

## A SUPRAMOLECULAR STRUCTURE OF PHOSPHORYLATED N-PHENYL-1,2,4-TRIAZOLE- 3-THIONE AND ITS CRYSTAL SOLVATE

A. I. Samigullina<sup>1\*</sup>, I. A. Krutov<sup>2</sup>,  
E. L. Gavrilova<sup>2</sup>, D. R. Islamov<sup>3</sup>, K. S. Usachev<sup>4</sup>,  
and A. T. Gubaidullin<sup>3</sup>

A comparative analysis of the molecular and crystal structures is performed for 5-[(diphenylphosphoryl)methyl]-4-phenyl-2,4-dihydro-3*H*-1,2,4-triazole-3-thione (**1**) in individual crystal (**1a**) and a crystal solvate with dimethylformamide (DMF) in the 1:1 ratio (**1b**). The crystals of both modifications have the identical geometries of the molecule of the key compound, and the crystals (despite their different crystal systems and unit cells parameters) are characterized by the formation of an identical one-dimensional supramolecular motif in them due to classical N–H...O hydrogen bonds and weaker noncovalent –C–H ... S interactions in crystal **1a** and CH ... N in crystal **1b**. A tetragonal packing of one-dimensional motifs oriented along the smallest unit cell parameter are observed in both cases. Solvate molecules are localized in zero-dimensional cavities in crystal **1b**. Despite a denser molecular packing in crystal **1b**, the solid-state phase transformation is observed for its polycrystalline sample, and the powder X-ray diffraction method shows that it partially transforms into form **1a** with time. The latter form is characterized by a less dense molecular packing in the crystal.

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### INTRODUCTION

The heterocyclic 1,2,4-triazole system is a unique heterocyclic platform [1–3] whose modification makes it possible to obtain a compound with a wide spectrum of the biological action, including antimicrobial, antibacterial, analgesic, anticancer, anti-inflammatory, etc., on its base [4–9]. Derivatives of 1,2,4-triazoles and 1,2,4-triazole-3-thiones are also used as insecticidal, herbicidal, antifungal, and plant growth regulating compounds [10, 11].

Such a wide spectrum of the biological activity stimulates the search for new synthetic approaches of obtaining polyfunctional compounds based on 1,2,4-triazoles in order to combine the pharmacological properties of separate fragments due to the synergetic effect. Our scientific group has previously elaborated the synthesis of new phosphorylated derivatives of 1,2,4-triazole-3-thiones (Scheme 1) with substitution at the N atom by heterocyclization of respective

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<sup>1</sup>Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, Russia; a\_samigullina@iopc.ru. <sup>2</sup>Kazan National Research Technological University, Kazan, Russia. <sup>3</sup>Arbuzov Institute of Organic and Physical Chemistry, RFC Kazan Scientific Center, Russian Academy of Sciences, Kazan, Russia. <sup>4</sup>Kazan Federal University, Institute of Fundamental Medicine and Biology, Kazan, Russia. Original article submitted August 26, 2020; revised September 29, 2020; accepted October 20, 2020.