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

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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 (lgβ=7.91). The compound of the 5,5'-disulfanediylbis(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 salthas 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.