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N-Phosphorylated Esters of Allophanic Acid

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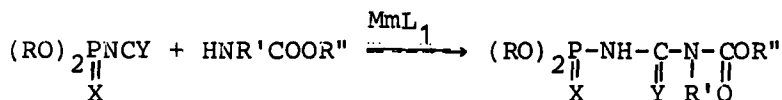
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N-PHOSPHORYLATED ESTERS OF ALLOPHANIC ACID

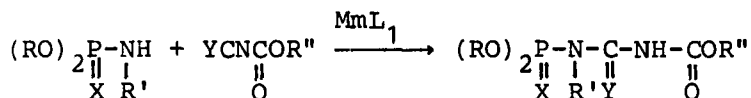
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4-Dialkylphosphoryl allophanates have been prepared by reactions of dialkylphosphoryl isocyanates and isothiocyanates with carbamates



and alkoxycarbonyl isocyanates and isothiocyanates with dialkylphosphoramides, both catalyzed by metal salts



Kinetic measurements of the reaction of methoxycarbonyl isothiocyanates with diisopropylphosphoramides were carried out. The structures of allophanates were confirmed by IR and ^{31}P spectroscopy. Mass spectra of N-phosphorylated allophanates were recorded and the observed fragmentation behavior was compared with that of allophanates, phosphoramides and N-phosphorylated carbamates. One of the pathways of fragmentation observed in mass spectra of allophanates is the skeletal rearrangement with N → O migration. High-resolution measurements were carried out ions discussed in the fragmentation of rearrangement. This pathway was observed for phosphoric carboxylic imides (1), and earlier by us for N-phosphorylcarbamates. The skeletal rearrangement is common in spectra of N-acylamides of phosphorus acid.

(1) V.Mizrahi, T.A.Modro, J. Org. Chem. 47, 3533 (1982).