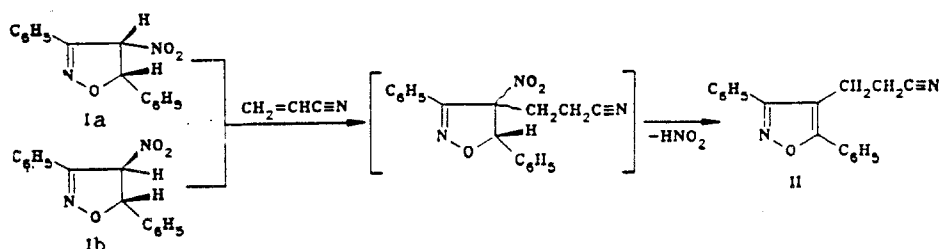


CYANOETHYLATION OF STEREOISOMERIC 4-NITRO-3,5-DIPHENYL-2-ISOXAZOLINES

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We have determined that *cis*- and *trans*-4-nitro-3,5-diphenyl-2-isoxazolines (Ia, b) react with acrylonitrile in the presence of an equimolar amount of KOH to form the previously unknown 3-(3,5-diphenylisoxazolyl-4)propionitrile (II). To all appearances the reaction includes the formation of 3-(4-nitro-3,5-diphenyl-2-isoxazolyl-4)propionitrile (IV), which by splitting out a molecule of nitrous acid is converted to isoxazolylpropionitrile (II).



The reaction was carried out in dioxane at 50-60°C and a 1:6 (I): acrylonitrile ratio. Potassium hydroxide, 40% aqueous solution, was added dropwise over 12 h with energetic stirring of the reaction mixture. At the end of the reaction the solvent and the excess acrylonitrile were removed in vacuum. The residue was extracted with absolute ether, the ether was evaporated, and the residue was crystallized from ethanol. The yield of nitrile (II) (mp 144-146°C) was ~70%. The IR spectrum (KBr) of (II) contains absorption bands in the regions of 2260 (C=N), 1610 (C=N), and 950 cm⁻¹ (N-O); the bands that are typical of the NO₂ group are not present. PMR spectrum (acetone-D₆): 2.8 (t, 2H, J = 7 Hz), 3.3 (t, 2H, J = 7 Hz), 7.3-7.9 ppm (m, 10H). Elemental composition (C, H, N) agreed with calculated values.

Regioisomeric *trans*-3,4-diphenyl-5-nitro-2-isoxazoline does not participate in cyanoethylation; under the above conditions it is completely decomposed to benzonitrile and a tarry residue.