REACTION OF SULFUR DICHLORIDE WITH N-CYANOAMIDINES

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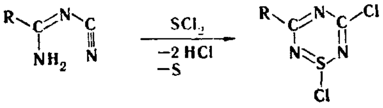
We have established that 1,3-dichloro-1,2,4,6-thiatriazines (II) are formed when a mixture of an N-cyanoamidine (I) with a fivefold excess of sulfur dichloride is heated for several hours.



Ia,b IIa,b

I, II a $R=CCl_3$; b $R=C_6H_5$

1,3-Dichloro-5-trichloromethyl-1,2,4,6-thiatriazine (IIa), with bp 81-86°C (0.04 mm) and n_D^{20} 1.6193, was obtained in 40% yield. Found: Cl 61.8; S 11.2%. $C_3Cl_5N_3S$. Calculated: Cl 61.7; S 11.1%. 1,3-Dichloro-5-phenyl-1,2,4,6-thiatriazine (IIb), with mp 93-95°C (from petroleum ether), was obtained in 45% yield. Found: Cl 28.6; S 12.5%; M 240 (by cryoscopy). $C_8H_5Cl_2N_3S$. Calculated: Cl 28.8; S 13.0%; M 246. The IR spectra of IIa,b (in CCl_4) contain absorption bands at 1518 (1494) and 1381 (1406) cm^{-1}, which are characteristic for the stretching vibrations of the thiatriazine ring [1]. The band of a nitrile group is absent in the spectra; this excludes the structure of the acyclic isomer $Cl_2S{=}N{-}CR{=}N{-}C{\equiv}N$. UV spectra (in n-hexane), λ_{max} (log ε): IIa 278 (3.79); IIb 259 nm (4.26). Chlorine nuclear quadrupole resonance spectrum of IIb: 35.341 ($C-^{35}Cl$), 27.853 ($C-^{37}Cl$), and 27.163 MHz ($S-^{35}Cl$).

LITERATURE CITED

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