ABSTRACT OF DOCTORAL THESIS

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"Study on the synthesis and properties of new 1,3,4-oxadiazole derivatives as components of micronutrient chelates"

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The subject of the work is research devoted to the synthesis of new, previously unknown in the literature, symmetrical and asymmetric derivatives of 1,3,4-oxadiazole equipped with bis(carboxymethyl)amine groups. Compounds of this type are classified as organic ligands that can participate in the formation of microelement chelates, which can be used, among others, in agriculture as artificial fertilizers.

1,3,4-Oxadiazole, belonging to the group of five-membered heterocyclic compounds, is composed of two nitrogen atoms and one oxygen atom. Many 1,3,4-oxadiazole derivatives have strong biological activity, thanks to which they are used in medicine and pharmacy as active substances. These include antibacterial, antifungal, antiviral, anticancer, anticonvulsant, anti-inflammatory and blood pressure-lowering properties. The desired biological activity of 1,3,4-oxadiazole derivatives is also used in agriculture, where many compounds based on the 1,3,4-oxadiazole ring have herbicidal, insecticidal and antifungal properties.

Microelement chelates are a combination of organic compounds containing amine and carboxyl groups, thanks to which they can form coordination bonds with metal ions, locking them in their structure. Fertilizers of this type are characterized primarily by high absorption of microelements by the plant, significantly reducing the need to use larger amounts of compounds that improve the yield of harvested crops. For this reason, these compounds are of interest to modern agriculture. Currently, micronutrient chelates based on organic ligands are used, such as ethylenediaminetetraacetic acid (EDTA), diethylenetriaminepentaacetic acid (DTPA), *N,N′*-bis(2-hydroxybenzyl)ethylenediamine-*N,N′*-diacetic acid (HBED), or iminodisuccinic acid (IDHA). A new alternative to the above-mentioned ligands that have been used for years may be derivatives based on a biologically active heterocyclic ring, such as 1,3,4-oxadiazole.

The doctoral thesis is divided into three parts. The first one presents information on the properties, applications and various methods of synthesis of 1,3,4-oxadiazole derivatives. The first part also contains basic information about micronutrient chelates and organic ligands currently used for the production of chelated fertilizers. The second part presents a detailed

discussion of the results related to the development of a synthetic path leading to the preparation of organic ligands based on 1,3,4-oxadiazole, previously unknown in the literature. This chapter is divided into two parts, the first of which focuses on the synthesis of alkyl, symmetrical derivatives of 1,3,4-oxadiazole, and the second on unsymmetrical derivatives containing a benzene ring in the 5-position. This chapter also contains a summary of the obtained research results. The third part presents detailed synthetic procedures for individual reactions as well as physicochemical and spectroscopic characteristics of the obtained intermediate and final products.

The synthetic path presented in this work leading to the preparation of symmetrical and unsymmetrical organic ligands based on 1,3,4-oxadiazole containing carboxymethylamine groups consists of several stages and uses commercially available reagents. The first fragment of research on the synthesis of symmetrical alkyl derivatives of 1,3,4-oxadiazole with different alkyl chain lengths. The second part focused on research related to the synthesis of unsymmetrical derivatives containing a benzene ring in the 5-position. In this part, reactions using microwave radiation were also carried out.

The developed synthetic methodology consists of five main stages. The first one involves obtaining the intended symmetrical or unsymmetrical *N,N'*-diacylhydrazine derivatives, starting from commercially available reagents, which are acid chlorides with different alkyl chain lengths, containing a bromine atom in the terminal position. The second stage is based on the cyclodehydration reaction of previously obtained diacylhydrazines to the title 1,3,4-oxadiazole derivatives. The next step is to convert commercially available iminodiacetic acid into its corresponding ester in order to increase its reactivity. Step 4 includes the substitution reaction of the obtained iminodiacetic acid ester with 1,3,4-oxadiazole derivatives containing a bromine atom in their structure. The last stage is to carry out the hydrolysis reaction in order to restore the carboxyl groups and obtain final compounds of the nature of an organic ligand, capable of coordinating metal ions. The structures of all the obtained connections were characterized using NMR spectroscopy (^{1}H- and ^{13}C-NMR) and high-resolution mass spectrometry (HRMS).