4-ANILINO-1,3-DIPHENYLIMIDAZOLIUM CHLORIDE

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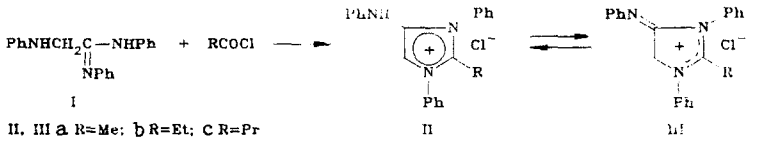
α-Aminoacid derivatives are widely used in the synthesis of various heterocyclic compounds [1, 2] but α-amino acid amidines have not been previously described up to this time. We have found that, in contrast to benzoylation [3], treatment of N^1,N^2-diphenyl-N-phenylglycinamidine (I) with aliphatic acid chlorides in pyridine produces the anilinoimidazolium chlorides II. In DMSO II exist in equilibrium with the imidazolinium chlorides III (70-80%).



The reaction takes place via the acyclic product of acylation at the amino or amido function with cyclization in the presence of HCl, as confirmed by model experiments.

The method known previously for obtaining 4-aminoimidazolium halides based on haloacetonitriles [4] does not lend itself to the synthesis of compounds with an arylamino group.

Compound IIa. Yield 87%, mp 253-255°C (from acetonitrile). IR spectrum (Nujol): 1530, 1620 (NC=CH-$\overset{+}{N}$=C), 1498, 1596 (C=C arom.), 3050, 3078 (=C-H arom.), 3158 (=C-$\overset{+}{H}$ ring), 3400 cm^{-1} (N-H). PMR spectrum (DMSO-d_6): 2.44 (3H, s, CH_3); 3.41 (1.6H, s, $CH_2\overset{+}{N}$); 6.62-8.05 (15H, 2H, m, $3C_6H_5$ + 0.2$\overset{+}{N}$=CH); 8.27 ppm (0.2H, br s, NH). m/z 325 (M − HCl).

Compound IIb. Yield 53%, mp 241-243°C (acetonitrile–ethyl acetate). IR spectrum (Nujol): 1532, 1628 (NC=CH-$\overset{+}{N}$=C), 1504, 1600 (C=C arom.), 3050, 3082 (=C-H arom.), 3158 (=C-H ring), 3400 cm^{-1} (N-H). PMR spectrum (DMSO-d_6): 0.81 (3H, t, CH_3, ^3J = 7 Hz); 2.71 (2H, q, CH_2C); 3.37 (1.6H, s, $\overset{+}{N}CH_2$); 6.57-7.89 (15.2H, m, $3C_6H_5$ + 0.2$\overset{+}{N}$=CH); 8.30 ppm (0.2H, br, s, NH). m/z 339 (M − CHCl).

Compound IIc. Yield 39%, mp 167-168°C (acetone). Spectral data similar to that for IIa, b.

Elemental analytical data for the synthesized compounds was in agreement with that calculated.

LITERATURE CITED

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