PO 16

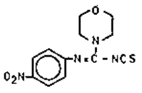
REACTIONS OF FORMAMIDINOYL ISOTHIOCYANATES. A NEW SYNTHESIS OF QUINAZOLINE DERIVATIVES

Š. Stankovský, A. Martvoň
Department of Organic Chemistry, Slovak Institute of Technology 880 37 Bratislava

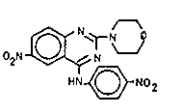
Heating of title compounds (I) give rise to isomerisation and dimerisation products — 3H -Quinazoline -4-thiones and substituted amidinoyl - tetrahydro- s- triazine-2,5-thiones respectively.

We have found, that N^1,N^1-(pentamethylene-3-oxo)-N^2-[4- nitrophenyl] formamidinoyl Isothiocyanate afford on heating not only mentioned products of isomerisation and dimerisation, but also 6-Nitro-4-[4-nitroanilino] quinazoline (II).

Aspects formation of this compound and some other reactions of Formamidinoyl Isothiocyanates will be discussed.



(I)



(II)

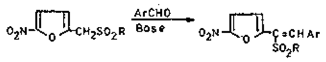
PO 17

REACTION OF 5-NITROFURFURYL SULPHONES WITH ALIPHATIC ALDEHYDES. NEW SYNTHESIS OF 5-NITROFURYL CYCLOPROPANES

D. Geisbacher, A. Jurášek and J. Kováč

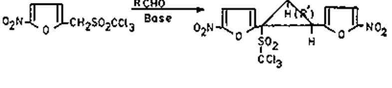
Department of Organic Chemistry, Slovak Technical University, 880 37 Bratislava

Condensation of 5-nitrofurfuryl sulphones with substituted aldehydes of the aryl, heteroaryl and aryl furyl series afforded the corresponding trisubstituted ethylenes.



R= $-CH_3$, $-CHCl_2$, $-CCl_3$, $-CF_3$ and $-C_6H_4X$

Reaction of 5-nitro-2-furfuryl trichloromethyl sulphone with aliphatic aldehydes led to 1-(5-nitro-2-furyl)-1-trichloromethyl sulphonyl-2-(5-nitro-2-furyl)-3-alkyl cyclopropanes, where alkyl is H, CH_3, C_2H_5 and C_3H_7 respectively. This reaction with aliphatic aldehydes is a consequence of their less reactivity and possibility of further cyclization with carbanions, due to less steric hindrance of the resulting ethylene.



The reaction mechanism and stereochemistry are discussed.

PO 18

^{19}F AND ^{1}H NMR SPETROSCOPY OF 2-ALKYL DERIVATIVES OF 3,3,4-TRIFLUOROXETANE

I. Hrušovský*, P. Trška, V. Dědek

Department of Organic Chemistry, Institute of Chemical Technology, 166 28 Prague 6

Department of Organic Chemistry, Slovak Institute of Technology, 880 37 Bratislava

^{19}F and ^{1}H NMR spectra of 2-alkyl and 2,2-dialkyl-3,3,4-trifluoroxetanes were analyzed. We have solved the problem of assignement of non-equivalent resonances of CF_2 group as well as the assignement of resonances of individual isomers. The determination of configuration and conformation was solved independently by the lanthanide shif reagent $Yb(FOD)_3$ separately for protons as well as for fluorine nuclei, the obtained results are confronted with results obtained by EHT quantum mechanical method for various puckering angles of oxetane ring.

Assignement of resonances of CF_2 group and determination of configuration was based on calculation of relative chemical shifts due to electrical fields at fluorine nucleus, as well as on relative signs and values of F—F coupling constants. A confirmation of this assignement was obtained based on ASIS, and on variable temperature studies.

All compounds were obtained by alkaline cyclization of fluorochloroalkanols, which were prepared by the radical addition of 1- and 2-alkanols to chlorotrifluoroethylene.

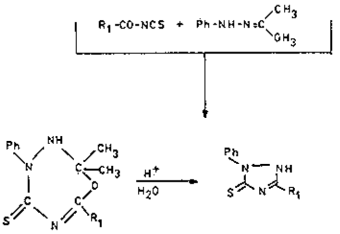
PO 19

SUBSTITUTED 2,3,4,5-TETRAHYDRO-1,3,4,6-OXATRIAZEPINE-5-THIONES

M. Uher*, Š. Kováč, A. Martvoň

Institute of Organic Chemistry, Slovak Technical University, 880 37 Bratislava, Jánská 1

Benzoyl- and 2-furoylisothiocyanates react with acetonephenylhydrazone to give oxatriazepinethiones which on hydrolysis afforded 1,2,4-triazoline-5-thiones.



This cycloaddition reaction has been found to not proceed with benzaldehydedephenylhydrazone.

The structure of compounds prepared was proved by spectral methods.