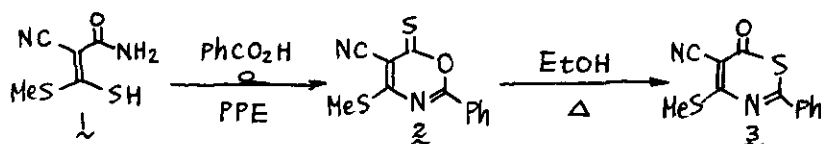


REACTION MECHANISM OF S,N-DOUBLE REARRANGEMENT

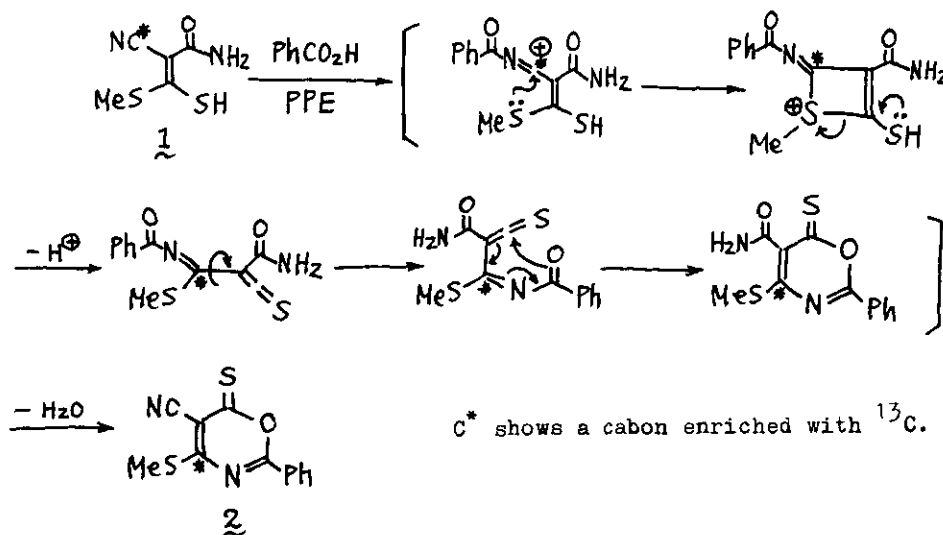
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In our continuing study on the chemistry of thiazines and related compounds, we found that 2-cyano-3-mercapto-3-methylthioacrylamide **1** reacted with benzoic acid in the presence of polyphosphate ester (PPE) to give 5-cyano-4-methylthio-2-phenyl-1,3-oxazine-6-thione **2**, which, on treatment with refluxing ethanol, underwent a ring-transformation to form the corresponding thiazine derivative **3**.



This novel condensation reaction involving an interchange of sulfur and nitrogen atoms was termed "S,N-double rearrangement".^{1,2} Herein, we present a reaction pathway which is explained on the basis of chemical reactions, ¹³C labeling, and crossover experiments.



References: (1) M.Yokoyama et al., J. Chem. Soc. Chem. Commun., 1981, 560.

(2) M.Yokoyama et al., J. Org. Chem., 1982, 47, 1090.