R1400D

ON ACYLATION OF 1H-3/5/-AMINO-5/3/-R-1,2,4-TRIAZOLES

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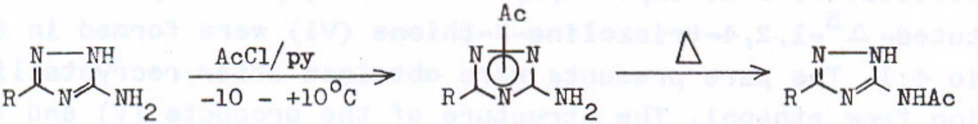
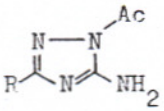
In connection with our biological research work different 1-type substituted amino-1,2,4-triazoles were acylated. If the acylation was carried out in pyridine at low temperatures ring-acylated 1,2,4-triazoles /2/ were formed. These products underwent a thermal rearrangement at elevated temperature into the exo-acylated derivatives /3/.



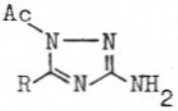
1 2 3

Ac = CH_3CO, PhCO, CO_2Me, CO_2Et, CH_3SO_2

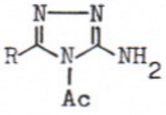
Structure 2 and 3 could be easily distinguished by their PMR spectra, but the position of the acyl-group on the triazole ring in 2 could not be located by this method.



2a

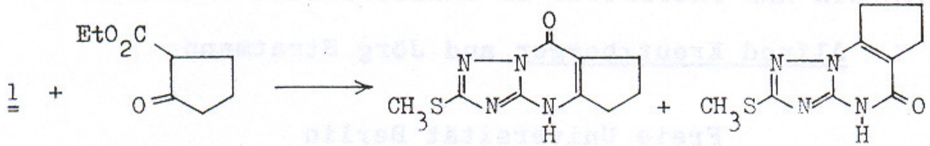


2b



2c

Fromamong the theoretically possible isomeric structures 2a, 2b and 2c the latter could be excluded by an independent synthesis. For deciding between structure 2a and 2b the UV spectra of compounds 2 and 3 were compared with the spectra of the isomers 5 and 6, formed in the reaction of 1 /R=SCH_3/ with 2-carboethoxy-cyclopentanone /4/.



R=SCH$_3$ 4 5 6

As the spectrum of 3 resembled that of 6, the other isomer must passes structure 5. The spectrum of the latter was in good agreement with that of the endo-acylated compounds 2, consequently their structure must be closely related. Accordingly 2a was suggested for the endo-acylated isomer.