

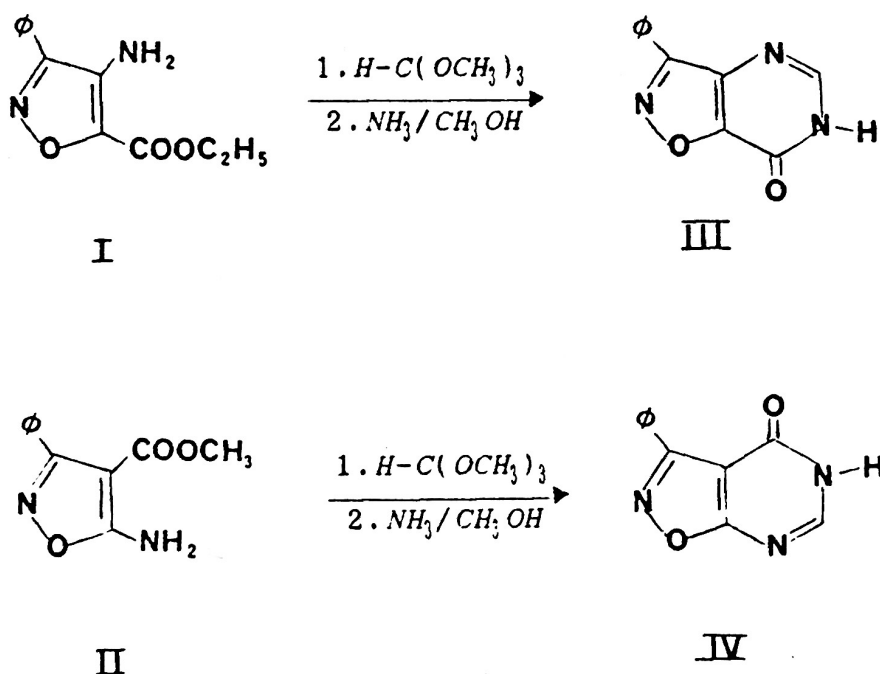
## ISOXAZOLO [4,5-d] AND ISOXAZOLO [5,4-d] PYRIMIDINONES

Synthesis and behaviour upon flash-vacuum pyrolysis

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The title compounds are conveniently prepared by a two step reaction starting with readily available 4(5)-amino-5(4)-alkoxycarbonyl isoxazoles, I and II. The first step involves the formation of imidates by the action of orthoesters on the aminoesters ; cyclisation of these intermediates is then performed by primary amines or hydrazines. The progress of these reactions is easily monitored by proton magnetic resonance.



The isomeric pyrimidinones, III - IV, are also easily differentiated by their 70 eV EI mass spectra which besides intense molecular ion peaks usually exhibit different fragmentation schemes.

Short contact time flash-vacuum pyrolysis has been applied to the pyrimidinones III in a 200-800° temperature range. Real time analysis of the products by tandem mass spectrometry indicate a quantitative isomerization at 700°. Although the nature of these isomers is not yet proved, MS data could be in agreement with a  $\alpha$ -ketoketenimine structure. Such a process is also observed for compounds IV, with moreover a fragmentation reaction at 800° yielding  $C_6H_5N=C=C=O$ , a cumulog of phenylisocyanate.