C-21

SYNTHESIS AND REACTIONS OF TRIFLUOROMETHYLTHIOSUBSTITUTED PYRIMIDINES

Alois Haas and Max Lieb*

Anorganische Chemie II, Ruhr-Universität Bochum, Postfach 102 148, D-4630 Bochum 1 (F.R.G.)

5-Trifluoromethylthio-2,4(6)-tri(di)halogeno-substituted pyrimidines have been synthesized by reaction of 5-Trifluoromethylthiosubstituted uracile and barbituric acid with POX_3 (X = Cl, Br). These pyrimidines are good starting materials for further nucleophilic exchange reactions; thus, 5-trifluoromethylthio-2,4(t)-tri(di)fluoro and 5-trifluoromethylthio-2,4(6)-tri(di)jodo compounds are synthesized by reaction with the corresponding alkali halides. In like manner alkoxy-, phenoxy-, anilino-, hydrazino- and amino-derivatives are formed. The latter derivatives can be substituted with Perhalogenomethylthio-functions $Cl_nF_{3-n}CS$ or converted into the isocyanates by reaction with oxalylchloride. Furthermore, CF_3S-functions can be introduced into the pyrimidine ring by Grignard reactions or by using $CuSCF_3$. Persubstituted CF_3S- and CF_3Se-pyrimidines are generated by reacting iodine-containing rings with $Hg(SCF_3)_2$ in the presence of an activated copper bronze.