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SYNTHESIS OF PYRROLO [1, 2-a] IMIDAZOLE AND PYRROLO-[1, 2-a] BENZIMIDAZOLE DERIVATIVES

P. M. Kochergin, A. A. Druzhinina, and R. M. Palei

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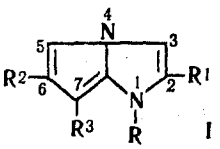
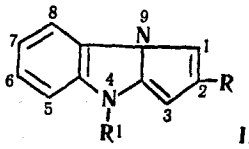
Little research has been done on pyrrolo [1, 2-a] imidazole (I) and pyrrolo [1, 2-a] benzimidazole (II) derivatives. Some compounds have been described; these are mainly 2, 3-dihydro derivatives of I [1-3], and 1, 2-dihydro derivatives of II [4-7].



I



II

We have now synthesized a number of compounds of types I and II. Reaction of 1, 2-dialkylimidazoles and 1, 2-dialkylbenzimidazoles with α-halogenoketones in acetone or benzene gives the corresponding quaternary salts. As Chichibabin [8] and other workers [9-11] have stated, in connection with synthesis of various condensed pyrrole derivatives, when these quaternary salts are heated with aqueous sodium bicarbonate, pyrrole ring closure occurs, with formation of I and II.

Ia: R=CH_3, R^1=R^3=H, R^2=C_6H_4 Br-p, mp 136° (isopropanol). Found: C 56.50; H 4.05; Br 29.15; N 9.52%. Calculated for $C_{13}H_{11}BrN_2$: C 56.75; H 4.03; Br 29.04; N 10.18%. Ib: R=C_2H_5, R^1=Cl, R^2=C_6H_5, R^3=H, mp 84-85° (ex EtOH). Found: C 68.29; H 5.45; Cl 14.96; N 11.54%. Calculated for $C_{14}H_{13}ClN_2$: C 68.66; H 5.35; Cl 14.48; N 11.44%. Ic: R=C_2H_5, R^1=Cl, R^2=C_6H_4Br-p, R^3=H, mp 149-150° (ex EtOH). Found: C 51.74; H 3.74; N 8.53%. Calculated for $C_{14}H_{12}BrClN_2$: C 51.95; H 3.74; N 8.66%. Id: R=n-C_2H_7, R^1=Cl, R^2=C_6H_4Br-p, R^3=CH_3, mp 99-100° (ex isopropanol). Found: C 54.19; H 4.60; N 8.09%. Calculated for $C_{16}H_{16}BrClN_2$: C 54.64; H 4.58; N 7.97%.

IIa: R=C_6H_4Br-p, R^1=CH_3, mp 155-156° (ex EtOH). Found: C 62.71; H 4.00; N 8.52%. Calculated for $C_{17}H_{13}BrN_2$: C 62.78; H 4.03; N 8.61%. IIb: R=$C_6H_4NO_2$-m, R^1=CH_3, mp 170.5-171.5° (ex dimethylformamide). Found: C 69.82; H 4.61; N 14.33%. Calculated for $C_{17}H_{13}N_3O_2$: C 70.09; H 4.49; N 14.42%. IIc: R=$C_6H_4NO_2$-p, R^1=CH_3, mp 180-182° (ex EtOH-dimethylformamide). Found: C 70.13; H 4.48%. Calculated for $C_{17}H_{13}N_3O_2$: C 70.09; H 4.49%. Id: R=C_6H_5, R^1=C_2H_5, mp 119-120° (ex EtOH). Found: C 82.72; H 6.28; N 10.61%. Calculated for $C_{18}H_{16}N_2$: C 83.04; H 6.19; N 10.76%. IIe: R=C_6H_4Br-p, R^1=C_2H_5, mp 123-124°, (ex EtOH). Found: C 63.85; H 4.37; Br 23.32; N 7.99%. Calculated for $C_{18}H_{15}BrN_2$: C 63.72; H 4.46; Br 23.65; N 8.26%. IIf: R=$C_6H_4NO_2$-p, R^1=C_2H_5, mp 118-121° (purified by precipitation from Me_2CO with petrol ether). Found: C 70.47; H 4.72; N 13.77%. Calculated for $C_{18}H_{15}N_3O_2$: C 70.81; H 4.95; N 13.76%.

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Ordzhonikidze All-Union Pharmaceutical Chemistry Research Institute, Moscow