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Study of the cobalt structure with nicotinamide

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Abstract

Conducted research on the chemical structure of cobalt crystals with nicotinamide (Coamide). Studies have been carried out on the study of crystallographic parameters, IR spectra and thermoanalytical parameters of the crystals obtained. In the course of the research it was revealed that, according to the schematic structure, coamide is a dimeric complex with an acidoligand in the internal environment.

Keywords: Coamide, crystals of cobalt with nicotinamide, crystallographic parametrs, IR spectr.

INTRODUCTION

Nowadays the native pharmaceutical industry directed mainly to the production of the medicinal preparations-generics, and introduction of the new original preparations into the manufacture requires high costs. However, synthesis, study of structure and biological activity of new chemical compounds similar by structure with known analogues with determined biological activity appeared to be one of actual and low costs in the world pharmacy.

The chemical substances, developed on the basis of the coordinative links between metal and organic ligand, have, as a rule, high biological activity with wide spectrum of therapeutic effect. In the list of these preparation there may be noted such drug compounds as cyanocobalamin, coamide, cobalt-30 and others. It is necessary to remember that in the last time in Tashkent Pharmaceutical Institute there was established school under the leadership of professor Asisov M.A. in the area of synthesis and study of biological characteristics of new coordinative substances of 3 metals with organic compounds[1].In the Introduction to the first issue of this monograph academician A.A.Grinberg said that the structure of some obtained bioactive compounds requires additional physical-chemical background. The modern instrumental supplementation of the pharmaceutical science allows more careful study of chemical structure of the previously synthesized complexes and etermination of the relationships between composition-structure-properties with purpose of modeling of their biological active centers.

Analysis of the foreign literature resources showed a number of researches on study of structure of chemical connections of cobalt with nicotinamide (NA), isonicotinamide [2].It was shown that the structure consists of cations$[Co(NA)2_{2(}H_2O)_4]^{-2+}$anions Cl^- , and in case [3] cations $[Co(NA)2_{2(}H_2O)_4]^{-2+}$ anions CH_3COO^-.
This article is devoted to the study of the structure of cobalt with nicotinamide.

MATERIALS AND METHODS

The cobalt crystals with nicotinamide from water solution of cobalt nitrate complex with nicotinamide were obtained at the room temperature. Crystallographic parameters of monocrystals were obtained and specified on the CCD-difractometer “Xcalibur Oxford Diffraction” (CuKά-irradiation, graphitic monochromator, in room temperature): triclinic crystals, pr.gr. P-1, $C_{44}H_{60}O_6N_2$, a=7.030(3) Å, b=8.380(4) Å, c=10.248(4) (14) Å, α=100.06(4)°, β=108.23(4)°, γ=95.70(4)°, V=556.9(5) $Å^3$, Z=2, $D_{выч.}$=1.596 г/см^3. The strategy of the collection of the experimental data was performed with use of program CrysAlisPro.

Integral intensities were measured with method of ω-scanning, monochromotised reflection from graphitic crystal. After data averaging of equivalent and removal

of week reflexions from 1,2σ(I) there was obtained working massive, containing of 397 reflexions. Adjustment for absorption was performed with method “multi-scan“ , in the package of program CrysAlisPro [4].The structure was decoded with direct method with use of complex of programs SHELXS-97 [5] and was corrected with full matrix method of the least squares [5].All non-hydrogen atoms were anisotropic précised. Oxygen atoms were obtained from the various synthesis and were précised isotropic. The final value of R-factor: R=0,163, (wR2=0.3855). Building of the molecular graphics was performed with program XP in the packet of programs SHELXTL-Plus [6].

The IK-spectra of the sample $[Co(NA)_2(H_2O)_4](NO_3)_2$ were photographed with use of IK-Furiye spectrometer IRTracer-100 in the complex with attachment of single-pulse exposure NPVO with prism diamond/ZnSeMIRacle 10 in scanning diapasone:4000-600cm-1. It should be noted that interpretation of the analogous contents of IK spectra of the complex was made with comparatively known preparation of cobalt-coamide.

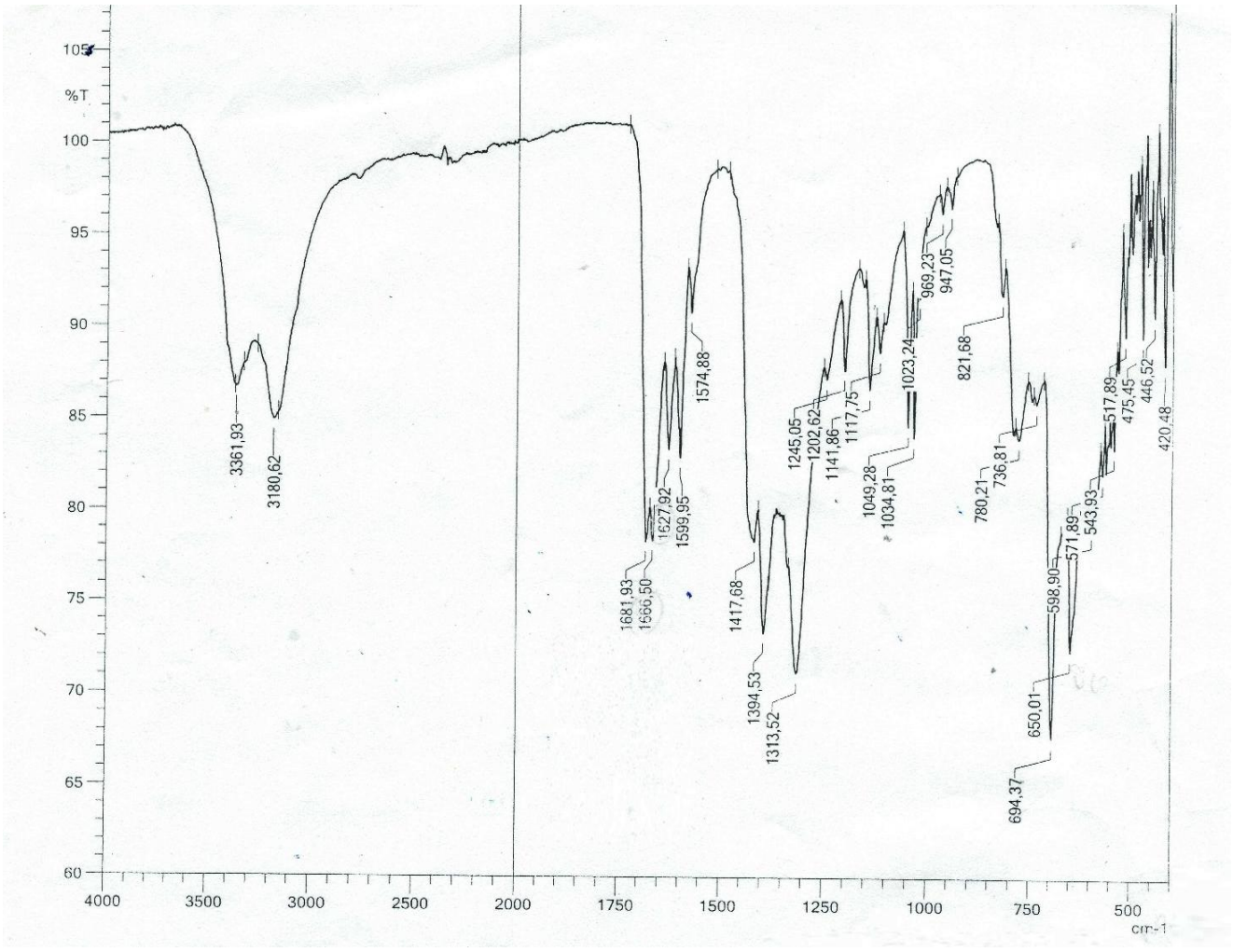

Figure 1: IK-spectra of the sample$[Co(NA)_2(H_2O)_4](NO_3)_2$

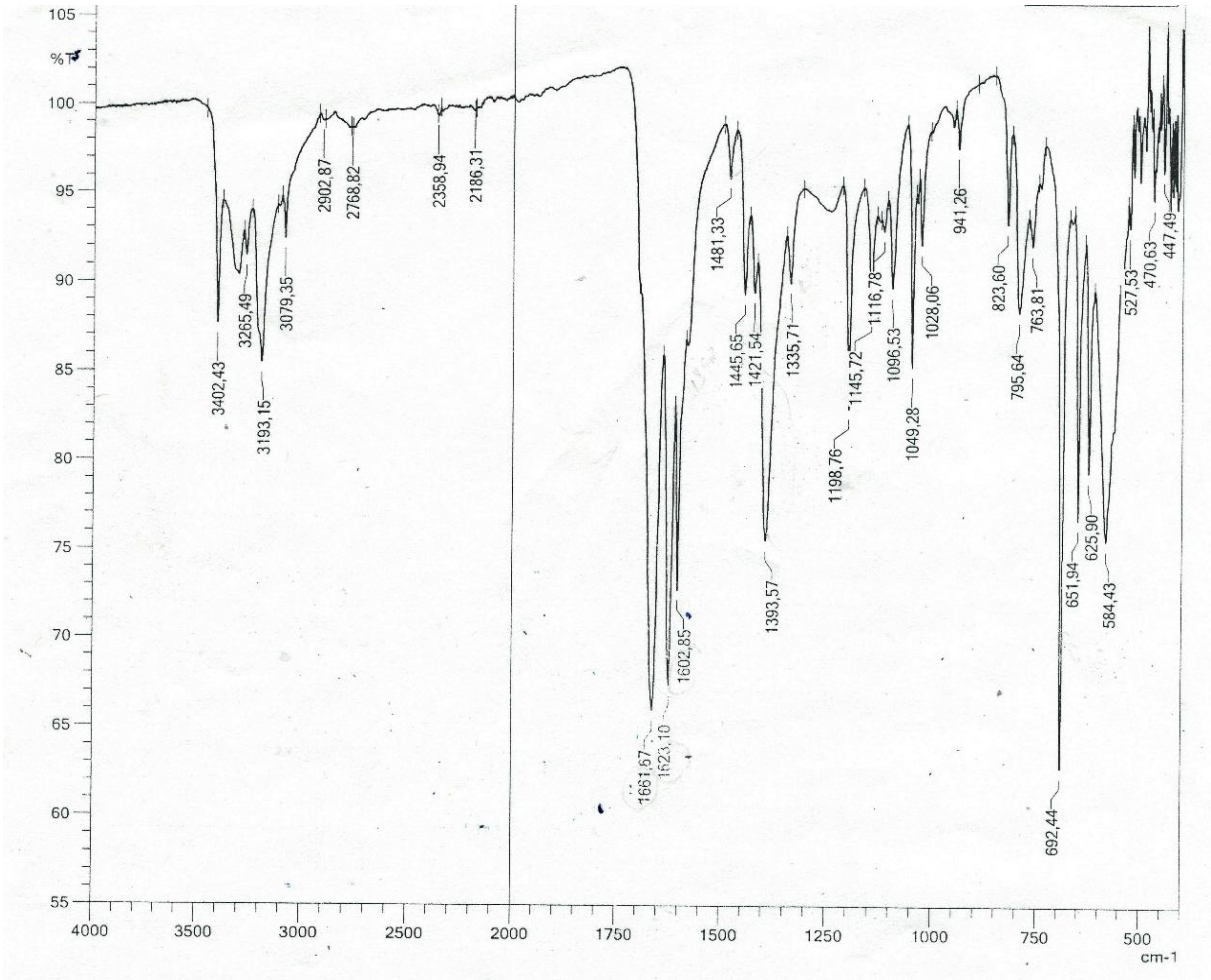

Figure 2: I-K-spectra of coamide.

Thermoanalytical investigations of the samples presented was performed on the device Netzsch Simultaneous Analyzer STA 409 PG (Germany), with thermopare of K-type (Low RG Silver) and aluminium crucibles. All measurements were performed in the inert nitrogenic atmosphere with velocity of nitrogen flow 50 ml/min. temperature diapason of measures was 25-300˚C, heating velocity was 5K/min. The quantity of the sample for one measurement was 5-10 mg. The Measurement system was calibrate with standard kit of substances KNO3, In, Bi, Sn Zn.

DISCUSSION OF THE RESULTS

The comparative analysis of the IK-spectrum of nitrogen and chloride acidocomplexes of cobalts with nicotinamide showed that the strips of valent fluctuations γ (Co) of complexes Co $(NO_3)_2$ and $CoCL_2$ were observed, respectively, also practically in 650 and 651 cm-1 (Fig.1.2), the frequencies of the fantail fluctuations C-C-H links in the pyridine ring of nicotinamide were observed in the nitrocomplex in 1142 cm-1, and in chloride complex in 1145 cm-1 [7]. The strips γ of ring are found in 1599 and 1597 -1, respectively. In the spectra the differential properties appeared in the middle IK area, that is , in the nitrate complex there were noted relatively intensive strips in 1599 and 1417 cm-1, which are characteristic for γas and γs.

Thus, the results of comparative analysis of IK-spectra of absorption with the most probability indicate about identity of coordinative ability of the nicotinamide molecules to the cobalt atom in the complexes.

Reconstructive analysis showed that crystals of the complex were built from discrete ions: of cations $[Co(NA)_2(H_2O)_4]^{2+}$ nitrate NO3 anions, as well as water molecules. Coordinational polyhedron of Co2+ ion is almost ideal octaedr N2O4, formed from 4 atoms of water oxygen in the equatorial and 2 atoms of cyclic nitrogen of the nicotinamide molecule in the axial positions (Fig.3) . Ions Co2+ were localized in the crystallographic centers of symmetry, independent part of the elementary cell consists of 0,5 ion of cobalt and one molecule of nicotinamide, two coordinationally connected water molecules and one unbound water molecule. In the complex

the lengths of equatorial links Co-O5 and Co-O6 account for 2.11(2), 2.12(2) A, respectively, the length of axial link Co-N1 was 2.13(2) A. Valence angles of cobalt ion are close to the ideal, which values were 90±1˚ for equatorial positions, 180±1˚ for axial. The rest values of the link lengths and valence angles in the nicotinamide molecule and nitrate ions were closed to the standard values.

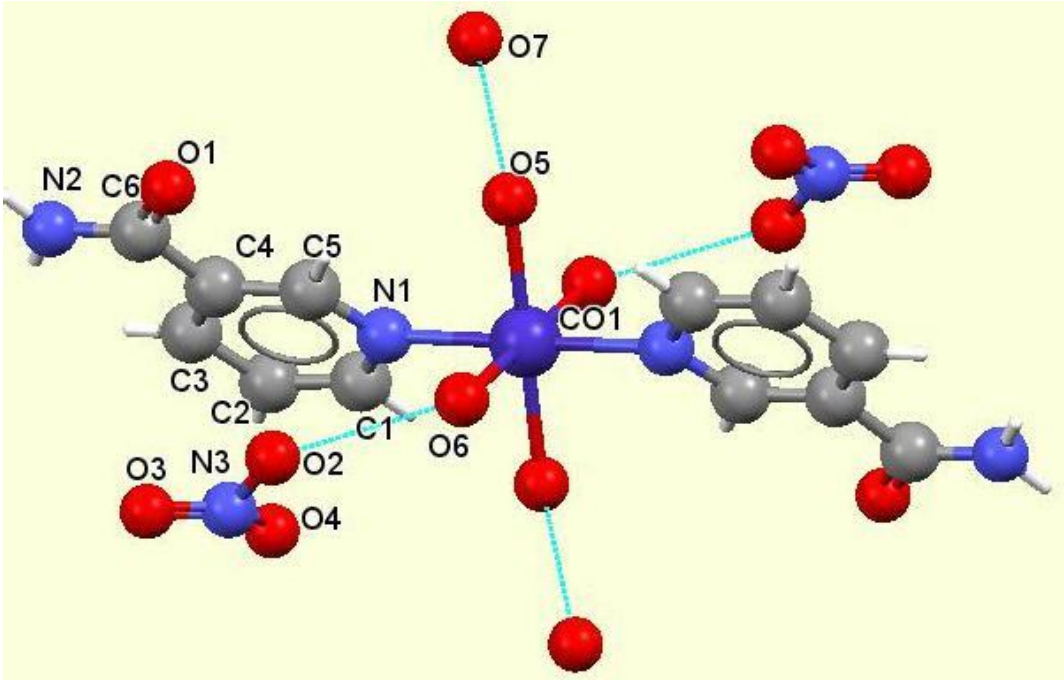

Figure 3: Molecular structure of the complex with numbering of non-hydrogenous atoms

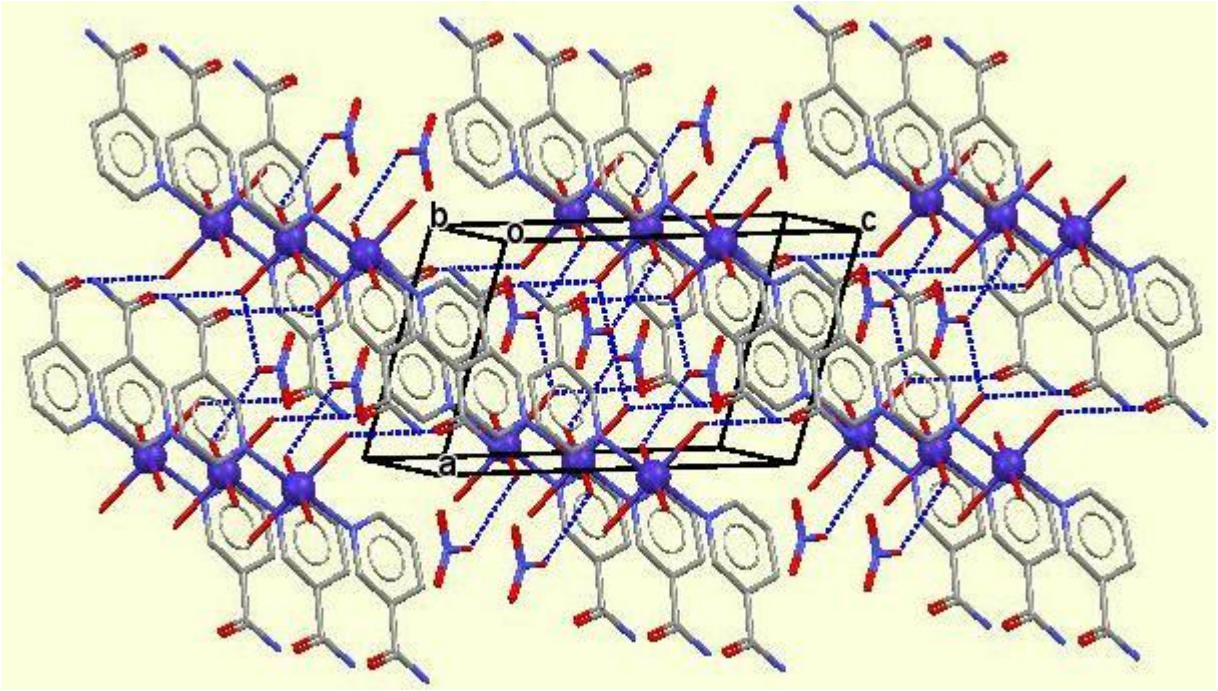

Figure 4: The complex crystalline structure

Crystal structure (Fig.4) is characterized by three-sized kit of hydrogen links between ions $[Co(NA)_2(H_2O)_4]^{2+}NO_3^-$, also unbound water molecules: every anion nitrate connected with two molecules of crystall water and one molecule of coordinationally connected water, molecule of the crystal water connected with molecules of nicotinamide. This is confirmed also by the results of the thermoanalytical researches. Besides, there were observed H-links between molecules of nicotinamide.

Thus, on the basis of the results obtained from investigations the correction may be introduced into the scheme of coamide building shown in the monograph [1]as dimmer complex with acidoligand in the internal medium.

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