

# Reaction of Aziridine with Cyanuric Acid

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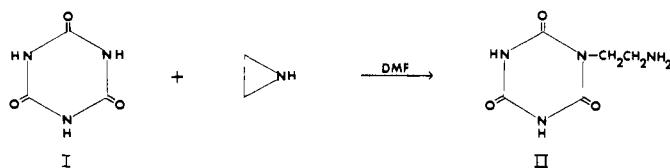
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The reaction of aziridine with cyanuric acid in dimethylformamide gives exclusively mono-2-aminoethyl isocyanurate when reacted in a 1 to 1 ratio.

BASE-CATALYZED condensation reactions of cyanuric acid are well known (1). However, aziridines, unlike epoxides, will not open under alkaline conditions. On the other hand, the presence of acid, which would make the aziridine more susceptible to nucleophilic attack, would also reduce the nucleophilicity of the cyanuric acid and would result in self-condensation of the aziridine.

The reaction of 1 mole of aziridine with 1 mole of cyanuric acid in dimethylformamide (with no added base or acid catalyst) gives an almost quantitative yield of mono-2-aminoethyl isocyanurate (II). Treatment of cyanuric acid with three molar equivalents of aziridine did not result in detectable amounts of bis or tris derivatives (fractional crystallization) but gave slightly reduced yields of II. This self-catalyzed reaction of cyanuric acid is unique in that it is, to the best of the author's knowledge, the only condensation reaction of cyanuric acid which stops at the mono adduct without using a large excess of cyanuric acid.

The cyanuric acid donates a proton to aziridine, and the resulting isocyanurate ion attacks the protonated aziridine to form the product.



The reaction stops at II for several reasons; II is insoluble in dimethylformamide under the conditions of the reaction, and the mildly alkaline monoaminoethyl derivative is too weak an acid to protonate aziridine.

To obtain the bis derivative, further reaction of II with aziridine was attempted in the presence of one equivalent of sulfuric acid (to block the —NH<sub>2</sub> group and dissolve the starting material). Only starting material (II) could be recovered.

## REACTION OF AZIRIDINE WITH CYANURIC ACID

To a magnetically stirred suspension of 17.5 grams (0.135 mole) of cyanuric acid in 200 ml. of dimethylformamide (DMF) was added dropwise a solution of 7.0 ml. of aziridine (0.135 mole) in 20 ml. of DMF over a period of 30 minutes. The reaction mixture was allowed to stir overnight.

The DMF-soluble material (6.3 grams) is crude starting material (same infrared spectrum as that of cyanuric acid). The DMF-insoluble material (14.4 grams) is mono-2-aminoethyl isocyanurate. A small amount of material was recrystallized from water and melts at 279–80°C., with decomposition, and its infrared spectrum is identical to that of the crude material. The literature value for the melting point of mono-2-aminoethyl isocyanurate is 280°C. with decomposition (2). Anal. Calcd. for C<sub>5</sub>H<sub>8</sub>N<sub>4</sub>O<sub>3</sub>: C, 34.88; H, 4.69; N, 32.55. Found: C, 35.08; H, 4.43; N, 32.96.

Based on unrecovered starting material, the theoretical yield is 14.9 grams. The actual yield was 14.4 grams or 97% of theoretical.

## LITERATURE CITED

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- (2) Schaefer, F.C., *J. Am. Chem. Soc.* **77**, 5922 (1955).

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