The reaction products were a 1-benzyl-3-(4-ethoxyphenyl)-6,7-dimethoxy-2-benzopyrylium salt (III), which was isolated in quantitative yield, and 4,4'-diflav-2-enyl (VI), which was isolated in 70% yield. The physical and spectral characteristics of salt III are identical to those of a sample obtained by the method in [1], and those of VI are identical to those described in [2].

The formation of salt III evidently proceeds through intermediate cation radical II, which captures a hydrogen atom from the chloroform used as the solvent.

4,4'-(1,2-Ethanediylidene)bis(4H-7-methoxyflavene) undergoes a similar reaction [3].

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MOLECULAR STRUCTURE OF 3-AMINO-1,2,4-TRIAZOLE

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3-Amino-1,2,4-triazole (also known under its technical names amizol, amitrole, etc.) can exist in several tautomeric forms, of which the most probable structures, according to the results of quantum-chemical calculations [1], are 3-amino-1H-1,2,4-triazole (I) and 3-amino-2H-1,2,4-triazole (II). We made an x-ray diffraction study of single crystals of this compound (with a $P2_1$ diffractometer, 387 nonzero independent reflections, and Mo emission) and established the lattice parameters $a = 9.29(1)$, $b = 10.64(3)$, $c = 3.73(2)$ Å, $\beta = 94.96(8)°$, and $z = 4$ and space group $P2_{1/n}$. A model of the structure was obtained by means of a complex of programs of Multan direct methods, and the result was refined up to an R factor of 0.057. Peaks above 0.24e $Å^{-3}$ were not observed on maps of the last differential Fourier synthesis. The ring configuration found (Fig. 1) is in agreement with the data for unsubstituted 1,2,4-triazole [2].

Since the hydrogen atom is localized on the nitrogen atom adjacent to the amino group, the molecule has the 3-amino-2H-1,2,4-triazole structure (II).

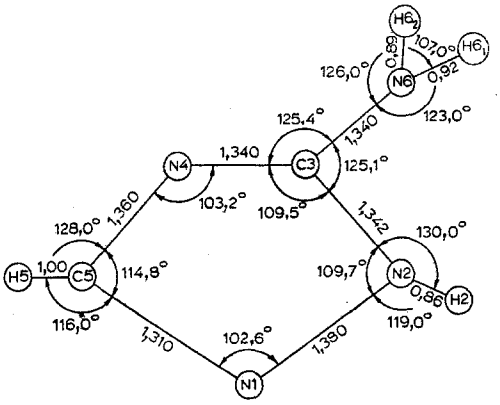

Fig. 1. Configuration of the triazole ring.

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