A study of the stereochemistry of five-membered heterocycles that contain either an endo- or an exocyclic phosphorus atom is of interest for many reasons. The main reason is to secure more profound stereochemical concepts regarding organophosphorus compounds that have generally theoretical value. At the same time, a study of the spatial structure of these heterocycles employing NMR is important for developing a number of operational problems, which have received little development, although papers in this direction have appeared in recent years [1-3].

In the present paper we studied the structure of 2,3-diphenyl-4-dimethoxyphosphonoisoxazolidine (III), the 1,3-dipolar cycloaddition product of dimethyl vinylphosphonate (II) to C,N-diphenylnitrone (I).

By analogy with 2-pyrazoline and 2-isoxazoline derivatives, the previously obtained isoxazolidine (III) [4] was assigned the structure with the phosphorus atom in the 5 position of the ring, although the data of the $^1$H and $^{31}$P NMR spectra, which prove its structure, are not given in [4]. Consequently, we made a more detailed study of the reaction of C,N-diphenylnitrone (I) with ester (II).

The structure of isoxazolidine (III) was established on the basis of the elemental analysis, the $^1$H and $^{31}$P NMR spectra, and the IR spectra. The chemical shift of $\delta_{31p}$ -29 ppm proves the phosphonate environment of the phosphorus atom. The IR spectrum of (III) has the following absorption bands ($\nu$, cm$^{-1}$): 1035, 1050 v. s. (P-O-C), 1190 m (P-O-CH$_3$), 1260 v. s. (P=O), 1492, 1602 m (C$_6$H$_5$). Absorption bands at 1559 cm$^{-1}$ ($\nu$C=N of starting nitrone) and 1620 cm$^{-1}$ ($\nu$C=O of ester (II)) are absent in the spectrum.

Besides the crystalline isomer (III), which, as is shown below, has the trans-configuration, the alternate liquid isomer is formed in the studied 1,3-bipolar cycloaddition reaction, which as yet could not be isolated in the pure state. However, employing NMR spectral "separation," some of its structural traits are discussed below. In addition, by chromatographing the reaction mixture we detected (via the IR spectra) small amounts of products in which the phosphorus atom is absent: the starting C,N-diphenylnitrone, benzaldehyde, and N-benzalaniline.

Starting with the reaction mechanism for the synthesis of 2,3-diphenyl-4-dimethoxyphosphonoisoxazolidine and the elemental analysis results it could be expected that the compound has one of the indicated structures (IIIa) or (IIIb).

Fig. 1. $^1$H NMR and $^1$H–{$^{31}$P} NMRD spectra of trans-2,3-diphenyl-4-methoxyphosphonoisoxazolidine (III) at 27°.