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Mixed LigandicCordination Magnesium Nitrate Compound with Some Acid Amides

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ABSTRACT. The synthesis of a complex compound of magnesium nitrate with nitrocarbamide and acetamidewas carried out. Using methods of vibrational spectroscopy and thermal analysis, methods for coordinating organic ligands and the thermal behavior of synthesized compounds are proved. The results of a quantum chemical calculation of a new mixed amide coordination compound are presented. Based on quantum chemical calculation, an energetically advantageous molecular geometry has been established.

KEYWORDS: Coordination, central atom, IR absorption spectra, thermal behavior, electronic energy, heat of formation.

I.INTRODUCTION

Currently, interest has increased in chelating compounds of nutrients with organic ligands exhibiting different types of biological activity. Of particular interest from such complexes are mixed ligand metal compounds with vitamins, which represent a new class of biologically active compounds. Nitrocarbamide and acetate acid amide in their composition contain donor atoms and contribute to the formation of coordination compounds with metal ions. In this case, the anion of organic acids, depending on the synthesis conditions, the nature of the metals and the composition of the complexes, exhibits diverse coordination methods. Studies of mixed amide complex compounds of metal salts with amides have been the subject of certain works [1,2]. In the literature there are no data on the complex compounds of magnesium nitrate with these amides.

II. SIGNIFICANCE OF THE SYSTEM

The synthesis of a complex compound of magnesium nitrate with nitrocarbamide and acetamidewas carried out. The study of literature survey is presented in section III, methodology is explained in section IV, section V covers the experimental results of the study, and section VI discusses the future study and conclusion.

III. METHODOLOGY

For the synthesis of the coordination compound, we chose the mechanochemical method, since it does not require scarce organic solvents. The synthesis was carried out according to the procedure [3]. The analysis of synthesized compounds for magnesium content was carried out according to [4]. Nitrogen was determined by the Dumas method, carbon and hydrogen with combustion in a stream of oxygen (Table 1). To establish the identity of the synthesized compound, X-ray diffraction patterns were recorded on a DRON-2,0 apparatus with a Cu anticathode. IR absorption spectra were recorded in the region of 400-4000 sm^{-1} on a Nicolet AVATAP-360 spectrometer. Thermal analysis was carried out on a F. Paulik-J.Paulik-L.Erdey system derivatograph at a speed of 9deg / min, and a weight of

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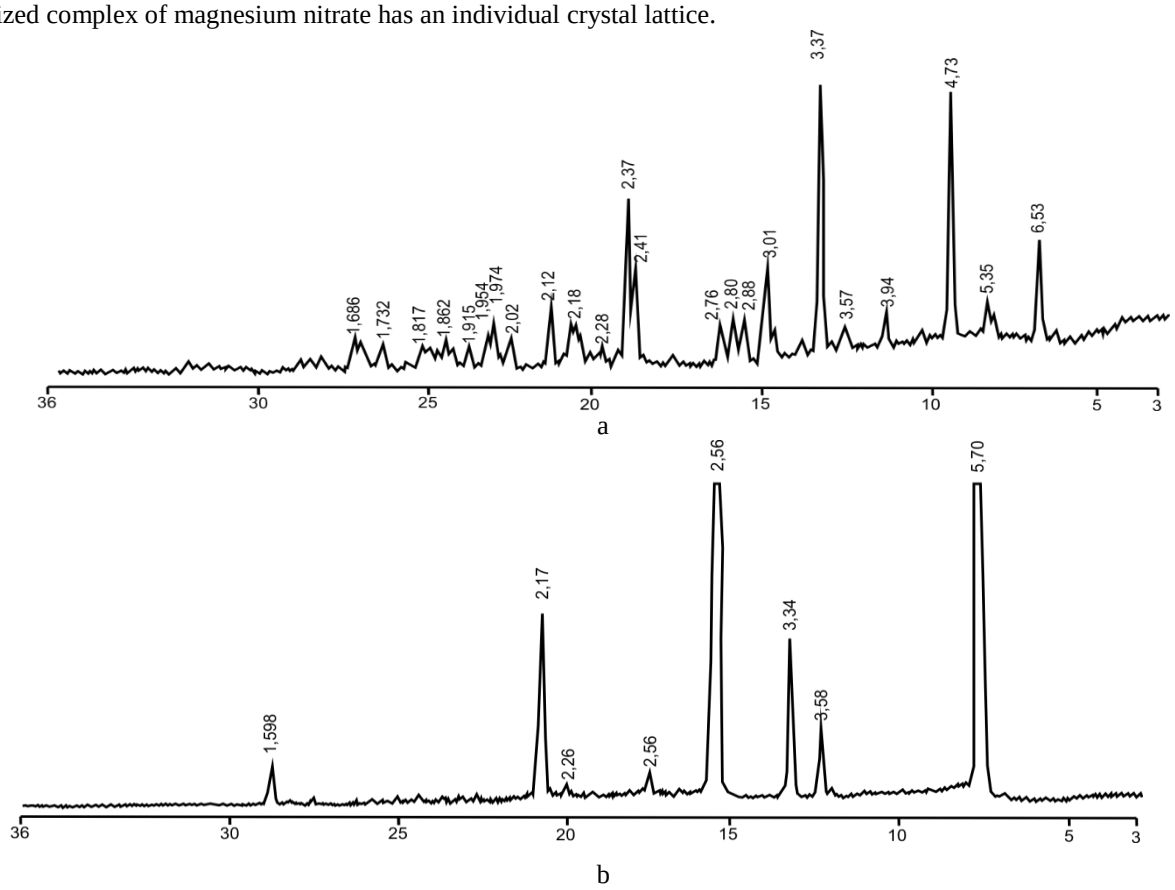
0,102-0,143 g. with sensitivity of galvanometers T-900, TG-200, DTA, DTG-1/10. Recording was carried out in atmospheric conditions. The holder was a platinum crucible with a diameter of 10 mm without a lid. $Al_2O_3$was used as a reference. In order to establish the energy parameters, as well as the geometry of the molecule, we performed a quantum chemical calculation of the molecule. The calculation was carried out in the HyperChem software package 8,07 using the semi-empirical method in the PM3 approximation, extended by the Hartree-Fock method with a convergence gradient of 0,0606 ccal / mol/ang. [five].

A compound of the composition $Mg(NO_3)_2 \cdot AA \cdot HTK$ was synthesized by stirring 2,5630 g (0,01 mol) $Mg(NO_3)_2 \cdot 6H_2O$ with 0,5972 g (0,01 mol) of acetamide and 1,0519 g of nitrocarbamide (0,01) in a ball mill at room temperature for 0,15-0,20 hours. The product yield is 84,0%.

IV. EXPERIMENTAL RESULTS

Comparison of the interplanar distances and relative intensities of the free molecules of nitrocarbamide, acetamide, magnesium nitrate hexahydrate and the coordination compound $Mg(NO_3)_2$ CH_3CONH_2 $NH_2COHNHNO_2$ H_2O showed that the new coordination compound differs significantly from similar starting compounds. Therefore, the synthesized complex of magnesium nitrate has an individual crystal lattice.



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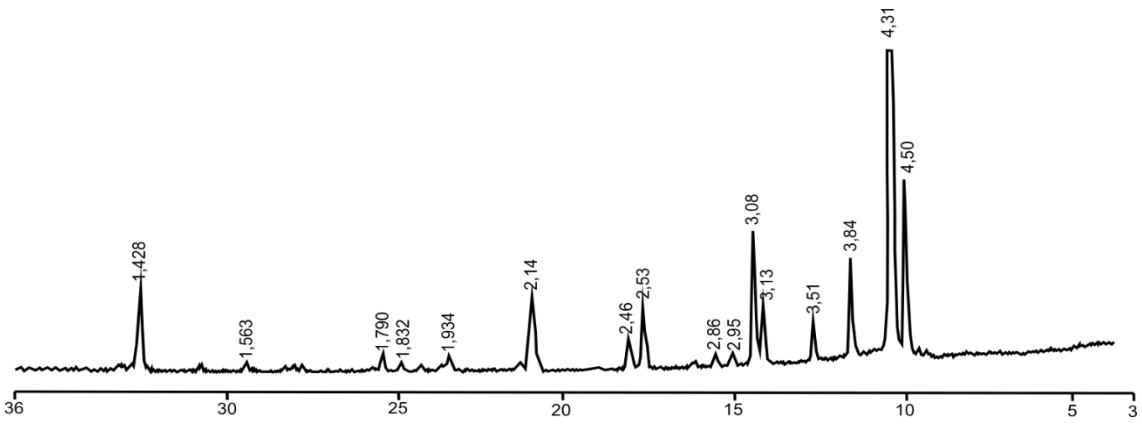

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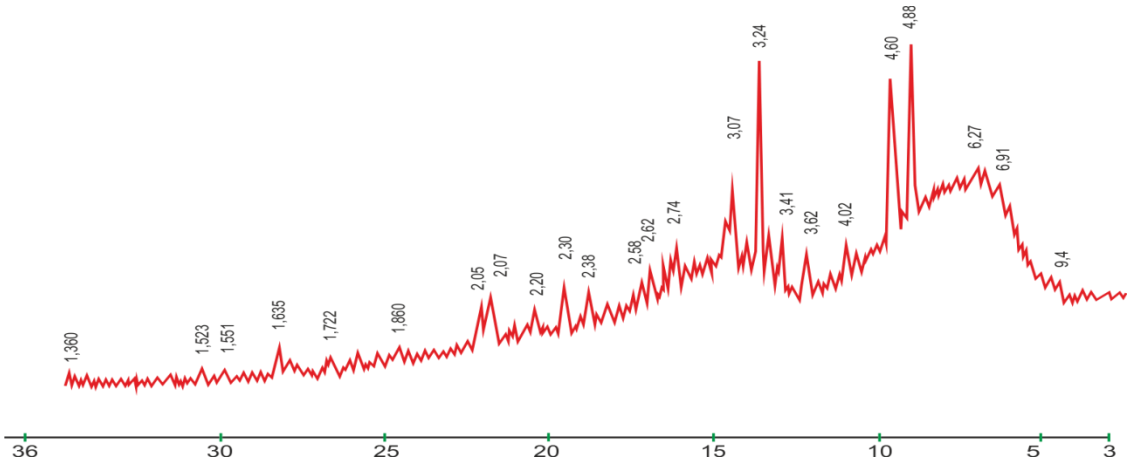

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Fig.1. X-ray diffraction pattern: a) $Mg(NO_3)_2$; b) CH_3CONH_2; c) $NH_2CONHNO_2$, g) $Mg(NO_3)_2$

Table 1
Results of an elemental analysis of mixed amideco-ordinates of magnesium nitrate

Connection	Me,%		N,%		S,%		C,%		H,%		Gross formula
	Naid	Calc	Naid	Calc	Naid	Calc	Naid	Calc	Naid	Calc	
$Mg(NO_3)_2 \cdot CH_3CONH_2 \cdot CONH_2NHNO_2$	8,03	8,11	28,29	28,38			2,07	12,16	2,77	2,70	$MgN_6C_3H_8O_9$

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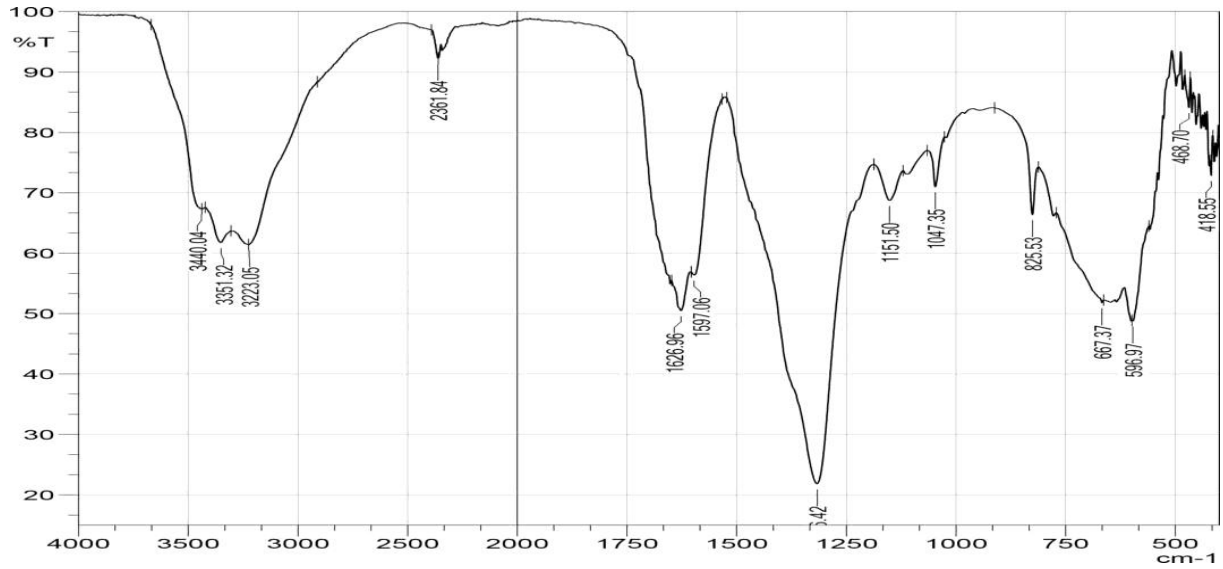

Fig.2. IR absorption spectrum of a mixed amide complex of magnesium nitrate with acetamide and nitrocarbamide.

The infrared absorption spectrum of a free nitrocarbamide molecule together with other frequencies has two characteristic frequencies at 1704-$\nu_{(CO)}$ and 1460-$\nu_{(CN)}$. The indicated frequencies undergo a change when the nitrocarbamide molecule is coordinated through the oxygen atom of the carbonyl group undergo a change. The bond stretching frequency C = O decreases and the second frequency increases. (Figure 2).

Table 2
Derivatographic data of thermolysis of a mixed amide complex of magnesium nitrate with acetamide and nitrocarbamide.

Connection	Effect Temperature Range°C	Peak effecta °C	Loss of mass%	Total loss of mass%	Nature of effects	Compounds formed
$Mg(NO_3)_2 \cdot CH_3CONH_2 \cdot \cdot H_2NCONHNO_2 \cdot H_2O$	80-120	108	0,00	0,00	Endothermic	$Mg(NO_3)_2 \cdot CH_3CONH_2 \cdot \cdot H_2NCONHNO_2$
	120-205	172	15,53	15,53	Endothermic	Thermolysis Product
	205-313	228	17,96	33,49	Endothermic	Thermolysis Product
	313-350	338	8,25	41,74	Endothermic	Thermolysis Product
	350-380	360	7,28	49,04	Endothermic	Thermolysis Product
	380-480	403	9,71	58,75	Endothermic	Thermolysis Product
	480-550	500	0,49	59,24	Endothermic	Thermolysis Product
	550-750	614	4,46	63,70	Endothermic	Thermolysis Product
	750-840	775	16,88	80,58	Endothermic	Thermolysis Product

Five endothermic effects were detected at 108, 172, 228, 338, 775 and four exothermic effects at 360, 403, 500, 614°C on the DTA curve of the compound $Mg(NO_3)_2CH_3CONH_2$ $H_2NCONHNO_2$. The nature of the first endoeffect is related to the polymorphic transformation of the compound $Mg(NO_3)_2CH_3CONH_2H_2NCONHNO_2$. The nature of the subsequent thermal effects is accompanied by a stepwise decomposition of the anhydrous compound. In the temperature ranges 80–120, 120–205, 205–313, 313–350, 350–380, 380–480, 480–550, 550–750, and 750–840°C, the mass loss, respectively, is 15,53; 17,96; 8,25; 7,28; 9,71; 0,49; 4,46; 16,88%. The total mass loss in the temperature range of 90-840 °C along the TG curve is 80,58%, which corresponds to the formation of magnesium oxide (table 2.).

Four tetrahedral structures and four octahedral environments with various methods for the coordination of acetate groups and the presence of intramolecular hydrogen bonds have been proposed for a complex compound of the

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composition $Mg(NO_3)_2CH_3CONH_2NH_2CONHNO_2H_2O$. Of the eight structures, a structure was found to be energetically favorable in terms of the heat of formation, where the central magnesium atom is surrounded by a tetrahedral site due to the monodentate coordination of nitrate fragments and donor-acceptor coordination of acetamide and nitrocarbamide molecules through the oxygen atom of the carbonyl group. Intramolecular hydrogen bonds are carried out due to the oxygen atoms of one nitrate group and the hydrogen of the amine group of acetamide. Another intramolecular bond is manifested due to the oxygen and hydrogen atoms of the nitrocarbamide molecule. (Fig. 3.4)

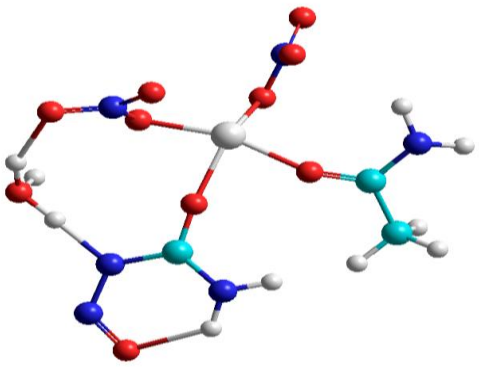

Fig.3. Spatial model of a molecule of magnesium nitrate with acetamide and nitrocarbamide of the composition $Mg(NO_3)_2 \cdot CH_3CONH_2 \cdot NH_2CONHNO_2 \cdot H_2O$.

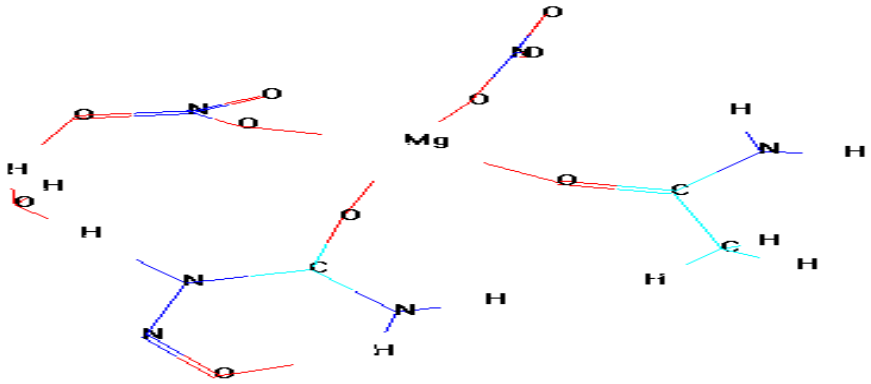

Fig.4. Designation of the formula of the molecule $Mg(NO_3)_2$ CH_3CONH_2 $NH_2COHNHNO_2$ H_2O

The lengths of bonds of electron-donating atoms with the central ion show that the distance of the donor atoms from the central atom depends on the radius of the atom. The bond lengths between the nitrogen atoms of nitrocarbamide and the central ion are approximately the same, while the bonds between oxygen and the central atom are much larger (Fig.5-6).

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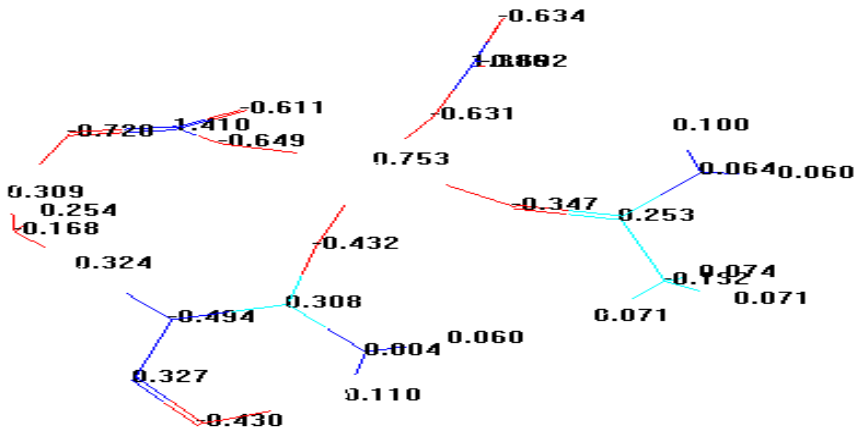

Fig.5.The distribution of charges on the atoms of a moleculeMg(NO$_3$)$_2$·CH$_3$CONH$_2$·NH$_2$CONHNO$_2$·H$_2$O

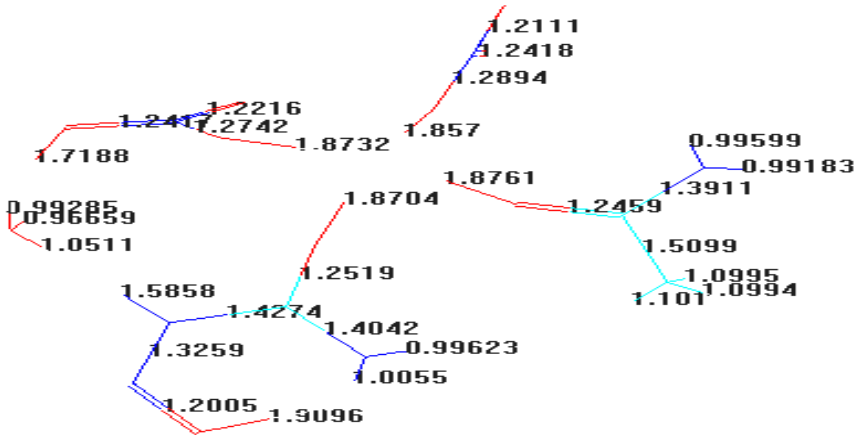

Fig.6. The bond lengths of the atoms of the molecule Mg(NO$_3$)$_2$·CH$_3$CONH$_2$·NH$_2$CONHNO$_2$·H$_2$O.

V. CONCLUSION AND FUTURE WORK

Synthesis conditions have been developed, a complex compound of magnesium nitrate with nitrocarbamide and acetamide has been isolated in the solid state. Using x-ray phase, vibrational spectroscopy, derivatographic analyzes, the individuality, methods of coordination of the molecules of nitrocarbamide, acetamide, nitrate fragments and the thermal behavior of the synthesized compound are proved. Based on quantum-chemical calculations, we established an energetically advantageous molecule geometry, based on the minimum formation energy, calculated energy parameters, determined the bond lengths between the atoms that make up the molecule. The central atom is surrounded by four oxygen atoms and has a geometric configuration of a distorted tetrahedron.

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