SYNLETT Spotlight 444

This feature focuses on a reagent chosen by a postgraduate, highlighting the uses and preparation of the reagent in current research.

Methallyl Isothiocyanate

Compiled by Maksym Fizer

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Introduction

Methallyl isothiocyanate (MAITC) is a flammable, colorless liquid with a boiling point of 169–170 °C (760 mm),1 a flash point of 57 °C, and a density of 0.993 g/cm³ at 25 °C. It has a special, onion-like odor and is insoluble in water. MAITC is a lachrymator and may be harmful if inhaled, swallowed, and absorbed through the skin; it may cause respiratory tract, skin and eye irritation.

MAITC is commercially available and can be synthesized by the reaction of methallyl chloride with an alkali metal thiocyanate or with ammonium thiocyanate to give methallyl thiocyanate which readily rearranges under heating (usually with distillation) to the desired product (Scheme 1).1 In addition, it is the product of the reaction of thiocyanogen with isobutylene.2

Abstracts

(A) Reaction with Arylhydrazines:
Richter and co-workers found that MAITC reacts with substituted arylhydrazines to 1,4- or 2,4-disubstituted thiosemicarbazides, depending on the reaction conditions and the nature of the aryl group.6 A derivative of methallyl thiosemicarbazide can be used as sensor element suitable for colorimetric detection of anions.7

(B) Derivatization of Heterocycles:
Merla and co-workers patented a method for the synthesis of substituted benzo[d]isoxazol-3-yl-N-methallyl thioureas which exhibit an strong affinity for the KCNQ2/3 K⁺ channel and which are suitable for relieving pain.8 MAITC is a reagent for the synthesis of thiourea-substituted spiro compounds which can be used for the production of producing pain-relief medicaments.9 A new thiourea derivative of 1,2,4-triazole has been synthesized and tested as a possible drug. It was shown that the thiourea with the endocyclic N-atom forms selectively.10

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Production of Substituted and Condensed Thiazoles:
Novel bicyclic thiazolopyrimidinone compounds, which inhibit HIV integrase, were synthesized using methylallyl thiourea. MAITC is a general reagent for the synthesis of thiazole compounds which have an excellent inhibitory action on melanin production and which are useful as skin whitening agents. The first step of the synthesis is the formation of N-aryl-N'-methylallyl-thioureas. The second stage is the cyclization to thiazoles by the action of hydrochloric acid in a steel tube.

Synthesis of Triazoles:
New 1,2,4-triazoles have been synthesized by the alkali cyclization of acyl thiosemicarbazides which can be obtained from MAITC and hydrazides. The obtained compound exhibited a stabilizing effect on cell membranes, and antioxidant activity with respect to erythrocytes under oxidative stress conditions was demonstrated.

Diaminothiadiazoles Formation:
Cyclization of substituted thiosemicarbazides with methylallyl isothiocyanate in the presence of acetic anhydride gave diaminothiadiazoles.

Synthesis of Polymers:
MAITC can be used to synthesize fluoropolymers via the formation of urethanes with an appropriate fluorinated alcohol under the action of water-soluble azo-initiator.

References