

- A 29 **Aktuelle Themen im Kontext der Entwicklung der modernen Wissenschaften:** der Sammlung wissenschaftlicher Arbeiten «ΛΟΓΟΣ» zu den Materialien der internationalen wissenschaftlich-praktischen Konferenz, Dresden, 23 Januar, 2019. Dresden : NGO «Europäische Wissenschaftsplattform», 2019. B. 9. 120 s.

ISBN 978-617-7171-80-4

Es werden Thesen von Berichten und Artikeln von Teilnehmern der internationalen wissenschaftlich-praktischen Konferenz «Aktuelle Themen im Kontext der Entwicklung der modernen Wissenschaften», am 23 Januar 2019 in Dresden vorgestellt.

Die Sammlung richtet sich an Studierende, Doktoranden, Bewerber, junge Berufstätige, Lehrer, Forscher und andere interessierte Personen sowie an ein breites Spektrum von Lesern.

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UDC 001 (08)

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ISBN 978-617-7171-80-4

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## **ABSCHNITT 21. CHEMISCHE WISSENSCHAFTEN**

### **A STUDY OF COMPLEX ALUMINUM-PHOSPHATES CATALYSTS BY METHOD OF INFRARED SPECTROSCOPY**

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The problem of finding new highly selective and active catalysts components converting natural gas into valuable products remains relevant and On Today. Development of the same criteria of scientific selection catalysts requires careful study of their physical and chemical properties.

The purpose of this study was to synthesize new complex catalytic systems based on nickel and manganese phosphate and explore their physical and chemical properties. Manganese nickel phosphat complex catalysts prepared by co-precipitation of the corresponding nitrate salts according to techniques [1].

Physico-chemical properties of samples were studied using XRD, DTA, IR-spectroscopic and chemical analysis methods. Defined surface acidity and distribution of active sites on it.

Found that the resulting series Manganese nickel phosphat catalysts in which nickel phosphate content varies from 0.5 to 99.5 wt. % Has high thermal and chemical stability.

IR spectra of the studied air-dry phosphate catalysts characterized by intense absorption in the region stretching ( $3460\text{--}3020\text{ cm}^{-1}$ ) and deformation ( $2360\text{--}1400\text{ cm}^{-1}$ ) vibrations of OH groups of molecules water. Valence and deformation vibrations of phosphate ion most evident in products of dehydration as distinct bands  $1110\text{--}350\text{ cm}^{-1}$ .

Typical symptoms of hydrogen bond in the vibrational spectra of water is low frequency slider, increasing intensity and expansion strip stretching vibration O-groups. These changes in the spectrum of water serve as a special criterion for participation in the formation of molecular hydrogen bond. The presence of five absorption bands ( $3460, 3230, 3050, 1640$  and  $1440\text{ cm}^{-1}$ ) show that water molecules, which are part of the original solid phase, energetically unequal [2-4]. We can assume the existence of structures in the data samples of three types of molecules hydrate water, which are characterized by different energies of the

hydrogen bond [5]. Hydrogen bond really affect the state of water in crystalline, in as much hard to find anhydrite in which water molecules would not take part in the formation of hydrogen bonds or salt anion, or from water molecules. Participation in the formation of hydrogen bond with the anion leads to reduction of O–H constant communication polarizing effect on the water are also making cations.

During heat treatment there is a gradual decrease in the intensity of the absorption bands in the valence and deformation vibrations of water molecules, even before their disappearance in products treating, calcining catalysts above  $T=973$  K leads to dehydration and the emergence of full spectrum typical phosphate anhydrous.

The complex nature of spectrum and the presence of several absorption maxima relating to degenerate valence orthophosphate vibrations caused by apparently twisting structure tetraedr by strong hydrogen bonds. Complications range of phosphate ion associated with the distortion of the tetrahedron in real crystals and lowering of symmetry may be due to one of the following reasons: low-symmetry environment; disturbance phosphate ion by water molecules forming the intermolecular hydrogen bonds; coordination phosphate ion with cations  $Al^{3+}$ . The energy of hydrogen bonds formed between water molecules and anion salt increases with increasing proton-acceptor ability and anion ion  $RO_4^{3-}$  is  $\sim 37.6$  kJ/mol.

Thus, orthophosphate tetrahedral anion has considerable proton-acceptor ability, and hydrated phosphates may form quite strong hydrogen bonds, especially in the presence of hydrate structure coordinated water molecules because the interaction of cations and anions can mutually reinforce each other.

A large quantity of splitting frequencies degenerate types of vibration and high intensity bands forbidden by symmetry oxy anion can serve as an indication of the formation of coordination bonds, as deviations from the ideal geometry ligand field coordinated central atom must be greater than for non-directional crystal field or hydrogen-bredge binding.

It is possible also that a significant expansion and absorption bands  $\nu_3$  та  $\nu_4$   $PO_4^{3-}$  ions can be explained as a consequence of the manifestation of adsorbed hydrogen bonds between water molecules and oxygen ions attacks.

Based on the data obtained can be assumed that the introduction of the alumina phosphorus ions formed surface structures that have different structure from other systems. This is confirmed by the results of the DTA and the Differential gravimetric analysis spectra. The formation of such surface structures in complex oxides increases the acidity of the surface and changing the catalytic activity.

Based on infrared spectroscopic analysis using quantum-mechanical method of Sokolov we calculated the energy of hydrogen bonds EH-called coordinated between the hydrogen atoms of water molecules and oxygen atoms of phosphate groups In the IR spectra of air-dried samples synthesized phosphates there is a clear long-wave shift of  $\nu(OH)$ . This picture shows, according to [4], the implementation of a hydrogen bond. Obviously this character changes the energy of the hydrogen bond in this series due to several factors: a decrease in the

strength of OH, and thus the long-wave shift of the absorption bands stretching vibration coordinated water molecules, called as the formation of coordination bonds  $\text{Me}^{n+} \leftarrow \text{O} < \begin{array}{c} \text{H} \\ | \\ \text{H} \end{array}$ , and hydrogen bond  $-\text{O}-\text{H} \dots \text{O}=\text{P}=\text{O}$ . Moreover, the formation of both types of communication leads to qualitatively the same direction shift  $\nu(\text{OH})$  of the absorption bands. The emergence in the infrared spectra of doublet located in the  $3000\text{--}3600\text{ cm}^{-1}$  may be an indication that the coordinated central atom of transition metal water molecules form two unequal laden with hydrogen bonds. From a quantitative point of view of energy these relationships are also different. In particular, the energy of one type of H-bond within  $30,37\text{--}31,63\text{ kJ/mol}$  communication, and the second – in the range  $38,54\text{--}40,89\text{ kJ/mol}$  to connection. This indicates the presence of certain structural differences in the structure studied polyhedra [6].

Thus, our IR studies of synthesized catalyst have shown that the spectra of synthesized catalysts identified bands, the occurrence of which is  $\nu(\text{OH} \dots \text{O})$  and  $\delta(\text{HOH})$  groups associated with water, which is manifested in the form (HOH) groups. One can assume that the presence of these groups leads to higher catalytic activity of catalyst K-6 compared with individual crystal structures phosphate obtained at  $T=1173\text{ K}$  binary complex phosphates obtained under mild conditions and fried only  $T=973\text{ K}$  are higher acidity of the surface due to interaction of water with the said active centers and the formation of acid Brensted centers [7, 8].

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