

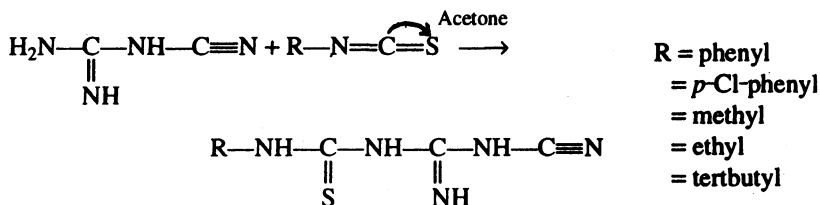
NOTE

A Novel Synthesis of Some Substituted Cyanoamidinothiocarbamides

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Certain reactions of dicyanodiamide with (1) phenyl isothiocyanate, (2) *p*-Cl-phenyl isothiocyanate, (3) methyl isothiocyanate, (4) ethyl isothiocyanate, and (5) tertbutyl isothiocyanate in acetone medium have been investigated.

Dicyanodiamide is an important organic compound due to its pharmacological, agricultural, industrial and biological activities.¹⁻⁹ It has been found as an intermediate in the synthesis of various hetero-acycles and heterocycles, and its derivatives. Dicyanodiamide has basic amino group at position 1 and cyano group at position 3. So it appeared interesting to investigate its chemistry. This molecule is therefore expected to produce varieties of nitrogen, nitrogen and sulphur containing compounds through its amino and cyano groups. The present communication describes the interaction of dicyanodiamide and alkyl/aryl isothiocyanate in acetone medium which are hitherto not known.



All chemicals used were of pure analytical grade. Phenyl-isothiocyanate, *p*-Cl-phenylisothiocyanate, methyl isothiocyanate, tertbutyl isothiocyanate were prepared as described.¹⁰

Cyanoamidinophenyl thiocarbamide (1a): A mixture of cyanoguanidine (4.2 g, 0.05 M) and phenyl isothiocyanate (5.8 mL, 0.05 M) was refluxed over a boiling water bath in acetone medium for 4 h. After filtering off the insoluble product (which is likely to be unreacted cyanoguanidine) the resultant filtrate was evaporated, then a needle-shaped yellowish product (C₉H₉N₃S) was isolated

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(yield 67%; m.p. 187°C m.f. C₉H₉N₅S); Calcd.: C 49.21, H 3.97, N 31.79, S 14.521%; Reqd.: C49.31, H 4.10, N 31.96, S 14.61%.

IR (KBr): $\nu_{\max} = 1360$ (s) cm^{-1} $\left(\begin{matrix} \text{N} \\ \text{N} \end{matrix} \right) \text{C}=\text{S}$ 1080 (s) (C=S stretching vibrations), 2850 (CN aliphatic sym. stretching), 1660 (s) (>C=NH (imino)), 1590–1565 (C=C stretching benzene ring).

UV (dioxane–water): λ_{\max} (log ϵ) = 200, 215, 270 nm.

Similarly 1b–e were synthesised (as depicted in Table-1).

TABLE -1
PHYSICAL DATA OF COMPOUNDS (1a–e)*

Compound No.	R	m.p. (°C)	Yield (%)
1a	Phenyl	187	67
1b	<i>p</i> -Cl-phenyl	147	78
1c	methyl	183	74
1d	ethyl	179	58
1e	tertbutyl	182	52

*All compounds gave satisfactory C, H, N and S analyses.

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