NOVEL SYNTHESIS OF 2-BENZYL-2-IMIDAZOLINES FROM 1-(PHENYLETHYNYL)-AZIRIDINE AND PRIMARY AMINES

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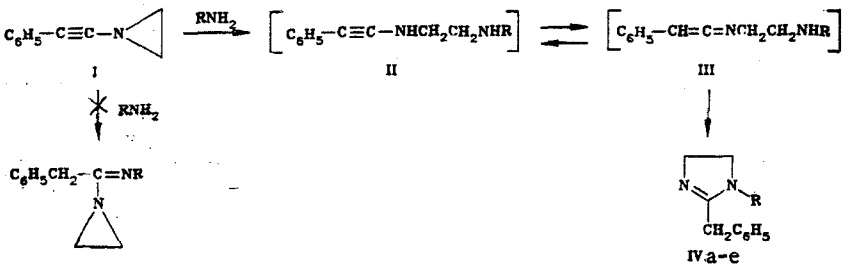
Primary amines add to the triple bond of ynamines to give N-alkylamidines [1].

We have found that the reaction between primary amines and 1-(phenylethynyl)aziridine (I) gives the 2-benzyl-2-imidazolines (IVa-e) by nucleophilic attack on the aziridine ring.



IV a R=H; b R=CH_3; c R=C_2H_5; d R=$CH_2CH_2C_6H_5$; e R=$CH_2CH=CH_2$

Cleavage of the aziridine ring by the amine is evidently accompanied by prototropic isomerization of the ynamine (II) to the ketenimine (III), followed by cyclization to the imidazoline (IV).

The imidazolines (IVa-e) were synthesized using an excess of the amine in acetonitrile or methanol, at room temperature. The progress of the reactions and the purities of the products were followed by GLC. The products (IVa-e), which were oils, were isolated by column chromatography.

2-Benzyl-2-imidazoline (IVa). Yield 64%, bp 65-66°C. According to [2], bp 66-67°C. IR spectrum: 1620 (C=N), 3200 cm^{-1} (NH). PMR spectrum ($CDCl_3$), δ: 3.30 (1H, br. s, NH), 3.56 (4H, s, ring CH_2), 3.6 (2H, s, CH_2), 7.24 ppm (5H, m, C_6H_5).

2-Benzyl-1-methyl-2-imidazoline (IVb). Yield 80%. IR spectrum: 1615 cm^{-1} (C=N). PMR spectrum ($CDCl_3$), δ: 2.67 (3H, s, NCH_3), 3.31 and 3.67 (2H each, m, ring CH_2), 3.58 (2H, s, CH_2), 7.2 ppm (5H, m, C_6H_5).

2-Benzyl-1-ethyl-2-imidazoline (IVc). Yield 95%. IR spectrum: 1610 cm^{-1} (C=N). PMR spectrum ($CDCl_3$), δ: 0.93 (3H, t, CH_3), 3.02 (2H, q, CH_2), 3.24 and 3.69 (2H each, m, ring CH_2), 3.56 (2H, s, $CH_2C_6H_5$), 7.18 ppm (5H, m, C_6H_5).

2-Benzyl-1-phenethyl-2-imidazoline (IVd). Yield 55%. IR spectrum: 1610 cm^{-1} (C=N). PMR spectrum ($CDCl_3$), δ: 2.56 and 3.24 (2H each, t, J = 8 Hz, $CH_2CH_2C_6H_5$), 3.27 and 3.67 (2H each, m, ring CH_2), 3.44 (2H, s, $CH_2C_6H_5$), 6.96 and 7.2 ppm (5H each, m, C_6H_5).

1-Allyl-2-benzyl-2-imidazoline (IVe). Yield 51%. IR spectrum: 1610 cm^{-1} (C=N). PMR spectrum ($CDCl_3$), δ: 3.31 and 3.67 (2H each, m, ring CH_2), 3.62 (2H, s, $CH_2C_6H_5$), 3.58 (2H, m, CH_2), 5.04-5.51 (3H, m, $CH=CH_2$), 7.2 ppm (5H, m, C_6H_5).

Mass spectrometric data supported the structures assigned to the compounds.

LITERATURE CITED

1. S. E. Tolchinskii, I. A. Maretina, and A. A. Petrov, Zh. Org. Khim., 17, 1807 (1981).
2. B. George and E. P. Papadopoulus, J. Org. Chem., 42, 441 (1977).

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