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Reaction of Isothiazolones with Amines

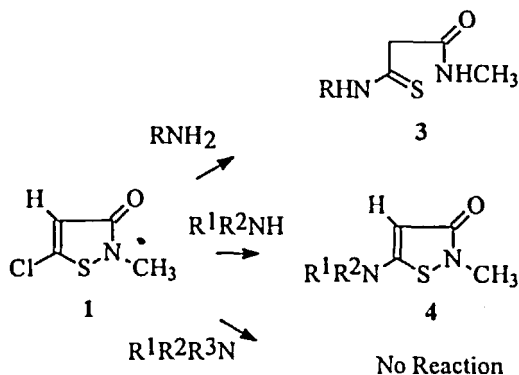
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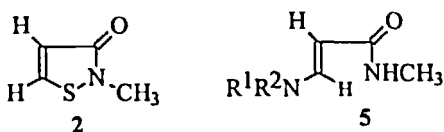
Keywords: isothiazolones; amines; reactions

Both 5-chloro-1-methylisothiazolone (**1**) and 1-methylisothiazolone (**2**) are widely used and very effective industrial microbicides. They are routinely used in water cooling towers, metal working fluids, cosmetics (shampoo, conditioners, etc.) to prevent the growth of microorganisms. In a number of these applications there are amines present which tend to degrade the isothiazolone molecule. To come up with a strategy to stabilize these molecules we have studied the reaction of molecules **1** and **2** with amines under different reaction conditions.

The reaction of **1** with primary amines results in the formation of the thioamide **3** as the major product. The reaction is slow at ambient temperature but is rapid in refluxing ethanol. The reaction is also accelerated by the addition of thiols. With secondary amines the product is the 5-amino-1-methylisothiazolone (**4**).



The reaction of **2** with primary amines also gives the thioamide **3** as the major product. If the reaction is carried out in the presence of a strained olefin, e.g. nobornylene, the formation of **3** is prevented and norbornane polysulfides are obtained. This indicates the presence of nucleophilic sulfur in the reaction pathway. The reaction of **2** with secondary amines, on the other hand, results in the loss of sulfur and the enamine **5** is obtained as the major product.



Neither **1** or **2** react with tertiary amines. Although when traces of sulfur are present, rapid degradation of the isothiazolones take place.

Based on the results of this study we have proposed reaction mechanisms for the above transformations. This mechanistic picture suggests that nucleophilic sulfur chains play an important role in these reactions.