YANGI O‘ZBEKISTON, YANGI TADQIQOTLAR JURNALI
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SYNTHESIS AND PHYSICO-CHEMICAL PROPERTIES OF BENZOIC ACID DERIVATIVES WITH 3d-METALS WITH MIXED LIGAND COMPLEXES

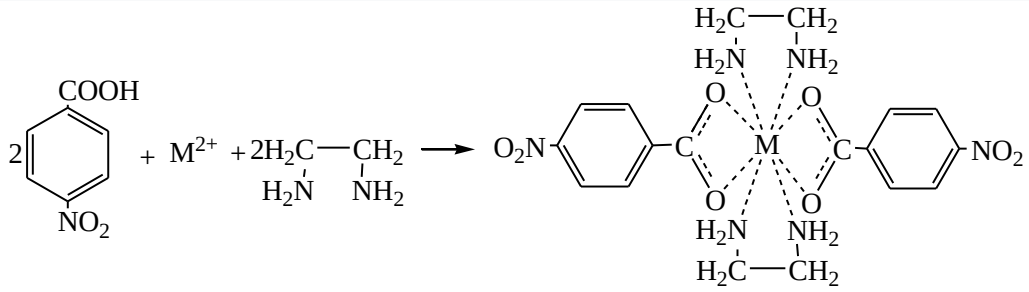
Boltayev Rakhmonbek O'tkirjonovich
master Bukhara State University
Email: raxmonbekboltayev6@gmail.com

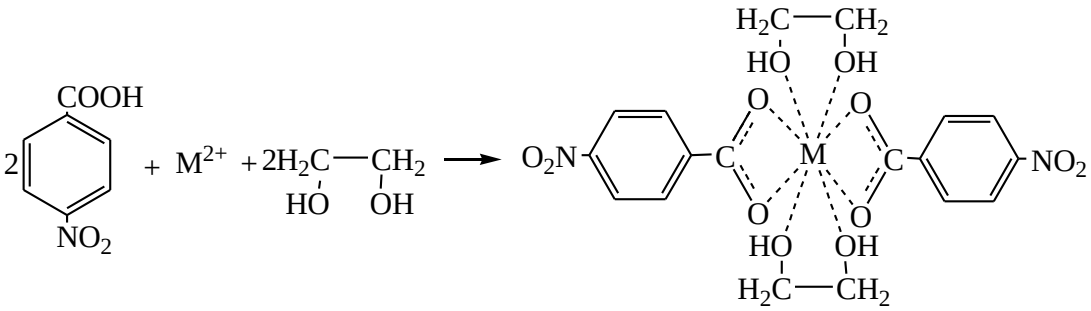
Abstract: *In this article, the structure and properties of complex compounds with mixed ligands of Ni(II), Cu(II), Zn(II) ions from various 3d metals based on benzoic acid derivatives were studied using modern physical and chemical research methods. Complex formation properties, geometry and physicochemical properties of various mono- and bidentate ligands obtained were studied.*

Key words: *benzoic acid, benzoic acid derivatives, mixed ligand, monodentate ligand, bidentate ligand, complex compound, infrared spectroscopy, symmetric and asymmetric vibrational frequency, valence vibration, quantum chemical calculation, molecular orbital, relaxation molecular orbital energy.*

Today, chemical scientists are interested in the synthesis and research of complex compounds of intermediate 3d metals such as Ni(II), Cu(II), Zn(II) with para-nitrobenzoic acid with mixed ligands such as diethylamine or ethanediol. Because such substances are widely used as fungicides, biocatalysts, medicinal substances in medicine, antimicrobial agents and plant growth stimulants, biologically active substances in agriculture. Intermediate metal ions researchers are paying attention to researching the dependence of centers of formation of complexes with ligands, energy parameters, electron density and coordination with 3d-central ion on various factors.

The reaction scheme for the formation of a complex compound can be expressed as follows:





M=Ni(II), Cu(II), Zn(II).

As a result of determining the "composition-structure-property" system in complex compounds, it is possible to predict the composition and properties of complex compounds, as well as the structure and electron distribution of the molecule. Based on this information, it is possible to draw preliminary conclusions and plan the synthesis of complex compounds. Quantum-chemical calculations of the synthesized complexes were carried out.

The coordination of monodentate and diethylamine or ethanediols through nitrogen and oxygen atoms was determined through the oxygen of the carboxyl group of para-Nitrobenzoic acid.

According to the results of the chemical analysis of the complex compound, it was determined that the metal ion is a substance with a unique complex composition consisting of molecules of a double core, mixed ligand (anions of para-nitrobezoic acid and dimethyl amine or ethanediol). Also, in order to study the method of coordination of ligands in each inner and outer sphere and the surrounding of the central ion, the IR-spectrum of the ligands in the complex and free state was compared and studied. The IR spectrum has the following absorption lines (cm1): 3090 (C-H, Ar), 2510–2995 (OH), 1660-1690 (C=O), 1600, 1575 (Ar), 1515, 1340 (para-NO2), 1290 (C-O, COOH). Absorption lines (1525, 1350 cm1) characteristic of the valence vibrations of the nitro group in the ligand were shifted to a lower frequency region (1515, 1340 cm1) in the obtained complex, and absorption lines in the region 1660-1690 cm–1 belonging to the C–O group are not present in the spectrum of the complex compound.

In the molecular orbitals of the complex compound (para-nitrobenzoic acid) (8) the share of r-orbitals of oxygen atoms is 36.12% and 37.03%, respectively. It was found that in the second band MO (EUuBMO-1= -6.6 eV) the share of d-electrons of Ni(II) atoms is large (54.92%). However, the second empty MO (EQBMO+1= -3.12 eV) is composed mainly of the relaxation orbitals of the para-nitrobenzoic acid molecule. The analysis of the energy of the frontier molecular orbitals and the electron density of states diagram showed that the energy of the lower relaxing molecular orbitals and the energy gap are very small. The

lower relaxing molecular orbital energy has a small value (-3.98 eV), which indicates that the complex has a high electron affinity and the molecule is prone to nucleophilic reactions.

In the charge distribution of atoms in the para-nitrobenzoic acid, dimethylamine and copper(II) complex, we can see that the lowest negative charges are localized in the carboxylate group of oxygen atoms, and the highest positive charge is localized in carbon atoms. At the same time, the negative charge on the oxygen atoms of the carboxylate group is 0.38-0.42 units, and the nitrogen group attached to the carbon of the aromatic ring in the para position has a negative charge of 0.34 units. Considering the para-nitrobenzoic acid molecule as a ligand, the coordination capabilities of the oxygen of the carboxyl group are higher compared to the competing oxygen atoms of the -NO2 group, and coordination is carried out at the expense of -COO-.

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