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ЭКСПЕРТНОЕ ЗАКЛЮЧЕНИЕ О ВОЗМОЖНОСТИ ОПУБЛИКОВАНИЯ

Руководитель-эксперт Федерального государственного бюджетного учреждения науки Института элементоорганических соединений им. А.Н.Несмеянова Российской академии наук, рассмотрев *статью* L. Kayukova, A. Vologzhanina, P. Dorovatovskii, E. Yergaliyeva, A. Uzakova and A. Duisenali «**N-N(+) Bond-Forming Intramolecular Cyclization of O-Tosyloxy β-Aminopropioamidoximes and Ion Exchange Reaction for the Synthesis of 2-Aminospiropyrazolilammonium Chlorides and Hexafluorophosphates**», подготовленную для печати в журнале *Int. J. Mol. Sci.*, подтверждает, что в материале *не содержатся* сведения, предусмотренные Постановлением Правительства РФ №1233 от 30.11.1994г. и на публикацию материала *не следует* получать разрешение *Минобрнауки и/или Президиума РАН*

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N-N(+) Bond-Forming Intramolecular Cyclization of O-Tosyloxy β-Aminopropioamidoximes and Ion Exchange Reaction for the Synthesis of 2-Aminospiropyrazolilammonium Chlorides and Hexafluorophosphates

Lyudmila Kayukova [1,*], Anna Vologzhanina [2,*], Pavel Dorovatovskii [3], Elmira Yergaliyeva [1], Asem Uzakova [1] and Aidana Duisenali [1]

[1] JSC A. B. Bekturov Institute of Chemical Sciences, 106 Shokan Ualikhanov St., Almaty 050010, Kazakhstan; erg_el@mail.ru (E.Y.); a7_uzakova@mail.ru (A.U.); duisenali-a@mail.ru (A.D.)
[2] A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, 28 Vavilova St., B-334, Moscow 119334, Russia
[3] NRC "Kurchatov Institute", 1 Kurchatova Pl, Moscow 123098, Russia; paulgemini@mail.ru
* Correspondence: lkayukova@mail.ru (L.K.); vologzhanina@mail.ru (A.V.); Tel.: +7-(705)-168-81-53 (L.K.)

Abstract: Our research area is related to the spiropyrazolinium-containingcompounds, which are insufficiently studied compared with pyrazoline-containing compounds. Nitrogen-containing azoniaspiromolecules have also been well studied. In drug design and other areas, they are a priori important structures, since rigid spirocyclic scaffolds with the reduced conformational entropy are able to organize a closely spaced area. Azoniaspirostructures are currently of wide practical interest as ionic liquids, current sources (membranes), structure-directing agents in organocatalysis, and in the synthesis of ordered ceramics. Our goal was the synthesis of 2-aminospiropyrazolilammonium chlorides and hexafluorophosphates. Our methodology is based on the tosylation of β-aminopropioamidoximes with six-membered N-heterocycles (piperidine, morpholine, thiomorpholine, and phenylpiperazine) at the β-position. 2-Aminospiropyrazolilammonium chlorides and hexafluorophosphates were obtained by the reaction of double ion substitution in the reaction of toluenesulfonates of 2-aminospiropyrazolinium compounds with an ethereal solution of HCl in ethanol and with ammonium hexafluorophosphate in ethanol in quantitative yields of 55–97%. The physicochemical characteristics of the synthesized compounds and their IR and NMR spectra are presented. The obtained salts were additionally characterized by the single-crystal XRD analysis. The presence of both axial and equatorial conformations of spirocations in solids was confirmed. 2-Aminospiropyrazolilammonium chlorides and hexafluorophosphates have weak in vitro antimicrobial activity on Gram-positive and Gram-negative bacterial lines.

Keywords: chlorides; hexafluorophosphates; spiropyrazolines; toluenesulfonates; X-ray diffraction analysis; in vitro biological screening

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1. Introduction

Our research area concerns spiropyrazolinium-containing compounds, which are insufficiently studied as compared with other azoniaspiroalkanes (Scheme 1). The latter possess numerous practical applications, which are described below. At the same time, pyrazoline derivatives, which belong to the family of nitrogen-containing heterocycles, have been the subject of a global diphenylpyrazoline market report by Market Strides (a global aggregator and publisher of market research reports). The diphenylpyrazoline market utilizes both pharmaceutical and industrial applications. The pharmaceutical industry is the largest end-user of diphenyl pyrazoline due to its various biological activities, including antioxidant, anti-inflammatory, anti-cancer, and anti-diabetic properties, as well as its ability to treat cardiovascular disorders. The industrial market covers textiles, detergents,

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Conflicts of Interest: The authors declare no conflict of interest.

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