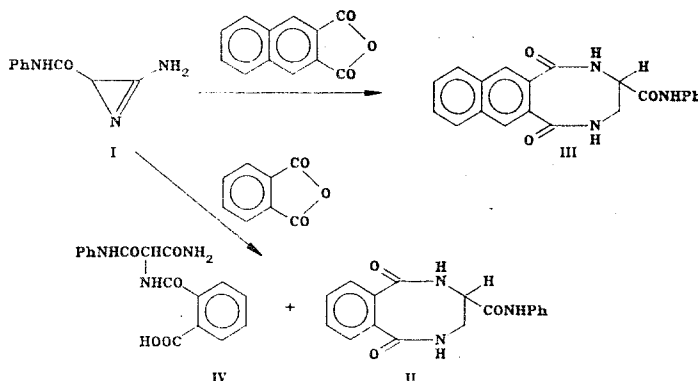


In a study of the reactivity of 2-amino-3-phenylcarbamoyl-1-azirine (I) with dicarboxylic acid anhydrides we have established for the first time that I reacts with phthalic and naphthalic anhydrides to form 3-phenylcarbamoyl-1,2,3,4,5,6-hexahydro-1,2,4H-2,5-benzodiazocin-1,4,6-trione (II) and 3-phenylcarbamoyl-1,2,3,4,5,6-hexahydro-1,3,4H-2,5-naphtho[2,3-f]-diazocin-1,4,6-trione (III), respectively. This opens a new route to the synthesis of a very difficultly available class of polycyclic nitrogen compounds. In the reaction of phthalic anhydride with I, N-(2-carboxybenzoyl)aminomalonic acid N-phenylamide (IV) was also isolated in 30% yield. Since this compound cannot be converted to II, the reaction mechanism for the formation of macrocycles II and III must be different from that described in [1].



Benzodiazocin II: yield 70%, mp 210°. IR spectrum (mineral oil): 1530-1658 (C=O), 3140-3285 cm^{-1} (NH). PMR spectrum (DMSO- D_6): 5.25 (1H, d, J = 8 Hz, CH-N), 7.1-7.92 (10H, m, C_6H_5 , NH), 8.88 (1H, d, J = 8 Hz, NH-C), 10.16 ppm (1H, s, NH). ^{13}C NMR spectrum (DMSO- D_6): 59.6 (CH), 120.8 (C_o), 125.0 (C_p), 129.3 ($\text{C}_{(10,7)}$), 129.9 (C_m), 131.4 ($\text{C}_{(9,8)}$), 136.1 ($\text{C}_{(6a,10a)}$), 139.7 (C_α), 166.4 (C=O), 169.4 ($\text{C}_{(1,6)}$), 169.6 ppm ($\text{C}_{(3)}$). Naphthodiazocin III: yield 79%, mp 208°. IR spectrum (mineral oil): 1530-1695 (C=O), 3270-3415 cm^{-1} (NH). PMR spectrum (DMSO- D_6): 5.32 (1H, d, J = 8 Hz, CH-N), 7.03-8.32 (12H, m, C_6H_5 , C_{10}H_8 , NH), 9.03 (1H, d, J = 8 Hz, NH-C), 10.19 ppm (1H, s, NH). ^{13}C NMR spectrum (DMSO- D_6): 59.6 (CH), 120.7 (C_o , $\text{C}_{(6a,12a)}$), 124.9 (C_p), 129.4 ($\text{C}_{(7,8,11,12)}$), 129.9 (C_m), 133.3 ($\text{C}_{(9,10)}$), 133.8 ($\text{C}_{(7a,11a)}$), 139.6 (C_α), 166.4 (C=O), 169.4 ($\text{C}_{(1,6)}$), 169.6 ppm ($\text{C}_{(4)}$). Amide IV: yield 30%, mp 251°. IR spectrum (mineral oil): 1530-1700 (C=O), 3140-3430 cm^{-1} (NH). PMR spectrum (DMSO- D_6): 5.32 (1H, d, J = 8 Hz, CH-N), 7.07-7.93 (11H, m, C_6H_5 , NH_2), 8.93 (1H, d, J = 8 Hz, NH-C), 10.15 (1H, s, NH), 12.26 ppm (1H, s, OH).

The elemental compositions of II-IV agree with the calculated values.

LITERATURE CITED

1. E. Schaumann, E. Kausch, and W. Walter, Chem. Ber., 108, 2500 (1975).