

P29. Antimicrobial Effect of 3d-Metal Coordination Compounds with 2,4-Pentanedione bis(4-Allylthiosemicarbazone)

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The aim of this work is the synthesis of chromium, manganese, cobalt, nickel, and copper coordination compounds with the product of condensation of 4-allylthiosemicarbazide and acetylacetone, determination of their composition, structure, physicochemical and antimicrobial properties.

The experiment showed that ethanolic solution of 4-allylthiosemicarbazide reacts with 2,4-pentanedione in 2:1 molar ratio forming a new white compound with composition C₁₃H₂₂N₆S₂ (HL). Monocrystals of this compound were obtained as a result of recrystallization from ethanol, and its crystal structure was determined by X-ray analysis. It was determined that the obtained product of condensation is 3,5-dimethyl-N-(prop-2-en-1-yl)-5-[2-(prop-2-en-1-ylcarbamoithiyl)hydrazinyl]-4,5-dihydro-1H-pyrazole-1-carbothioamide. Its formation apparently can be explained in the following way. At first, the process of condensation of one molecule of 4-allylthiosemicarbazide to one carbonyl group of acetylacetone takes place. After that the second carbonyl group condensates simultaneously to a new molecule of 4-allylthiosemicarbazide and thiocarbamidic nitrogen atom forming the resultant compound HL. The NMR study of the powder of this compound also confirmed its structure.

The experiments showed that chlorides, nitrates, acetates, and perchlorates of these metals react with the HL forming colored solutions. After cooling of these solutions synthesized coordination compounds MLX (M = Cu²⁺, Ni²⁺, Mn²⁺; X = Cl⁻, NO₃⁻, ClO₄⁻), M(L-2H) · 2H₂O (M = Cu²⁺, Ni²⁺, Mn²⁺), MLX₂ (M = Cr³⁺, Co³⁺, X = Cl⁻, NO₃⁻) precipitate. The structure of two coordination compounds of nickel Ni(L)X (X = NO₃⁻, ClO₄⁻) were determined using the X-ray analysis. It was determined that in the process of forming these coordination compounds the pyrazolic cycle is breaking up and the compound HL transforms into 2,4-pentanedione bis(4-allylthiosemicarbazone). It acts in the composition of complexes as a tetradentate monodeprotonated ligand.

Biological research showed that synthesized coordination compounds show bacteriostatic and bactericidal activity for tested gram-positive and gram-negative microorganisms in the range of concentration 0.03-10.0 mg/mL. It was shown that the nature of the central atom has a main influence on the antimicrobial activity of these complexes. Depending on the nature of the central atom of homotypic complexes the biological activity changes in the following way Cu > Ni > Co ≥ Mn ≥ Cr. Synthesized compounds manifest the best activity towards the standard strains of gram-positive microorganisms (*Staphylococcus aureus*, *Enterococcus faecalis*).

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