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Coordination Compounds of Barium Nitrate Strontium with Formamid and Carbamid

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Abstract Mixed-ligand coordination compounds of barium and strontium nitrates with formamide and carbamide have been synthesized. The composition, individuality, and coordination methods of formamide, carbamide and nitrate fragment molecules of coordination compounds were established, and the thermal behavior of the obtained complexes was studied.

Keywords Physicochemical analysis methods, IR absorption spectra, X-ray phase analysis, Coordination compounds, Synthesis, Composition, Thermal behavior

1. Introduction

Developing the synthesis of new chemical compounds with effective properties for use in agriculture is one of the urgent tasks of modern chemistry. mixed-ligand complex compounds of metals, possessing a number of specific properties, have found wide application in various sectors of the national economy. The use of substances containing donor atoms of aliphatic and carboxylic acid amides, in particular formamide (FA), carbamide (K), as ligands contributes to the formation of coordination compounds containing macroelements [1].

Numerous works by authors such as Yunusov D.Kh., Mukumova G.Zh., Kuzmin N.E., Palkin K.K., Parpiev N.A., Azizov T.A., Azizov O.T., Suleymanova G.G., Azizzhanov Kh.M., Khasanov Sh.B. and others have been devoted to the synthesis and study of mixed-amide complex compounds of metal nitrates. There is no data in the literature on mixed-ligand coordination compounds of barium nitrate.

Our goal is to synthesize the coordination compounds of barium and strontium nitrates with formamide and carbamide. Establishing the composition, individuality, and coordination methods of formamide, carbamide, and nitrate fragment molecules. Study of the thermal behavior of synthesized compounds.

2. Research Objects and Methods

For the synthesis of coordination compounds, we chose a mechanochemical method, as it does not require scarce organic solvents and allows for the synthesis of complexes of various compositions with a high yield in a short time. The synthesis was carried out according to the method [2].

The analysis of the synthesized compounds for magnesium and calcium content was carried out according to [3]. Nitrogen was determined by the Dumas method [4], carbon and hydrogen with combustion in oxygen current (Table 1). To establish the individuality of the synthesized compounds, diffractograms were taken on a DRON-2.0 device with a Cu-anticathode [5]. IR absorption spectra were recorded in the region of 400-4000 cm^{-1} on the AVATAP-360 spectrometer of the "Nicolet" company. Thermal analysis was carried out on a derivatograph of the F.Paulik, J.Paulik, L.Erdey system [6] at a rate of 9 deg/min and a sample of 0.102-0.143 g. at the sensitivity of galvanometers T-900, TG-200, DTA, DTG-1/10. The recording was carried out under atmospheric conditions. The holder was a 10 mm diameter platinum crucible without a lid. Al_2O_3 was used as a standard.

A complex compound of the composition $Ba(NO_3)_2 \cdot 2HCONH_2 \cdot 2CO(NH_2)_2$ was synthesized by mixing 1.3056 g (0.005 mol) of barium nitrate with 0.4504 g (0.01 mol) of formamide and 0.6008 g (0.01 mol) of carbamide in an agate mortar at room temperature for 3 hours. The product yield is 92.01%.

During the synthesis of a complex compound with the composition $Sr(NO_3)_2 \cdot 2HCONH_2 \cdot 2CO(NH_2)_2$, 1.065 g (0.005 mol) of strontium nitrate was ground with 0.4504 g (0.01 mol) of formamide and 0.6008 g (0.01 mol) of carbamide in an agate mortar at room temperature for 3 hours. The complex yield is 98.94%.

3. Results and Their Discussion

Comparison of the interplanar distances and relative intensities of barium and strontium nitrate, formamide, carbamide and coordination compounds of the compositions $[Ba(NO_3)_2 \cdot 2HCONH_2 \cdot 2CO(NH_2)_2]$, $[Sr(NO_3)_2 \cdot 2HCONH_2 \cdot 2CO(NH_2)_2]$ showed that the new coordination compounds

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differ significantly from each other and from similar initial compounds. Consequently, the synthesized barium and strontium nitrate complexes have individual crystal lattices (Table 1).

In the IR absorption spectrum of the free formamide molecule, two frequencies are observed at 1692, 1316 cm^{-1}, corresponding mainly to the valence vibrations of the C=O and C-N bonds. The IR absorption spectrum of the uncoordinated carbamide molecule is characterized by several frequencies. Of these, at 1680 and 1466 cm^{-1}, bands corresponding to the valence vibrations of the C=O and C-N bonds are observed. With the transition to a coordinated state, i.e., in mixed amide coordination compounds, the C=O frequency decreases by 8-23 cm^{-1}. While the C-N frequency value increases by 6-10 cm^{-1}, indicating the coordination of amides through the oxygen atom of the carbonyl group. The 3200-3400 cm^{-1} bands confirm the presence of crystallization water in the molecule. (Fig. 1,2).

The thermal behavior of the synthesized compounds was investigated. On the heating curve of the $Ba(NO_3)_2$ 2HCON H_2 $2CO(NH_2)_2$ derivative, five endothermic effects were observed at 115, 178, 205, 336, 372 ℃, and five exothermic effects at 435, 520, 546, 680, 816 ℃.

The nature of the subsequent thermal effects is accompanied by the stepwise decomposition of the anhydrous compound. In the temperature range of 140-180; 180-285; 285-360; 360-390; 390-448; 448-530; 530-591;591-748;748-850oC, respectively, the mass loss is 14.52; 18.55; 3.23; 0.97; 2.02; 28.44; 12.71; 0.40; 0.20% respectively. The total mass loss in the temperature range of 60-850 ℃ along the TG curve is 83.4%.

The thermal behavior of the complex compound $Sr(NO_3)_2$ 2HCONH $2CO(NH_2)_2$ is characterized by six exothermic effects at 110, 143, 183, 208, 345, 800 ℃ and five endothermic effects at 297, 410, 425, 450, and 600 ℃. The first two endoeffects correspond to the stepwise removal of water with the formation of thermolizing products of the $Ba(NO_3)_2$ $2HCONH_2$ $2CO(NH_2)_2$ and $Sr(NO_3)_2$ 2HCON H_2 $2CO(NH_2)_2$ compositions in the temperature range of 145-191; 191-250; 250-320; 320-388; 388-417; 417-436; 436-460; 460-650; At 650-820 ℃ mass loss is respectively 6.94%; 8.98; 2.04; 4.08; 0.82; 1.22; 1.22; 46.31 and 12.05.

Table 1. Results of elemental analysis of mixed amide coordination compounds of barium and strontium nitrates with formamide and carbamide

Compounds	Me, %		N, %		C, %		H, %	
	Found.	Calc.	Found.	Calc.	Found.	Calc.	Found.	Calc.
$Ba(NO_3)_2 \cdot 2HCONH_2 \cdot 2CO(NH_2)_2$	28,84	29.08	23.19	23.77	9.83	10.19	3.02	3.18
$Sr(NO_3)_2 \cdot 2HCONH_2 \cdot 2CO(NH_2)_2$	20.19	20.86	26.39	26.54	11.18	11.37	3.18	3.55

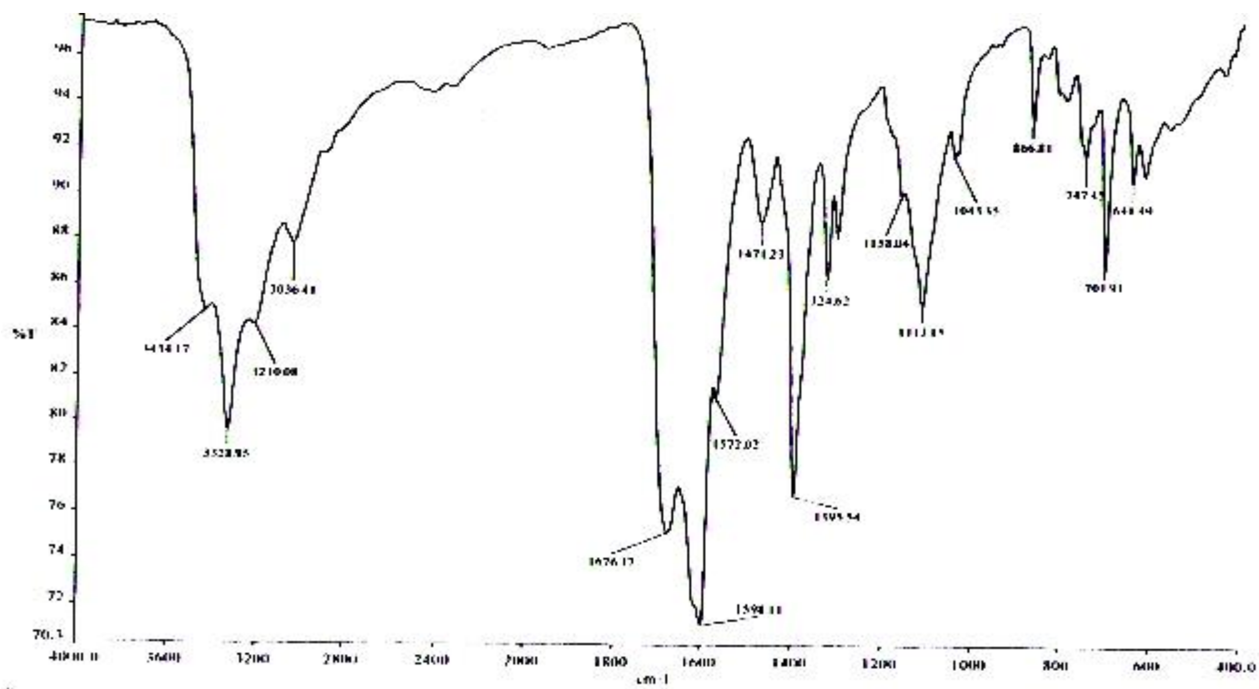

Figure 1. IR absorption spectrum of the mixed amide complex compound of barium nitrate with formamide and carbamide - $Ba(NO_3)_2$ $2HCONH_2$ $2CO(NH_2)_2$

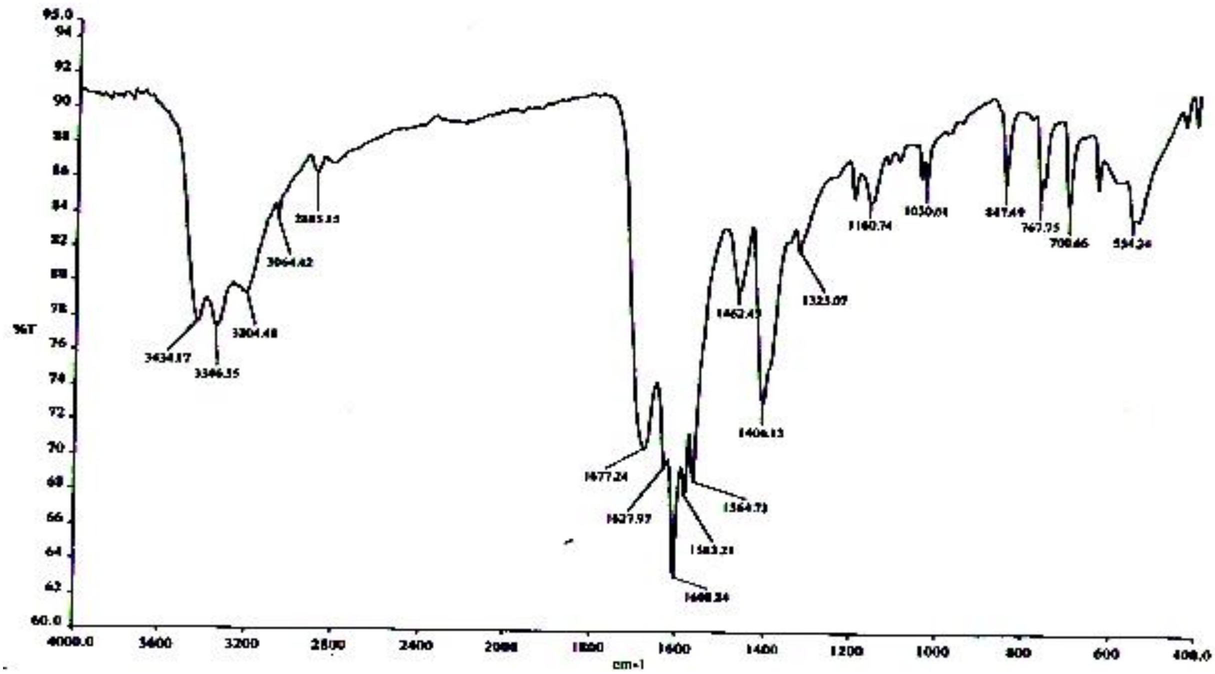

Figure 2. IR absorption spectrum of the different amide coordination compound strontium nitrate with formamide and carbamide

Table 2. Interplanar distances and relative intensities of barium nitrate, strontium, and their amide complexes lines

Compounds	d, Å	I/%	d, Å	I/%	d, Å	I/%	d, Å	I/%	d, Å	I/%
$Ba(NO_3)_2$	16.94	2	4.50	3	2.84	11	2.00	2	1.581	1
	15.96	3	4.38	48	2.79	25	1.977	4	1.571	1
	15.63	1	4.26	21	2.73	6	1.967	3	1.551	4
	14.21	2	4.22	17	2.71	7	1.942	6	1.534	3
	13.04	2	4.03	3	2.64	28	1.922	10	1.513	2
	12.59	2	3.94	17	2.57	8	1.890	2	1.494	2
	11.91	2	3.70	19	2.52	3	1.866	10	1.481	3
	11.30	3	3.58	5	2.48	3	1.841	4	1.427	3
	8.61	63	3.52	64	2.42	11	1.797	2	1.403	2
	6.55	25	3.44	14	2.38	5	1.773	4	1.381	3
	6.03	2	3.29	30	2.33	7	1.744	3	1.360	1
	5.74	11	3.27	28	2.26	3	1.723	1	1.333	2
	5.35	2	3.18	14	2.25	3	1.699	5	1.320	1
	5.09	8	3.13	13	2.21	2	1.678	3	1.308	1
	4.87	1	3.07	9	2.17	28	1.649	7	1.292	2
	4.66	18	2.97	100	2.11	8	1.637	4		
	4.52	3	2.88	3	2.04	6	1.601	1		
$Sr(NO_3)_2$	15.63	1	4.67	1	2.89	4	2.02	2	1.637	1
	15.09	1	4.44	17	2.86	6	1.985	2	1.613	2
	14.12	2	4.27	2	2.84	8	1.972	2	1.572	2
	12.89	2	4.07	1	2.77	1	1.967	3	1.563	3
	12.31	2	3.98	23	2.74	2	1.943	5	1.537	2
	11.30	1	3.86	100	2.65	2	1.907	4	1.506	4
	9.80	1	3.79	50	2.59	56	1.890	1	1.479	1
	9.18	1	3.76	55	2.50	12	1.861	4	1.460	1
	8.86	1	3.52	36	2.42	1	1.849	3	1.451	1
	8.35	1	3.44	5	2.35	5	1.811	9	1.418	1
	7.61	16	3.34	1	2.28	7	1.792	1	1.400	2

Compounds	d, Å	I/%	d, Å	I/%	d, Å	I/%	d, Å	I/%	d, Å	I/%
	6.87	39	3.25	1	2.24	2	1.774	1	1.384	1
	6.47	1	3.18	1	2.21	6	1.747	2	1.375	1
	5.95	1	3.12	1	2.18	4	1.732	2	1.363	1
	5.59	5	3.02	7	2.11	1	1.701	3	1.344	1
	5.25	1	2.97	1	2.08	4	1.689	2	1.319	1
	5.06	1	2.92	3	2.06	5	1.665	4	1.311	1
$Ba(NO_3)_2 \cdot 2HCONH_2 \cdot 2CO(NH_2)_2$	15.52	4	5.08	2	2.75	45	1.934	5	1.566	2
	14.69	14.70	4.96	2	2.67	12	1.910	6	1.552	1
	14.21	4	4.75	2	2.64	14	1.897	3	1.541	2
	13.35	4	4.51	13	2.58	27	1.890	3	1.533	6
	11.60	2	4.37	2	2.53	2	1.862	2	1.516	3
	11.30	3	4.19	28	2.47	21	1.837	9	1.496	2
	11.13	4	4.10	61	2.42	7	1.811	6	1.480	2
	10.86	3	3.86	90	2.38	6	1.782	2	1.460	2
	10.02	2	3.79	28	2.30	13	1.764	2	1.408	5
	9.71	2	3.70	5	2.23	2	1.754	2	1.405	3
	9.34	2	3.65	5	2.19	2	1.718	4	1.371	3
	8.02	100	3.50	5	2.16	3	1.684	5	1.348	2
	7.26	2	3.39	22	2.14	12	1.682	7	1.332	1
	7.07	2	3.34	5	2.10	2	1.658	11	1.326	2
	6.49	2	3.22	12	2.07	3	1.642	5	1.309	3
	6.15	15	3.11	17	2.02	2	1.632	4	1.301	1
	5.95	2	3.04	14	2.00	2	1.616	7	1.289	3
	5.47	10	2.99	10	1.989	1	1.589	2		
	5.15	6	2.89	41	1.961	6	1.576	2		
$Sr(NO_3)_2 \cdot 2HCONH_2 \cdot 2CO(NH_2)_2$	15.09	1	4.48	22	2.91	6	2.00	3	1.613	2
	13.27	2	4.32	4	2.87	10	1.976	7	1.577	2
	11.30	5	4.19	2	2.79	13	1.951	5	1.569	2
	11.02	6	4.12	3	2.66	4	1.935	2	1.542	2
	10.24	2	3.96	100	2.62	45	1.914	4	1.525	1
	9.26	1	3.83	57	2.50	26	1.890	1	1.511	3
	8.68	2	3.73	4	2.42	1	1.868	3	1.460	2
	7.69	16	3.65	6	2.39	3	1.819	9	1.454	2
	6.94	42	3.56	43	2.37	5	1.797	1	1.439	1
	6.24	2	3.47	6	2.30	9	1.769	1	1.421	1
	6.12	2	3.39	2	2.25	2	1.754	1	1.402	1
	5.95	1	3.32	1	2.21	6	1.741	2	1.378	1
	5.83	1	3.25	1	2.19	3	1.708	3	1.326	1
	5.66	5	3.20	2	2.15	1	1.696	3	1.321	2
	5.20	2	3.14	2	2.09	4	1.675	4		
	5.06	2	3.05	11	2.08	5	1.654	2		
	4.97	2	3.00	3	2.04	2	1.632	1		

4. Conclusions

For the first time, various ligand coordination compounds of barium and strontium nitrates with formamide and carbamide have been synthesized. The composition, individuality, and coordination methods of ligands and nicotinic fragments have been established. The coordination nodes of complex compounds are formed with the participation of nitrate groups and have the configuration of a distorted octahedron. The research results can serve as reference data for researchers and students.

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