

Accepted Manuscript

Spectroscopic and structural investigation of interaction of 5-mercapto-3-phenyl-1,3,4-thiadiazole-2-thione potassium salt with molecular iodine



Victoria A. Ivolgina, Margarita S. Chernov'yants

PII: S1386-1425(18)30277-4
DOI: doi:[10.1016/j.saa.2018.03.069](https://doi.org/10.1016/j.saa.2018.03.069)
Reference: SAA 15941

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received date: 16 November 2017
Revised date: 1 February 2018
Accepted date: 25 March 2018

Please cite this article as: Victoria A. Ivolgina, Margarita S. Chernov'yants, Spectroscopic and structural investigation of interaction of 5-mercapto-3-phenyl-1,3,4-thiadiazole-2-thione potassium salt with molecular iodine. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Saa(2017), doi:[10.1016/j.saa.2018.03.069](https://doi.org/10.1016/j.saa.2018.03.069)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Spectroscopic and structural investigation of interaction of 5-mercapto-3-phenyl-1,3,4-thiadiazole-2-thione potassium salt with molecular iodine

Victoria A. Ivolgina, Margarita S. Chernov'yants.

Department of Chemistry, Southern Federal University, Zorge St. 7, 344090 Rostov-on-Don, Russia

Abstract

The interest in the study of heteroaromatic thioamides which are known to exhibit antithyroid activity is stimulated by the variety and an unusual structure their complexes with molecular iodine.

The directions of dithiones investigation are diversity enough, however a few works are devoted to the study them as the potential thyreostatics. The ability of 5-mercapto-3-phenyl-1,3,4-thiadiazole-2-thion potassium salt to form the outer-sphere charge-transfer complex in dilute chloroform solution, coordinating 2 iodine molecules has been studied by UV-vis spectroscopy ($\lg\beta=7.91$). The compound of the 5,5'-disulfanediylobis(3-phenyl-1,3,4-thiadiazole-2(3H)-thione) - product of irreversible oxidation of 5-mercapto-3-phenyl-1,3,4-thiadiazole-2-thione potassium salt has been isolated and characterized by X-ray diffraction. Intermolecular interactions between sulfur atoms are observed with very short interatomic distance, shorter than sum of van der Waals radii. The contact between heterocyclic sulfur and heterocyclic nitrogen is also slightly short – 3.169 Å (0.053 Å less than vdW radii sum).

This investigation constitutes a starting point for study of novel antithyroid drugs in future.

Download English Version:

<https://daneshyari.com/en/article/7668968>

Download Persian Version:

<https://daneshyari.com/article/7668968>

[Daneshyari.com](https://daneshyari.com)