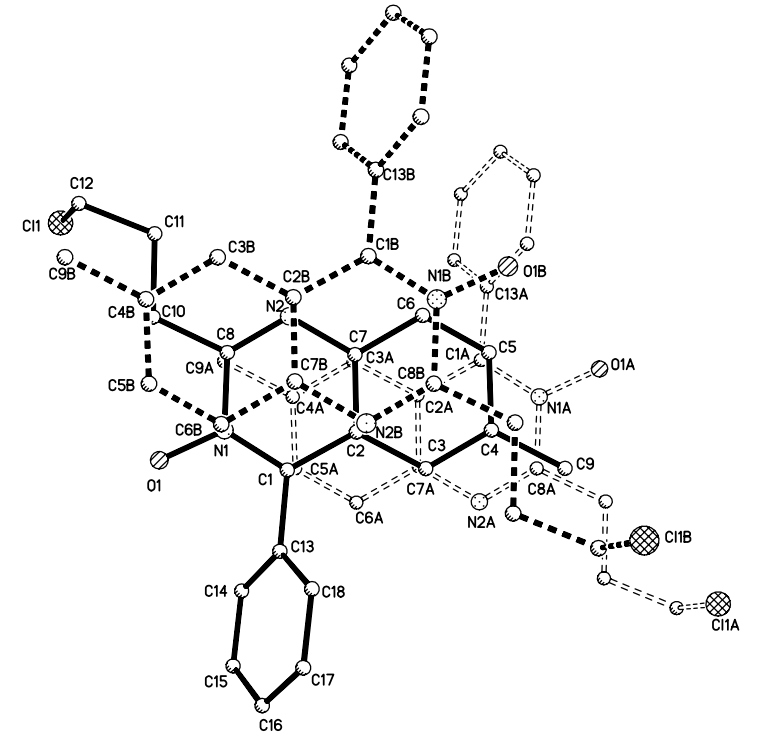
Fig. 2. Molecular packing of **3** in the crystal.

The molecular packing in the crystal is shown in Fig. 2. The major feature in the molecular packing is the formation of stacks parallel to the *a*-axis. A stacking interaction is noted between the parallel aromatic quinazoline systems and dimerization is clearly evident. The distance between the planes is 3.578 and 3.455 Å. The overlap of the aromatic systems of the base molecule (**O**) and molecules **A** (-*x, -y*-1, 1-*z*) and **B** (1-*x, -y*-1, 1-*z*) in a stack is shown in Figs. 3*a* and 3*b*. It is seen from Fig. 3*a*, that the character of the overlap of the quinozoline systems in the "dimers" (**O-B**) differs from the overlap of the molecules **O-A.**

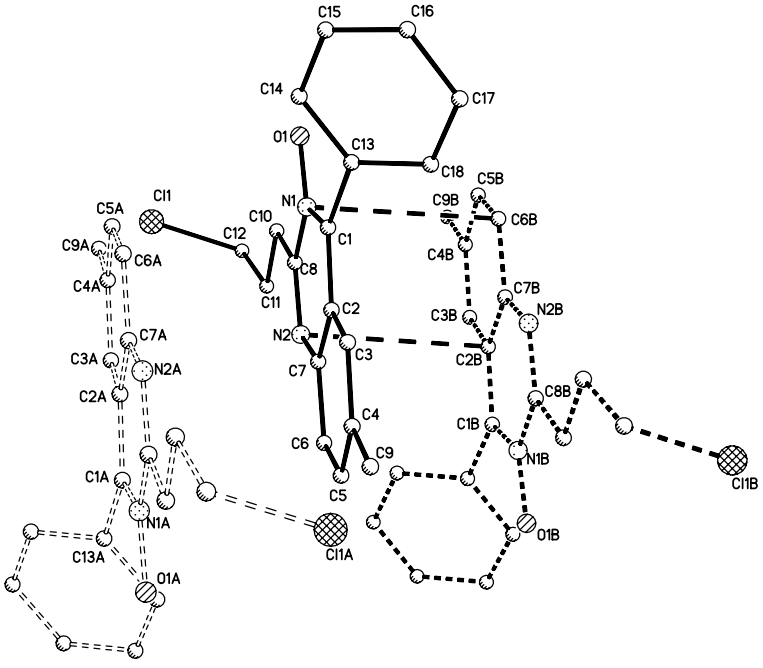
Although the area of overlap of the systems is the same in both pairs of molecules (**O-A** and **O-B**), molecule **B** is displaced such that the center of the benzene ring of molecule **B** is located under $C_{(8)}$ of the base molecule, while the methyl group ($C_{(9A)}$) is found in the **O-A** pair. Fig. 3*b* demonstrates the different displacement of molecules **A** and **B** relative to the central molecule. The shortest interatomic distances in the "dimer" are $N_{(1)}...C_{(6B)}$ (3.460) and $N_{(2)}...C_{(2B)}$ (3.457 Å) and the shortest distances between the "dimers" are $C_{(1)}...C_{(5A)}$ (3.649) and $C_{(7)}...C_{(3A)}$ (3.565 Å).

EXPERIMENTAL

The IR spectra were taken on a Specord IR-75 spectrometer for chloroform solutions. The UV spectra were taken on an SF-56 spectrometer for ethanol solutions (c $3 \cdot 10^{-3}$ mol/l); the cell path length was 10 mm. The mass spectra were taken on an MKh-1321 mass spectrometer with direct inlet of the sample in the ion source. The ionizing electron energy was 70 eV. The ionization chamber temperature was 150°C. Mass spectra were also taken on a VG 7070 EQ mass spectrometer (ionization was accomplished using an argon atom beam at 10 kV). The ^{1}H NMR spectra were taken on a Varian VXR-300 spectrometer at 300 MHz in DMSO-d_6 with TMS as the internal standard.



a



b

Fig. 3. Arrangement of molecules in **3** in stacks (*a, b*).

The *syn* isomer of the oxime of 2-amino-5-methylbenzophenone (**1**) was prepared according to our previous procedure [5].

4-Chlorobutyryloximine of 2-(4-Chlorobutyryl)amino-5-methylbenzophenone (*anti* isomer) (2) and 2-(3-Chloropropyl)-6-methyl-4-phenylquinazoline 3-Oxide (3). A solution of 4-chlorobutyryl chloride (10 ml, 0.089 mol) in 1,4-dioxane (10 ml) was added dropwise to a stirred solution of compound **1** (10 g, 0.044 mol) in 1,4-dioxane (70 ml) cooled to <10°C, stirred for 3 h, poured into water, and extracted with chloroform. The chloroform extract was evaporated. The orange oily residue was crystallized from benzene to give 2.29 g (33%) quinazoline 3-oxide **3**, mp 140-144°C. UV spectrum (EtOH), λ_{max}, nm (log ε): 232 (4.08), 261 (4.27), 312 (3.64), 355 (3.57). Mass spectrum, *m/z*: 312 $[M]^+$. IR spectrum, ν, cm^{-1}: 2985 (CH), 1600 (C=N), 1300 (N–O). ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 7.86-7.09 (8H, m, Ar–H); 3.82 (2H, t, *J* = 6.7, CH_2Cl); 3.25 (2H, t, *J* = 7.2, N=C–CH_2); 2.40 (3H, s, CH_3); 2.36 (2H, q, *J* = 7.0, CH_2–C$\underline{H_2}$–CH_2). Mother liquor chromatograhed on the silica gel column using benzene as the eluent. Yield of the compound **2** 2.84 g (30%) (oil). UV spectrum (EtOH), λ_{max}, nm (log ε): 239 (4.38), 323 (3.52). Mass spectrum (FAB), *m/z*: 434 $[M]^+$. IR spectrum ν, cm^{-1}: 3265 (NH), 2945 (CH), 1745 (O–C=O), 1675 (NH–C=O), 1595 (C=N). ^{1}H NMR spectrum, δ, ppm (*J*, Hz): 10.19 (1H, s, NH); 7.85-6.94 (8H, m, Ar–H); 3.58 (2H, t, *J* = 6.5, NHCO–CH_2–CH_2–C$\underline{H_2}$Cl); 3.55 (2H, t, *J* = 6.5, OCO–CH_2–CH_2–C$\underline{H_2}$Cl); 2.53 (2H, t, *J* = 7.2, NHCO–C$\underline{H_2}$); 2.30 (2H, t, *J* = 7.2, OCO-C$\underline{H_2}$); 2.25 (3H, s, CH_3); 1.99 (2H, q, *J* = 6.9, NHCO–CH_2–C$\underline{H_2}$–CH_3); 1.91 (2H, q, *J* = 6.9, OCO–CH_2–C$\underline{H_2}$-CH_3).

X-Ray Diffraction Structural Analysis. Unit cell parameters of triclinic crystals of **3** grown in benzene at 100(2) K: *a* = 7.5514(3), *b* = 9.5772(4), *c* = 10.5746(5) Å, *V* = 752.19(6) $Å^3$, d_{calc} = 1.381 g/cm^3, space group *P*-1, M_r = 312.79, *Z* = 2, wavelength 0.71073 Å, *F*(000) 328, α = 81.0500(10), β = 84.6750(10), γ = 88.9510(10)º, GOOF 1.000. θ_{max} = 30º. Index range: $-10 \le h \le 10$, $-13 \le k \le 13$, $-14 \le l \le 14$; 9804 measured reflections, 4353 independent reflections (R_{int} = 0.0214). *R*-factor ($I>2\sigma(I)$): R_1 = 0.0355, wR_2 = 0.0889. *R*-factor (over total set): R_1 = 0.0430, wR_2 = 0.0941; $\Delta\rho_{max}$ 0.388, $\Delta\rho_{min}$ –0.279 $eÅ^{-3}$.

The unit cell parameters and experimental data for the compound studied were obtained on a Bruker SMART APEX2 CCD diffractometer using MoKα radiation and a graphite monochromator. The structure was solved by the directly method and refined anisotropically relative to F^2 by the method of least squares for the non-hydrogen atoms using the SHELXTL-98 program package [14]. The hydrogen atom positions were calculated geometrically.

The coordinates of the non-hydrogen atoms and their equivalent isotropic temperature parameters for **3** may be obtained from the authors (e-mail: wizard@homei.net.ua).

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