

Mononuclear Nickel(II) and Copper(II) Coordination Compounds with Ligands Based on Acetyl(benzoyl)acetone S-Methylisothiosemicarbazones and 8-Quinolinecarboxaldehyde. Synthesis and Crystal Structure

M. A. Cocu^a, P. N. Bourosh^{b, *}, V. Ch. Kravtsov^b, O. S. Danilescu^{a, c}, and I. I. Bulhac^a

^a Institute of Chemistry, Moldova State University, Chisinau, Republic of Moldova

^b Institute of Applied Physics, Moldova State University, Chisinau, Republic of Moldova

^c Technical University of Moldova, Chisinau, Republic of Moldova

*e-mail: pavlina.bourosh@ifm.md

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Abstract—Template condensation of S-methylisothiosemicarbazones of acetyl- or benzoylacetone with 8-quinolinecarboxaldehyde in the presence of nickel(II) and copper(II) ions gave four new mononuclear coordination compounds [NiL¹]I (I), [CuL¹]II (II), [NiL²]III (III), and [CuL²]IV (IV). The chemical composition of the products was confirmed by elemental analysis, IR spectroscopy, and mass spectrometry, and the crystal structure of compounds I and II was determined by X-ray diffraction analysis (CCDC nos. 2266386, 2266387). X-ray diffraction study revealed a square planar coordination environment of the central ion of the cationic Ni(II) complex and square pyramidal geometry for the molecular Cu(II) complex.

Keywords: nickel(II), copper(II), coordination compound, S-methylisothiosemicarbazones, X-ray diffraction analysis

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INTRODUCTION

Transition metal complexes with Schiff bases with azomethine nitrogen donor atoms containing heterocyclic substituents attract considerable attention of researchers because of their unique properties and versatile applications in various fields [1].

The use of various diamine derivatives or dicarbonyl compounds in which the terminal groups are identical in functional properties as the initial blocks gives rise to various symmetrical systems. The use of hydrazine derivatives such as thio- and semicarbazides, thio- and semicarbazones, and S-alkylated thiosemicarbazones may afford asymmetric systems belonging to open-ring Schiff bases [2–11]. These compounds exhibit various biological activities, including antiviral, cytostatic, antibacterial, anticancer, and antifungal activities and catalytic activity towards a wide range of compounds [2].

It is also known that transition metal complexes based on quinoline derivatives (in particular, quinoline carboxaldehydes) exhibit bactericidal, insecticidal, fungicidal, and antitumor properties [12–15]. A combination of two active moieties, thiosemicarbazone or S-alkylisothiosemicarbazone ones, with a quinoline moiety in one molecule appears promising

for the preparation of biologically active compounds. There are a number of known 3d-metal complexes based on semi- and thiosemicarbazones of 8-quinolinecarboxaldehyde and its structurally diverse derivatives [10, 11, 16–19], including complexes able to inhibit cancer cell growth, which may allow, in the future, the use of these compounds as antitumor agents [10, 19]. Study of coordination compounds containing 8-quinolinecarboxaldehyde thiosemicarbazone [10, 16–18, 20–24] has shown that the nature of the anion and substituents in the chalcogen semicarbazide moiety of the ligand influences the composition and structure of the complexes. Thus, it is of interest to study asymmetric systems of transition metal complexes based on S-alkylisothiosemicarbazones of various β -diketones and quinolinecarboxaldehydes, which have diverse structures and useful properties.

This paper describes procedures for the synthesis and results of studies of four new asymmetric mononuclear nickel(II) and copper(II) complexes, [NiL¹]I (I), [CuL¹]II (II), [NiL²]III (III), and [CuL²]IV (IV), with ligands obtained by the reaction of acetyl- or benzoylacetone S-methylisothiosemicarbazone hydroiodide with 8-quinolinecarboxaldehyde.

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