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Mixed-Ligand Coordination Connection of Calcium Nitrate with Carbamide and Nicotinamide

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ABSTRACT. The mixed amide complex compounds of calcium nitrate with someacidamides were synthesized. The composition, personality, methods of coordination of nitrate groups, urea molecules, nicotinamide are established. Using methods of vibrational spectroscopy and thermal analysis, methods for coordinating organic ligands, the environment of the central ion, and the thermal behavior of the synthesized compounds are proved. Comparison of the interplanar distances and relative intensities of calcium nitrate, ligand molecules and synthesized complexes showed that the new coordination compounds differ from each other, as well as from the starting components. Therefore, the compounds have an individual crystal lattice.

KEYWORDS. Central atom, elemental analysis, IR absorption spectra, X-ray phase analysis, personality, thermal behavior

I.INTRODUCTION

In the world, obtaining coordination compounds of transition and alkaline-earth ions based on polydentate ligands and determining their properties is of practical and theoretical importance. At present, high efficiency is achieved through the use of these coordination compounds as medicines in medicine, biologically active substances in industry, and chemical preparations: stimulants, pesticins, mineral fertilizers, as well as defoliants and desiccants in agriculture [1,2]. Research is currently underway in the world to develop the development of conditions for the synthesis of highly effective and complex-acting stimulants. In this regard, an important task is to justify the creation of stimulants that increase the yield of plants, accelerating physiological processes, including the development of optimal conditions for synthesis and production; determination of the composition and structure of coordination compounds of calcium ions with magnesium with polydentate organic ligands - amides; determination of the nature of the coordination bond in the coordination of ligands to the central ion and in the mutual substitution of ligands, as well as determination of the thermal stability of the synthesized compounds [3]

II. SIGNIFICANCE OF THE SYSTEM

The mixed amidecomplex compounds of calcium nitrate with some acid amides were synthesized. 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 coordination compounds, we have chosen the mechano-chemical method, since it does not require deficient organic solvents and allows for a short time to synthesize different types. The synthesis was carried out according to the technique [4].

The analysis of synthesized compounds for the content of magnesium was carried out as agreed. Nitrogen was determined by the Dumas method [5], carbon and hydrogen with combustion of oxygen in the current (Table 2). To

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establish the individuality of synthesized compounds, the diphractogramm was removed on the installation of DRON-2.0 with Cu-anticode [7]. IR absorption spectra were recorded in the region of 400–4000 sm^{-1} on an AVATAP-360 spectrometer from Nicolet. Thermal analysis was performed on a derivative of the F. Paulik–J. Paulik–L. Erdey system [8] at a speed of 9 degrees/min, and a hitch of 0,102–0,143 g. with sensitivity of galvanometers T-900, TG-200, DTA, DTG-1/10. Recording was carried out under atmospheric conditions. The holder was a 10 mm plate crucible without a lid. As a standard, Al_2O_3 was used [4].

To determine the optimal conditions for carrying out the reactions, we carried out mechano-chemical reactions in a ball mill with a length of 0,1; 0,15; 0,2; 0,25 and 0,3 hours when using 1 and 2 working bodies. After each synthesis, the X-ray diffraction patterns of the obtained coefficients were removed and the comparison with the diffraction patterns of the original ligands was removed. It is defined that diphractogramm the connections received lasting reaction 0,2; 0,25 and 0.3 hours are excellent from diphractogramm initial substances and are identical between themselves, proceeding from this optimum conditions of carrying out mechano-chemical reactions in a spherical mill the following conditions are accepted: duration of reaction of 0,15-0,2 hours, number of working bodies 1 (steel sphere with a diameter of 20 mm). [10]

The complex $Ca(NO_3)_2{\bullet}CO(NH_2)_2{\bullet}NC_5H_4CONH_2$ was synthesized by intensive mixing of 2,3609 g (0,01 mol) $Ca(NO_3)_2{\cdot}4H_2O$ with 0,6031 g (0,01 mol), 22 (0,01 mol) of nicotinamide in a ball mill at room temperature for 0,15-0,20 hours. The yield of the product is 86,0%.

IV. EXPERIMENTAL RESULTS

Comparison of interplanar distances and relative tetrahydrate intensity nitrate of calcium, a carbamide, nicotinamide, and complexes on their basis showed that new coordination connections differ between themselves, an also from initial components, therefore, of connection have an individual crystal lattice. Results in table 1 [9].

Table 1

Interplanar spacings and relative intensities of nicotinamide, carbamide with calcium nitrate lines.

Connection	d,Å	I,%	d,Å	I,%	d,Å	I,%	d,Å	I,%	d,Å	I,%
$NC_5H_4CONH_2$	20,78	6	4,57	9	3,06	5	2,36	1	1,893	6
	18,50	8	4,46	14	3,03	5	2,30	20	1,851	4
	16,44	9	4,37	11	2,93	11	2,25	4	1,799	8
	15,63	9	3,92	42	2,84	4	2,22	2	1,737	5
	11,02	1	3,86	9	2,79	3	2,18	10	1,694	2
	7,58	5	3,76	12	2,72	6	2,16	5	1,675	1
	6,53	5	3,55	7	2,64	12	2,09	1	1,642	1
	5,92	100	3,48	23	2,57	10	2,06	2	1,623	1
	20,78	6	4,57	9	3,06	5	2,36	1	1,893	6
	18,50	8	4,46	14	3,03	5	2,30	20	1,851	4
	16,44	9	4,37	11	2,93	11	2,25	4	1,799	8
	15,63	9	3,92	42	2,84	4	2,22	2	1,737	5
$CO(NH_2)_2$	17,21	2	4,37	2	3,02	12	2,20	4	1,770	2
	16,08	3	3,98	100	2,80	27	2,15	2	1,736	1
	15,29	3	3,56	10	2,49	42	2,01	1	1,660	5
	13,86	2	3,25	2	2,46	5	1,980	18	1,557	1
	12,59	1	3,14	3	2,33	1	1,827	6		
$Ca(NO_3)_2{\cdot}CO(NH_2)_2$ $\cdot NC_5H_4CONH_2{\cdot}H_2O$	15,73	17	5,18	8	3,11	2	2,10	3	1,511	2
	15,19	13	5,06	2	3,07	2	2,03	2	1,506	2
	13,36	4	4,82	2	2,99	8	2,02	4	1,492	2
	11,59	3	4,71	3	2,90	6	1,982	18	1,479	1
	10,75	13	4,48	2	2,82	4	1,943	6	1,467	1
	10,25	1	4,38	2	2,77	5	1,906	2	1,459	2
	9,58	1	4,25	5	2,71	2	1,877	3	1,446	1
	8,75	1	4,14	2	2,69	2	1,840	2	1,409	5
	8,51	1	3,94	23	2,66	2	1,803	3	1,388	2

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Connection	d,Å	I,%	d,Å	I,%	d,Å	I,%	d,Å	I,%	d,Å	I,%
	8,02	2	3,86	4	2,62	3	1,779	1	1,380	2
	7,74	2	3,68	3	2,58	3	1,687	2	1,371	1
	7,35	1	3,57	2	2,50	8	1,658	1	1,343	1
	7,14	2	3,45	12	2,41	35	1,643	1	1,333	2
	6,79	1	3,43	8	2,39	2	1,633	1	1,318	1
	6,42	3	3,36	11	2,33	5	1,620	1	1,312	2
	6,31	2	3,32	4	2,25	2	1,606	1		
	5,81	100	3,29	6	2,21	1	1,586	2		

Table 2
Results of an elemental analysis of mixed amide co-ordinates of calcium nitrate

Connection	Me,%		N,%		S,%		C,%		H,%	
	Fin	Cal	Fin	Cal	Fin	Cal	Fin	Cal	Fin	Cal
$Ca(NO_3)_2 \cdot CO(NH_2)_2 \cdot NC_5H_4CONH_2 \cdot 0{,}5H_2O$	11,19	11,27	23,57	23,66			23,57	23,66	3,17	3,10

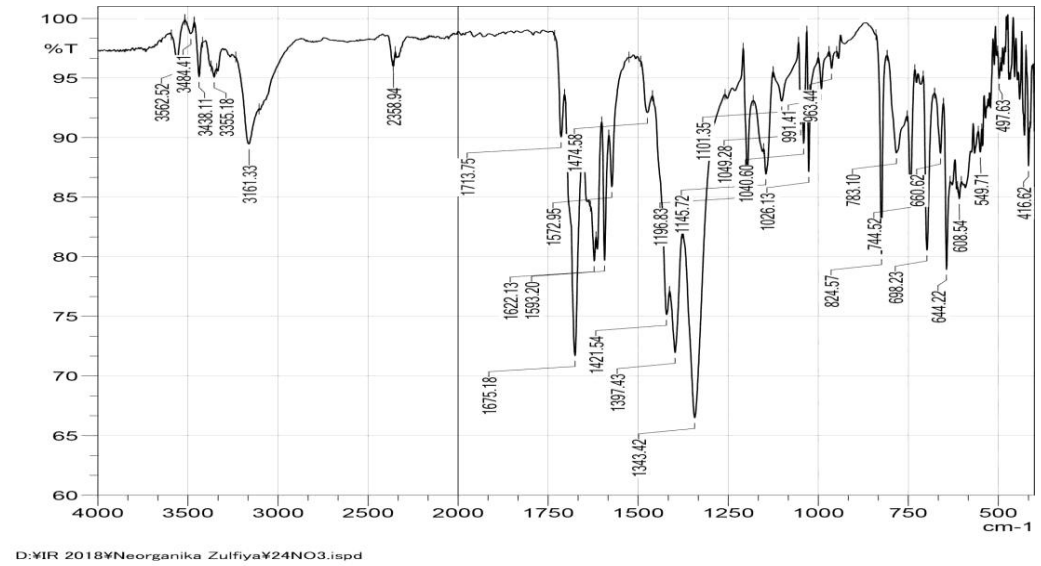

Figure 1.IR absorption spectrum of a mixed amide complex of calcium nitrate with carbamide and nicotinamide.

The infrared absorption spectrum of a free urea molecule is characterized by several frequencies. Of these bands, at 1686 and 1318 cm^{-1}, bands corresponding to stretching vibrations of the C = O and C – N bonds are observed. In the case of complexes, the first band decreases by 6-35 cm^{-1}, and the frequency of the second bond increases by 12-28 cm^{-1}, this confirms the presence of a coordination bond between the central ion and oxygen atoms of the carbonyl group of the molecule (Figure 1).

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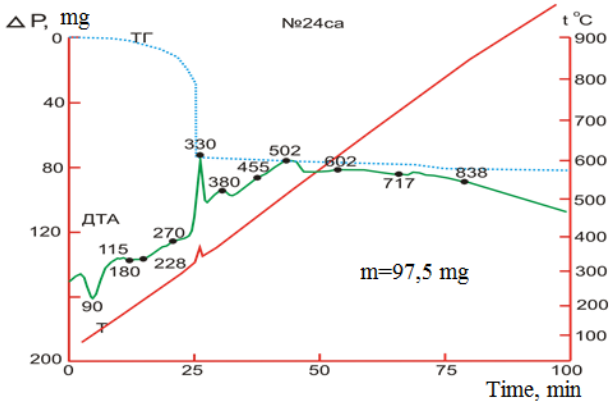

Figure 2. Connection program $Ca(NO_3)_2 \cdot CO(NH_2)_2 \cdot NC_5H_4CONH_2$

At the same time, the heating of the complex $Ca(NO_3)_2$ CO $(NH_2)_2 \cdot NC_5H_4CONH_2$ was found to have four endothermic effects at 90, 115, 180, 270 and a temperature of 350, 52, and a total of 350, which is accurate to 45, which is specific to a temperature of 350, a total of 350, a total of 45, a total of 45, a total of 52, of which, The manifestation of the first endo-effect is made possible by the removal of one water molecule. The nature of the subsequent thermal effects is accompanied by a stepped decomposition of the irrelevant coefficients. Losing masks in the range of 50-92 °C is 6,1%, 6,1% is calculated. In temperature ranges 92–153, 153–210, 210–310, 310–357, 357–686, 686–830°C, the weight of the mixture is adequately 12,39; 29,36: 9,17; 5,05; 5,96; 16,78%. The total decrease in masks at intervals of 60–746 °C for TG is 86,94%, which corresponds to the formation of calcium oxide (Figure 2).

V. CONCLUSION AND FUTURE WORK

X-ray phase analysis of the starting ligands, magnesium and calcium nitrates, as well as synthesized homogeneous and mixed ligand compounds, is a little different.

Based on the infrared spectroscopy data, the carbamide was coordinated with the central atom through the oxygen of the carboxylic acid group a ofnicotinamide through the heterohydroxide of pyridine. By the method of differential thermal analysis, the thermal behavior of synthesized coordinated compounds was established and the products of thermolysis were identified.

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