REACTION OF 2-AMINO-3-PHENYLCARBAMOYLAZIRINE WITH ACID CHLORIDES

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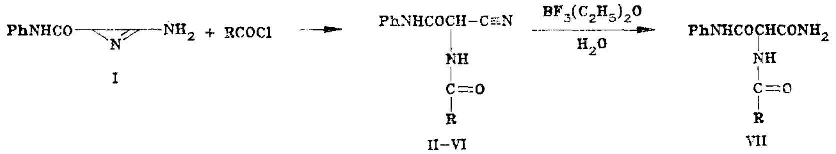
According to the literature, 2-dimethylaminoazirines react with carboxylic acid chlorides to form N-acylamidines [1]. In an investigation of the reactivity of 2-amino-3-phenylcarbamoylazirine (I), which contains a primary amino group, in the reaction with the carboxylic acid chlorides, regardless of the presence or absence of triethylamine, we observed a reaction leading to the formation of N-acylaminomalononitriles (II-VI) — an extremely poorly accessible class of acyclic compounds.



II R=CH_3; III R=Ph; IV, VII R=PhCH=CH; V R=CH_2=CH; VI R=$PhCH_2$

For the compounds synthesized, we give: compound, yield, %, mp, °C: (II), 80, 189; (III), 70, 166.5-167; (IV), 83, 186-187; (V), 68, 141-142; (VI), 76, 189. The IR spectra of compounds (II-VI) (in Nujol) showed bands of the stretching vibrations of C=O groups (1620-1720 cm^{-1}), C≡N groups (2250 cm^{-1}), and NH groups (3060-3400 cm^{-1}). In the PMR spectra ($DMSO-D_6$) of compounds (II-VI), compared with the spectra of the initial compound (I), the signals of the protons of COCHNH groups (d, 1 H, 5.6-5.9 ppm, J = 8 Hz), and the doublet signal of the protons of CHNH groups (9.2-9.7 ppm, J = 8 Hz) had appeared, and in the ^{13}C NMR spectra ($DMSO-D_6$) of compounds (III) and (IV) the signal of the carbon atom of the C≡N group at about 117.5 ppm and the signals of two carbonyl carbon atoms at about 162 and 167 ppm.

The mass-spectrometric analysis of compounds (II-VI) showed the presence of M^+ with masses corresponding to the empirical formulas (II-VI). The results of the elementary analyses of compounds (II-VI) corresponded to the calculated figures. The structure of the phenylcarbamoyl-N-acylaminomalononitriles (II-VI) was confirmed by the hydrolysis of compound (IV) under the action of boron trifluoride etherate to phenylcarbamoyl-N-cinnamoylaminomalonamide (VII), the physicochemical characteristics of which were identical with those of an authentic sample.

LITERATURE CITED

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