2-OXOOXAZOLOPYRIDINES.

1. SYNTHESIS OF ALKYL N-(2-OXO-3-PYRIDYL)CARBAMATES

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A convenient method is proposed for the synthesis of new derivatives of the pyridine series, alkyl N-(2-oxo-3pyridyl)carbamates (IIa-i, IVa-j), in the reaction of 7-trifluoromethyl-5-phenyl-2-oxooxazolo[5,4-b]pyridines (I, IIIa-j) with alcohols.

Alkyl carbamates of the pyridine series exhibit fungicidal, herbicidal [1], and anticancer [2] activity and are inhibitors of leucocytic elastase [3, 4]. They are obtained by the acylation of 3-aminopyridines with chlorocarbamates [2, 5], from 3-aminocarbonylpyridines in the Curtius [3, 6] or Hofmann reaction [2, 7, 8], and by the oxidation of 3-formamidopyridines with lead tetraacetate [9].

While continuing the investigations in [10, 11], we developed a preparative method for the synthesis of alkyl N-(2-oxo-3-pyridyl)carbamates (IIa-i) (Table 1) and (IVa-j) (Table 2) from 2-oxooxazolopyridines (I, IIIa-j). When the oxooxazole (I) [10] is boiled in a mixture of DMFA and the corresponding alcohol the oxazolone ring is cleaved with the formation of the carbamates (IIa-i). Higher-boiling alcohols (butyl, *iso*-amyl) form the carbamates (IIc-e) without the addition of DMFA. The effect of temperature shows up clearly in the reaction of the oxooxazole (I) with ethylene glycol. At 95-100°C the hydroxyethyl derivative (IIi) was formed, but on boiling 3-amino-2(1H)-pyridone (V) was isolated [11].

Like other oxooxazoles [12], after prolonged boiling (12 h) with water compound (I) also gives the aminopyridone (V). This reaction takes place rather more quickly (9 h) in the presence of sulfuric acid.



If 2-oxooxazolopyridine (I) is regarded as a cyclic carbamate, its reaction with alcohols can be assigned to the transesterification reactions. This was confirmed by experiments. A side reaction takes place when the carbamate (II)(R = Et) [11], for example, is heated with isoamyl alcohol in the presence of triethylamine and gives compound (IIe). Thus, both the oxooxazole (I) and the alkyl N-(3-pyridyl)carbamate (II) (R = Et) undergo esterification.

The oxazolone ring in the 1-substituted derivatives (IIIa-j) obtained earlier [11] is more stable in reactions with alcohols. The carbamates (IVa-j) could only be obtained by boiling the oxooxazoles (IIIa-j) with alcohols in the presence of bases.



Riga Technical University, Riga LV-1048. Latvian Institute of Organic Synthesis, Riga LV-1006. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 2, pp. 241-249, February, 1997. Original article submitted October 15, 1996.



Fig. 1. A general view of the molecule of compound (IVa).



Fig. 2. An *ac* projection of the structure of compound (IVa). The dotted lines show the intermolecular N-H…O hydrogen bonds.

The structure of the oxopyridylcarbamates (IIa-i, IVa-j) was confirmed by the data from the PMR and IR spectra and by x-ray crystallographic analysis. It should be noted that in the PMR spectra of compounds (IVa-j), in contrast to (IIa-i), in deuterochloroform and DMSO-d₆ solutions there are a series of additional signals corresponding to another rotational isomer, which could not be detected by chromatography.

In order to establish the structure of compound (IVa) objectively we undertook a complete x-ray crystallographic analysis of its crystals. A three-dimensional model of the molecule of compound (IVa) with the designations of the atoms is shown in Fig. 1. The bond lengths and bond angles in the structure of compound (IVa) are given in Table 3. The planar sixmembered heterocyclic ring has geometry characteristic of 2(1H)-pyridines [13, 14]. The departures of the O₍₁₎, N₍₂₎, C₍₁₆₎, and C₍₇₎ atoms from the plane of the heterocycle are 0.051(3), -0.080(3), 0.123(6), and -0.163(4) Å respectively. The dihedral angle between the planes of the heterocycle and the phenyl substituent is $32.5(2)^{\circ}$, whereas the dihedral angle between the heterocycle and the plane of the urethane group C₍₁₃₎, N₍₂₎, C₍₁₄₎, O₍₂₎, O₍₃₎, and C₍₁₅₎ is $81.3(1)^{\circ}$. The large value of the angle is due to presence of the oxo- and trifluoromethyl groups at positions 2 and 4 of the heterocycle. In this connection the length of the C₍₃₎-N₍₂₎ bond [1.424(5) Å] is substantially larger than the standard value of 1.355 Å [for bonds of the $C(sp^2)$ -N(sp^2) type] [15]. This indicates the absence of conjunction between the heterocycle and the urethane group. The lengths of the C-F bonds in the structure are reduced (standard length of the C-F bond 1.336 Å [15]) on account of the significant librational thermal vibrations of the fluorine atoms [16]. [The equivalent isotropic temperature factors B_{eq}^{iso} for the $F_{(1)}, F_{(2)}$, and $F_{(3)}$ atoms are 10.8(3), 9.1(2), and 8.4(2) Å respectively.] The other bond lengths are close to the standard values.

Figure 2 gives the projection of the unit cell of the crystal onto the zx plane. An intermolecular $N_{(1)}$ — $H_{(1)}$ — $O_{(1)}$ hydrogen bond characteristic of 2(1H)-pyridones was found in the crystal structure of compound (IVa). The length of the hydrogen bond is 2.825(6) Å $[H_{(1)}$ — $O_{(1)} = 2.15(4)$ Å, angle $N_{(1)}$ — $H_{(1)}$ — $O_{(1)} = 169(4)$ °]. This is rather shorter than statistical mean of 2.89 Å [17] for hydrogen bonds of the NH—O type. These hydrogen bonds link the molecules in the crystal lattice

(IIa-i)
Compounds
of
Characteristics
Ξ.
TABLE

IABLE		Isues of Compour	(11a-1) sui						
Com-	۲	Molecular	H .O	ound %/	%	mp, °C	PMR spectrum, σ , ppm, DMSO	IR spectrum,	Yield, %,
ninod			υ	н	z			5	
	2	3	4	5	9	7	60	6	10
lįa	CH ₃	C ₁₄ H ₁₁ F ₃ N ₂ O ₃	<u>53,78</u> 53,85	<u>3.55</u> 3,55	8.89 8,97	218219 decomp.	3,61 (3H, s, CH ₃); 6,81 (1H, s, 6-H); 7,50 (3H, m, Ph); 7,83 (2H, m, Ph); 8,75 (1H, s, NH); 12,50 (1H, NH)	3230, 31022800, 1716, 1670, 1632, 1580	90,9 A, 81,8 B
qu	C ₃ H _{7-i}	C ₁₆ H ₁₅ F ₃ N ₂ O ₃	<u>56,29</u> 56,47	<u>4.46</u> 4,44	8.23 8,23	214215 decomp.	1,19 (6H, d, 2CH3); 4,81 (1H, m, CH); 6,81 (1H, s, 6-H); 7,50 (3H, m, Ph); 7,83 (2H, m, Ph); 8,58 (1H, s, NH); 12,44 (1H, NH)	3258, 31002800, 1710, 1654, 1630, 1582	83,3 A, 83,3 B
IIC	C4H9	C ₁₇ H ₁₇ F ₃ N ₂ O ₃	<u>57.58</u> 57,63	4.75	7,91	177179 decomp.	0,80 (3H, t, CH3); 1,031,83 (4H, m, (CH2)2); 4,03 (2H, t, CH2); 6,81 (1H, s, 6-H); 7,50 (3H, m, Ph); 7,83 (2H, m, Ph); 8,67 (1H, s, NH); 12,46 (1H, NH)	3254, 30852870, 1710, 1670, 1632, 1580	84,0 A
pII	C4H9-i	C ₁₇ H ₁₇ F ₃ N ₂ O ₃	<u>57.44</u> 57,63	4.64 4,84	8.21 7,91	189190 decomp.	0,89 (6H, d, 2CH3); 1,87 (1H, m, CH); 3,78 (2H, d, CH2); 6,78 (1H, s, 6-H); 7,47 (3H, m, Ph); 7,78 (2H, m, Ph); 8,62 (1H, s, NH); 12,38 (1H, NH)	3226, 31862860, 1718, 1648, 1620, 1566	76,0 A
	C ₅ H ₁₁ - <i>i</i>	C ₁₈ H ₁ 9F ₃ N ₂ O ₃	58,70 58,70	5.21 5,19	<u>7,61</u>	174175 decomp.	0,89 (6H, d, 2CH3); 1,071,93 (3H, m, CH2, CH); 3,734,18 (2H, m, CH2); 6,78 (1H, s, 6-H); 7,49 (3H, m, Ph); 7,78 (2H, m, Ph); 8,62 (1H, s, NH); 12,56 (1H, NH)	3270, 31842802, 1716, 1654, 1632, 1582	84,6 A, 96,2 B, 77,3 C

TABLE	E 1. (Continued	(p							
Com-	~	Molecular	E 10	ound %/ alculated 9	20	mp, °C	PMR spectrum. a. nom. DMSO	IR spectrum,	Yield, %,
bunod			υ	н	z			5	וונכוווסת
1	2	£	4	S	9	1	60	0	01
Πf	CH(CH ₂) ₄ CH ₂	C ₁₉ H ₁₉ F ₃ N ₂ O ₃	<u>59,99</u>	<u>5.03</u> 4,78	7.38	203205 decomp.	0,922,03 (10H, m, (CH2)4, CH2); 4,56 (1H, CH1; 6,78 (1H, s, 6-H); 7,50 (3H, m, Ph); 7,81 (2H, m, Ph); 8,57 (1H, s, NH); 12,39 (1H, NH)	3270, 31002800, 1712, 1666, 1630, 1582	69,3 A
Шg	CH₂C ≡ CH	C ₁₆ H ₁₁ F ₃ N ₂ O ₃	<u>56.92</u> 57,15	<u>3.32</u> 3,30	8.07 8,33	211212 decomp.	2,62 (1H, t, J = 2,5 Hz, CH); 4,72 (2H, d, J = 2,5 Hz, CH); 6,56 (1H, s, 6-H); 7,47 (3H, m, Ph); 7,69 (2H, m, Ph); 8,11 (1H, s, NH); 12,42 (1H, NH)	3310, 3226, 31022800, 2138, 1716, 1658, 1632, 1582	79,2 B
ЧIJ	CH ₂ CH ₂ OCH ₃	C ₁₆ H ₁₅ F ₃ N ₂ O ₄	<u>53.84</u> 53,94	4,25	7,86	189191 decomp.	3.35 (3H, s, CH3); 3,61 (2H, m, CH2); 4,25 (2H, m, CH2); 6,56 (1H, s, 6-H); 7,47 (3H, m, Ph); 7,69 (2H, m, Ph); 8,11 (1H, s, NH); 12,47 (1H, NH)	3262, 31002800, 1714, 1670, 1630, 1580	88,0 B
ш	СН2СН2ОН	C ₁₅ H ₁₃ F ₃ N ₂ O ₄	52.38 52,64	<u>3.87</u> 3,83	2.98 8,18	210211 decomp.	3,60 (2H, m, CH2); 4,06 (2H, t, CH2); 4,72 (1H, OH); 6,79 (1H, S, 6-H); 7,50 (3H, m, Ph); 7,83 (2H, m, Ph); 8,78 (1H, S, NH); 12,51 (1H, NH)	3370, 3226, 31822890, 1714, 1642, 1616, 1578	79,2 B

12			Malacular	ш, † (/% puno	1			Vield
	×	2	Ferring 1		alculated	%	ູດ m	IR spectrum, cm ⁻¹	ĥ
mmod			lormuta	σ	н	z			9
IVa	CH ₃	сн,	C ₁₅ H ₁₃ F ₃ N ₂ O ₃	55.12 55,22	4.02 4,02	<u>8.56</u> 8,58	213214	31822882, 1718, 1648, 1622, 1580	96,0
٩٧١	CH ₃	C ₂ H ₅	C ₁₆ H ₁₅ F ₃ N ₂ O ₃	56.33 56,47	<u>4,44</u> 4,44	8.23 8,23	177178	31822864, 1714, 1648, 1622, 1580	76,2
IVc	CH ₃	C ₃ H ₇ -i	C ₁₇ H ₁₇ F ₃ N ₂ O ₃	<u>57,59</u> 57,63	<u>4.89</u> 4,84	7,91	160161	32122602, 1710, 1654, 1622, 1562	75,0
PVI	CH ₃	C5H ₁₁ -i	C19H ₂₁ F ₃ N ₂ O ₃	<u>59.34</u> 59,68	5.54 5,54	7,33	170171	31962702, 1712, 1652, 1618, 1578	84,6
IVd	C ₂ H ₅	C ₂ H ₅	C ₁₇ H ₁₇ F ₃ N ₂ O ₃	<u>57,63</u>	<u>4.77</u> 4,84	7,91	124126	32022840, 1714, 1646, 1618, 1580	77.8
IVe	C ₃ H ₇	C ₂ H ₅	C ₁₈ H ₁₉ F ₃ N ₂ O ₃	<u>58.51</u> 58,69	5,13 5,18	7,61	142144	32022945, 1710, 1646, 1618, 1578	69,5
IVf	C4H9	C ₂ H ₅	C ₁₉ H ₂₁ F ₃ N ₂ O ₃	<u>59,68</u> 59,68	<u>5,54</u>	7,33	120122	30282846, 1718, 1646, 1620, 1580	78,3
IVg	C ₅ H ₁₁ -n	C ₂ H ₅	C ₂₀ H ₂₃ F ₃ N ₂ O ₃	<u>60,68</u> 60,60	5.85 5.85	1.07	124125	31002802, 1722, 1650, 1622, 1578	76,6
μνι.	CH ₂ CH-CH ₂	C ₂ H ₅	C ₁₈ H ₁₇ F ₃ N ₂ O ₃	<u>58.95</u> 59,02	<u>4.60</u> 4,68	<u>7,65</u>	113115	31982862, 1714, 1646, 1632, 1620, 1578	69,6
iV	СН ₂ Рh	C ₂ H ₅	C ₂₂ H ₁₉ F ₃ N ₂ O ₃	63.23 63,46	<u>4.58</u> 4,59	<u>6.73</u> 6,73	188190	32002890, 1720, 1644, 1620, 1565, 1538	89,2

TABLE 2. Characteristics of Compounds (IVa-j)

Bond	δ, Å	Angle	ω, deg
·····			
C(2)-N(1)	1,372(5)	N(1)-C(2)-C(3)	115,5(4)
C(6)-N(1)	1,351(7)	N(1)-C(2)-O(1)	120,9(4)
C(3)-C(2)	1,439(6)	C(2)-N(1)-C(6)	126,2(4)
O(1)-C(2)	1,244(6)	N(1)C(6)C(5)	117,8(4)
C(4)C(3)	1,365(7)	N(1)-C(6)-C(7)	118,4(4)
N(2)—C(3)	1,424(5)	C(2)-C(3)-C(4)	119,1(4)
C(5)-C(4)	1,413(7)	C(2)C(3)-N(2)	117,1(4)
C(16)—C(4)	1,497(7)	C(3)-C(2)-O(1)	123,6(4)
C(6)-C(5)	1,365(6)	C(3)-C(4)-C(5)	121,4(4)
C(7)C(6)	1,472(6)	C(3)-C(4)-C(16)	120,9(4)
C(8)C(7)	1,380(7)	C(4)-C(3)-N(2)	123,8(4)
C(12)—C(7)	1,398(6)	C(3)-N(2)-C(13)	118,7(4)
C(9)—C(8)	1,390(7)	C(3)-N(2)-C(14)	122,8(4)
C(10)C(9)	1,361(8)	C(4)-C(5)-C(6)	119,6(5)
C(11)C(10)	1,378(9)	C(5)-C(4)-C(16)	117,7(5)
C(12)-C(11)	1,390(7)	C(4)-C(16)-F(1)	112,4(5)
C(13)—N(2)	1,457(7)	C(4)-C(16)-F(2)	113,2(5)
C(14)-N(2)	1,357(5)	C(4)-C(16)-F(3)	114,0(5)
O(2)—C(14)	1,341(6)	C(5)-C(6)-C(7)	123,7(4)
O(3)C(14)	1,207(6)	C(6)-C(7)-C(8)	121,1(4)
C(15)-O(2)	1,453(7)	C(6)-C(7)-C(12)	120,6(4)
F(1)C(16)	1,308(7)	C(7)-C(8)-C(9)	120,4(5)
F(2)—C(16)	1,308(8)	C(8)-C(7)-C(12)	118,2(4)
F(3)C(16)	1,296(7)	C(7)-C(12)-C(11)	120,8(5)
		C(8)C(9)C(10)	120,9(6)
		C(9)-C(10)-C(11)	120,0(5)
		C(10)-C(11)-C(12)	119,7(5)
		C(13)-N(2)-C(14)	117,4(4)
		N(2)-C(14)-O(2)	111,3(4)
		N(2)C(14)O(3)	124,3(4)
		C(14)-O(2)-C(15)	116,1(4)
		O(2)-C(14)-O(3)	124,3(4)
	1	$F_{(1)}-C_{(16)}-F_{(2)}$	106,0(6)
		F(1)-C(16)-F(3)	105,4(5)
	1	F(2)-C(16)-F(3)	105,0(5)

TABLE 3. Bond Lengths (δ) and Bond Angles (ω) in the Structure of (IVa)

into centrosymmetric dimers. The remaining intermolecular contacts are formed at distances not less than the sum of the van der Waals radii of the contacting atoms [18].

The alkyl N-(2-oxo-3-pyridyl)carbamates and also the oxazole (I) react with amines and give the respective ureas. The urea (VI) was obtained when compound (II) (R = Et) was boiled with isobutylamine.



Other compounds of this series will be covered in a separate communication.

EXPERIMENTAL

The IR spectra were recorded on a Specord 71A instrument in paraffin oil (1800-1500 cm⁻¹) and hexachlorobutadiene (3600-2000 cm⁻¹). The PMR spectra were recorded in DMSO-d₆ on a Bruker WH-90/DS spectrometer at 90 MHz with TMS as internal standard. The individuality of the compounds was checked by TLC on Silufol UV-254 plates.

Atom	x	у	2
N(1)	0,6210(3)	0,5341 (6)	0,4751(2)
C(2)	0,6428(3)	0,3867(7)	0,5354(2)
C(3)	0,7403(3)	0,2909(7)	0,5551 (2)
C(4)	0,8003(3)	0,3392(7)	0,5105(3)
C(5)	0,7722(3)	0,4957(8)	0,4501 (3)
C(6)	0,6820(3)	0,5963(7)	0,4339(2)
C(7)	0,6496(3)	0,7747(7)	0,3769(2)
C(8)	0,6803(4)	0,7836(9)	0,3113(3)
C(9)	0,6516(4)	0,9568(9)	0,2592(3)
C(10)	0,5932(4)	1,1214(9)	0,2720(3)
C(11)	0,5618(4)	1,1174(8)	0,3372(3)
C(12)	0,5890(3)	0,9436(7)	0,3892(3)
O(1)	0,5808(2)	0,3411(5)	0,5694(2)
N(2)	0,7666(3)	0,1425(5)	0,6190(2)
C(13)	0,7209(6)	-0,0742(9)	0,6094(4)
C(14)	0,8181(3)	0,2054(8)	0,6921 (3)
O(2)	0,8464(2)	0,4160(5)	0,6941(2)
O(3)	0,8379(3)	0,0856(6)	0,7480(2)
C(15)	0,9092(6)	0,4961(13)	0,7684(4)
C(16)	0,8977(4)	0,2254(10)	0,5235(4)
F(1)	0,8899(3)	0,0117(7)	0,5265(4)
F(2)	0,9389(3)	0,2649(7)	0,4689(2)
F(3)	0,9641 (3)	0,2799(9)	0,5877(2)
H(1)	0,574(3)	0,570(6)	0,470(2)
H(5)	0,812(3)	0,521(7)	0,421 (3)
H(8)	0,720(4)	0,686(8)	0,301(3)
H(9)	0,670(4)	0,960(8)	0,215(3)
H(10)	0,568(3)	1,227(8)	0,235(3)
H(11)	0,521(4)	1,250(8)	0,351 (2)
H(12)	0,567(3)	0,936(6)	0,434(2)
H(131)	0,757(4)	-0,168(10)	0,642(3)
H(132)	0,662(8)	-0,064(17)	0,586(6)
H(133)	0,726(5)	-0,125(11)	0,559(4)
H(151)	0,970(6)	0,454(12)	0,771 (4)
H(152)	0,869(5)	0,467(12)	0,810(5)
H(153)	0,907(6)	0,658(14)	0,775(4)

TABLE 4. Atomic Coordinates with the Standard Deviations in the Molecule of Compound (IVa)

The yields, melting points, elemental analyses, and PMR and IR spectra of compounds (IIa-i, IVa-j) are given in Tables 1 and 2.

Alkyl N-(2-Oxo-4-trifluoromethyl-6-phenyl-3-pyridyl)carbamates [3-Alkoxycarbonylamino-4-trifluoromethyl-6phenyl-2(1H)-pyridones] (IIa-f). Method A. We boiled 0.2 g of the oxooxazole (I), 3 ml of the respective alcohol, and 3 ml of DMFA for 2 h. The mixture was cooled and treated with water. The precipitate was recrystallized from a 4:1 mixture of ethanol and water.

Method B. We boiled 0.1 g of compound (I) and 25 ml of methyl (7 h), isopropyl (3 h), and 10 ml of isoamyl (2 h) alcohols. The respective compounds (IIa, b, e) were obtained.

Compounds (IIg, h, i) were obtained by heating 0.2 g of (I) and 5 ml of the respective alcohol at 95-100 °C for 3.5 h [for (IIg, i)] and 5 h [for (IIh)] respectively.

Method C. We boiled 0.1 g of previously obtained [11] 4-trifluoromethyl-6-phenyl-3-ethoxycarbonylamino-2(1H)pyridone (II) (R = Et) and 10 ml of isoamyl alcohol in the presence of triethylamine for 2 h. Compound (IIe) was obtained. It did not give a melting depression in a mixed melting test with samples obtained by methods A and B.

Alkyl N-Substituted N-(2-Oxo-4-trifluoromethyl-6-phenyl-3-pyridyl)carbamates (IVa-j). We boiled 0.1 g of 1-alkyl-7-trifluoromethyl-5-phenyl-2-oxo-1(H)-oxazolo[5,4-b]pyridines (IIIa-j), 5 ml of the respective alcohol, and 0.04 g of potassium hydroxide for 2 h. The mixture was cooled and diluted with water, and hydrochloric acid was added to pH 6-7. The precipitate was recrystallized from a mixture of ethanol and water (4:1).

X-Ray Crystallographic Analysis of the Molecule of (IVa). Single crystals of compound (IVa), grown from methanol, belong to the monoclinic system. The crystal lattice parameters were as follows: a = 14.140(3), b = 6.089(1), c = 18.053(3) \dot{A} , $\beta = 107.50(1)^\circ$; V = 1482.5(5) \dot{A}^3 , F(000) = 672, $\mu = 0.13$ mm⁻¹, $d_{calc} = 1.462(1)$ g/cm⁻³, Z = 4, space group P2₁/c.

The intensities of 1962 unique nonzero reflections were measured on an automatic Syntex P2₁ four-circle diffractometer (molybdenum radiation, $\lambda = 0.71073$ Å, graphite monochromator) by a $\theta/2\theta$ scan to $2\theta_{max} = 45^{\circ}$. In the calculations we used 1232 reflections with $|F| > 4\sigma_{\rm F}$. The structure was interpreted by the method in [19]. The refinement was made by least-squares treatment in full-matrix approximation using the software in [20]. All the hydrogen atoms were localized by a difference synthesis and were refined isotropically. The final divergence factor was R = 0.0609. The atomic coordinates are given in Table 4.

3-Amino-4-trifluoromethyl-6-phenyl-2(1H)-pyridone (V). We boiled 0.1 g of the oxooxazole (I) in 20 ml of water or in 20 ml of dilute sulfuric acid (pH 2-3) for 12 and 9 h respectively. The mixture was cooled, and the precipitate was recrystallized from a 4:1 mixture of ethanol and water. The yield was 94.4 and 96.0% respectively.

Compound (V) was obtained with a 59.3% yield by boiling 0.3 g of oxooxazole (I) with 5 ml of ethylene glycol for 2 h. The obtained compounds did not give a melting point depression with the previously synthesized 3-aminopyridone (V) [11].

Isobutyl N-(2-Oxo-4-trifluoromethyl-6-phenyl-3-pyridyl)urea (VI) ($C_{16}H_{16}F_3N_3O_2$). We boiled 0.15 g of the carbamate (II) (R = Et) and 10 ml of isobutylamine for 3 h. The mixture was cooled and diluted with water. The precipitate was recrystallized from ethanol. We obtained 0.13 g (83.3%) of the product; mp 254-255°C. IR spectrum, cm⁻¹: 3310, 2966, 1660, 1634, 1578. PMR spectrum (DMSO-d₆, δ , ppm): 0.89 (6H, d, 2CH₃); 1.69 (1H, m, CH); 2.92 (2H, t, CH₂); 6.67 (1H, s, 6-H); 6.75 (1H, t, NH); 7.50 (3H, m, Ph); 7.75 (2H, m, Ph; 1H, NH); 12.39 (1H, NH).

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