TETRAHALOSUBSTITUTED CONDENSED INDOLES

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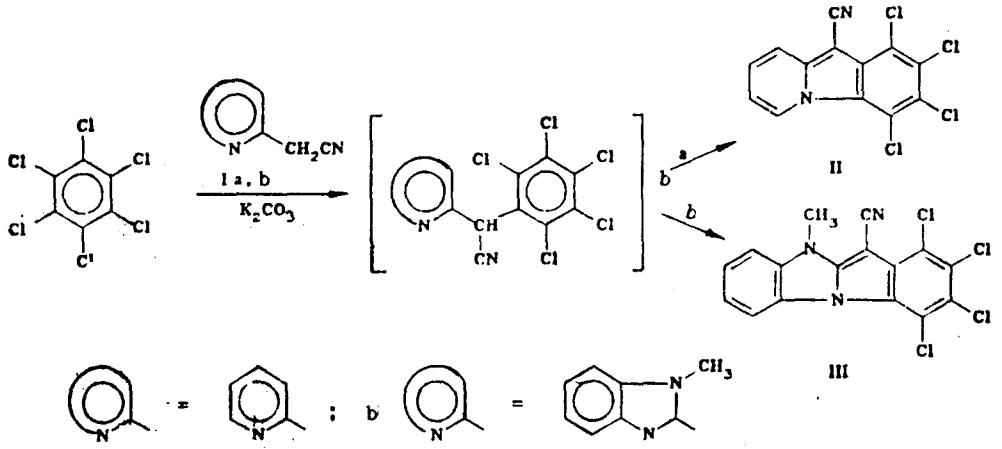
Nucleophilic replacement of the halogen atoms in hexachlorobenzene by carbanions has not been studied. We have found that when hexachlorobenzene reacts with carbanions generated from 2-azahetarylacetonitriles (Ia, b) for 2-3 h in boiling DMFA in the presence of K_2CO_3, two nucleophilic substitutions occur in succession: first, attack by the carbanion to form α-pentachlorophenyl-2-azahetarylacetonitriles, and then replacement of chlorine in the ortho position by the nitrogen of the heterocycle, so that tetrahalosubstituted condensed azahetareno[*a*]indoles (II) and (III) are formed.



1,2,3,4-Tetrachloro-10-cyanopyrido[1,2-*a*]indole (II, $C_{13}H_4Cl_4N_2$). Mp 276°C (from DMFA), R_f 0.63 (Silufol UV-254, 9:1 benzene–ethanol). IR spectrum (KBr): 2200 cm^{-1} (C≡N). UV spectrum (in propanol-2-), λ_{max}, nm (log ε): 204 (4.42), 270 (4.74), 325 (3.95), 338 (3.93), 372 (3.84), 392 (3.93), 413 (3.95), 439 (3.76). PMR spectrum (100 MHz, DMSO-D_6, TMS): 7.18 (1H, t, 7-H), 7.65-7.80 (2H, m, 8-H, 9-H), 9.62 ppm (1H, d, 6-H). Yield 97%).

10-Methyl-1,2,3,4-tetrachloro-11-cyanoindolo[1,2-*a*]benzimidazole (III, $C_{16}H_7Cl_4N_3$). Mp >310°C (from DMFA), R_f 0.58 (Silufol UV-254, 9:1 benzene–ethanol). IR spectrum (KBr): 2200 cm^{-1} (C≡N). UV spectrum (in propanol-2), λ_{max}, nm (log ε): 207 (4.40), 262 (4.53), 330 (4.23). PMR spectrum (100 MHz, DMSO-D_6, 373 K, TMS), 7.33-7.75 (3H, m, 7-H, 8-H, 9-H), 8.62 ppm (1H, d, 6-H). Yield 98%. Elemental composition of the synthesized substances agreed with the calculated values. Compound (III) is a derivative of a new heterocyclic system, indolo[1,2-*a*]benzimidazole.

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