

THE DISTRIBUTION OF THE EFFECTIVE CHARGE IN THE COORDINATION COMPOUNDS OF THE SALTS OF MANGANESE CHLORIDE WITH ACETAMIDE

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Abstract: at the present stage one of the main directions of chemistry is the synthesis of new compounds possessing a wide range of useful qualities. A special place in the implementation of this direction is occupied by a new class of different ligand coordination compounds that can combine the useful properties of the original components with newly acquired ones. The study of processes and products of interaction of three important classes of chemical compounds: amides, inorganic acids, d-metal salts is very relevant, which is connected with the possibility of obtaining a new class of different ligand coordination compounds.

Keywords: coordination compounds, metal salts, effective charge, acetamide.

РАСПРЕДЕЛЕНИЕ ЭФФЕКТИВНОГО ЗАРЯДА В КООРДИНАЦИОННЫХ СОЕДИНЕНИЯХ СОЛЕЙ ХЛОРИДА МАРГАНЦА С АЦЕТАМИДОМ

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Аннотация: на современном этапе одним из основных направлений химии является синтез новых соединений, обладающих широким спектром полезных качеств. Особое место в реализации этого направления занимает новый класс разнолигандных координационных соединений, которые могут сочетать полезные свойства исходных компонентов с вновь приобретенными. Исследование процессов и продуктов взаимодействия трёх важных классов химических соединений: амидов, неорганических кислот, солей d-металлов является весьма актуальным, что связано с возможностью получения нового класса разнолигандных координационных соединений.

Ключевые слова: координационные соединения, соли металлов, эффективный заряд, ацетамид.

Today, one of the most important areas of modern chemistry and chemical technology is the chemistry of coordination compounds with organic ligands. Among them, a special place belongs to coordination compounds based on bio metals and amides, which play an important role in various biochemical processes, as well as promising as analytical, organic reagents, starting materials in the chemical industry, they are also "good" objects for fundamental research [1].

Complex compounds of d-elements halides with nitrogen- and oxygen-containing ligands are a traditional area for studying the behavior of ligands and the metal-ligand bond. D-element salts are electron-withdrawing agents capable of joining organic and inorganic molecules at places of excessive electron density created by free

pairs of electrons from donor atoms or π -electrons of multiple bonds. This ability of d-element halides to form donor-acceptor bonds with a large number of chemically passive molecules containing O, N donor atoms underlies their catalytic activity, similar in character to the catalytic activity of protonic acids [2].

Coordination compounds containing amides, metal salts and mineral acids are of interest not only from a practical point of view, but they are very interesting for fundamental studies, since the conjugation of an unshared pair of electrons of the nitrogen atom and π -electrons of the carbonyl group is expressed in the characteristic physical and chemical properties of substances [3].

Manganese is an element of the subgroup of the seventh group of the fourth period of the periodic system of chemical elements of DI Mendeleev with atomic number 25. For manganese (II), the coordination number is six, which corresponds to the octahedral arrangement of the bonds. The structure of the high-spin octahedral complexes Mn (II) corresponds to the following electron configuration: $[s_s^{cb}]^2[s_p^{cb}]^6[s_d^{cb}]^4[p_d]^3[s_d^{pa3p}]^2$. Actively participates in the process of biochemical oxidation due to a change in the degree of oxidation.

The calculations were carried out using the semi-empirical quantum-chemical method PM3, which is included in the packages of MOPAC 7 and HyperChemPro 6.0. As the studied objects in the study of the structure of acetamide complexes of manganese, $MnCl_2 \cdot CH_3CONH_2$ and $MnCl_2 \cdot 4CH_3CONH_2$ (Figures 1, 3). One of the parameters characterizing the electronic structure of molecules is the effective charge on atoms (q).

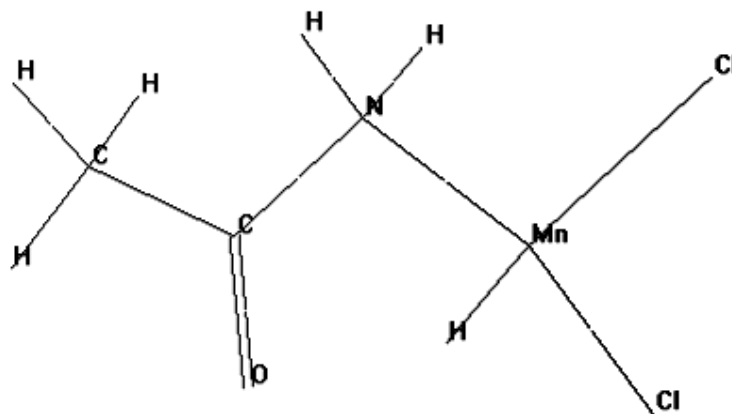


Fig. 1. Structural model of the $MnCl_2 \cdot CH_3CONH_2$ molecule

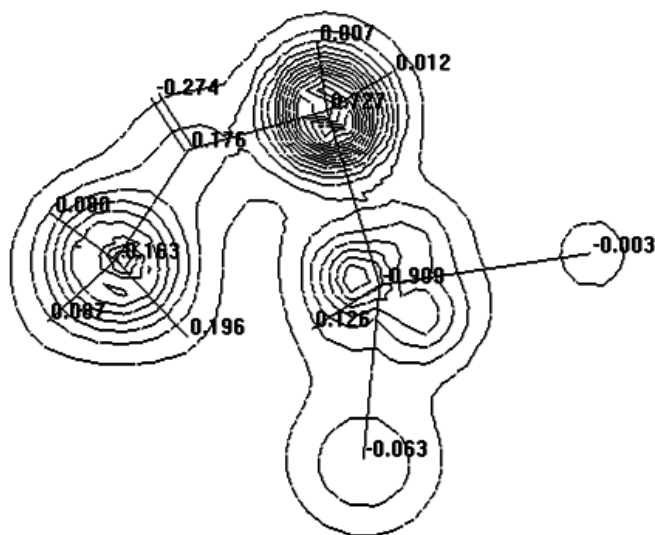


Fig. 2. The distribution of the effective charge in the $MnCl_2 \cdot CH_3CONH_2$ molecule

A comparative analysis of the electron distribution in the molecules of the compounds studied shows that the largest total negative charge is concentrated on the oxygen atoms of the carbonyl group. Figure 2 and Figure 4 show the distributions of the effective charges of molecules of manganese salts with acetamide.

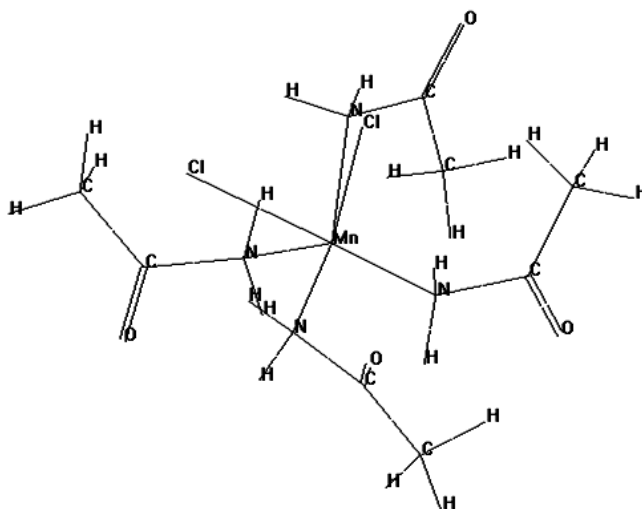


Fig. 3. Structural model of the $\text{MnCl}_2 \cdot 4\text{CH}_3\text{CONH}_2$ molecule

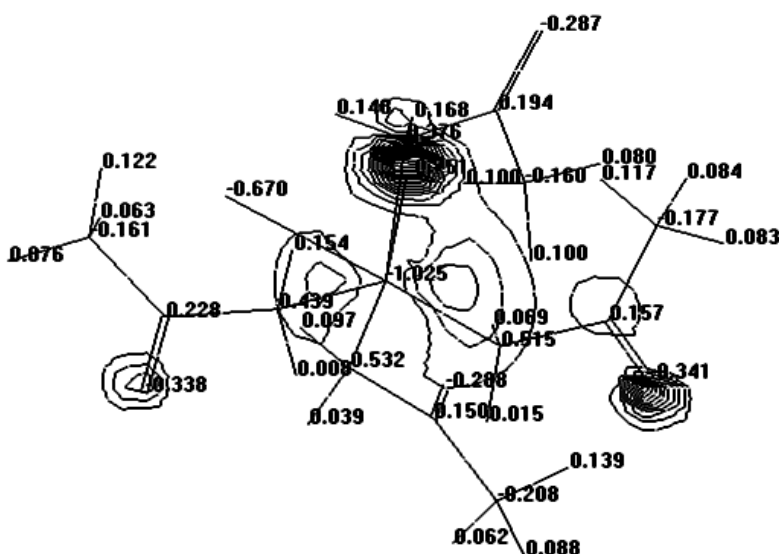


Fig. 4. The distribution of the effective charge in the $\text{MnCl}_2 \cdot 4\text{CH}_3\text{CONH}_2$ molecule

The concentration of positive effective charge is observed on the nitrogen atoms of the amino group of the model molecules of manganese coordination compounds. The largest positive effective charge for the nitrogen atom, which is in the molecule $\text{MnCl}_2 \cdot \text{CH}_3\text{CONH}_2$, $q \text{ N} = +0,727$ unit of charge (Fig. 1), and the smallest positive effective charge in the molecule $\text{MnCl}_2 \cdot 4\text{CH}_3\text{CONH}_2$, $q \text{ N} = +0,376$ unit of charge (Fig. 2). Thus, with the complication of the spatial structure of the models, not only a decrease in the absolute value of the positive effective charge on the nitrogen atom of the amino group is observed, but also an increase in the absolute value of the negative effective charge of the carbonyl oxygen atom.

Apparently, this is due to the complication of the geometric structure of the molecules (with the increase in the number of acetamide molecules connected to the central atom of the manganese complex), and this in turn affects the magnitude of the effective charges, the first ionization potential and the dipole moment of coordination compounds. The change in the above-mentioned quantities leads to a change in the electronic structure of the investigated models.

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