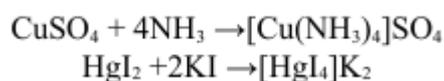


The complex in biological systems

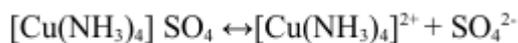
Plan

1. Definition of complex compounds. Werner's theory.
2. Basic concepts: complexing ligands, coordination number capacity. Geometry coordination complex ion.
3. Nomenclature.
4. The nature of the chemical bond.
5. Isomerism, stability, classification.
6. Iron, cobalt - mild bio-complexity and zinc compounds.
7. Complex ions as antidotes.
8. The concept of homeostasis metal-ligand.

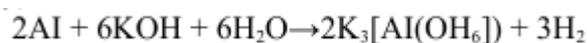
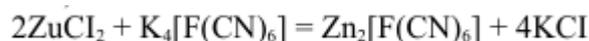
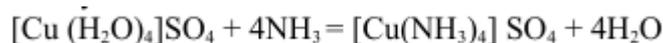
1. Oxides, salts, acids are formed from atoms by or chemical bond between them, are those of the first order. However, there are substances that are formed as a result of the connection between the neutral molecules without binding the emergence of new electronic pairs.



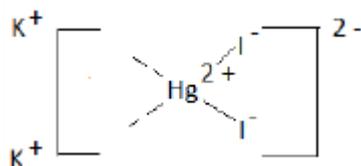
This molecule dissociates the highest order and they



Molecular compounds formed ion complex capable existence as a solution and in crystals - called complex. Complex compounds obtained by reactions, replacement, exchange and oxidation - reduction.



To explain why is joining some simple molecules others, Werner introduced the concept of main and side valence.



By joining two main valence ions and by side - two and formed ion complex which is not dissociated.

2. Basics of coordination theory of Werner (1893).



The centerpiece of the complex compound takes complexing - positively charged ion (usually a metal d elements)

2. Around complexing ligands are (adenty), is ions of opposite sign or neutral molecule Cl^- , CN^- , H_2O^0 ; NH_3^0 number that shows how many ligands holds complexing, called the coordination number.

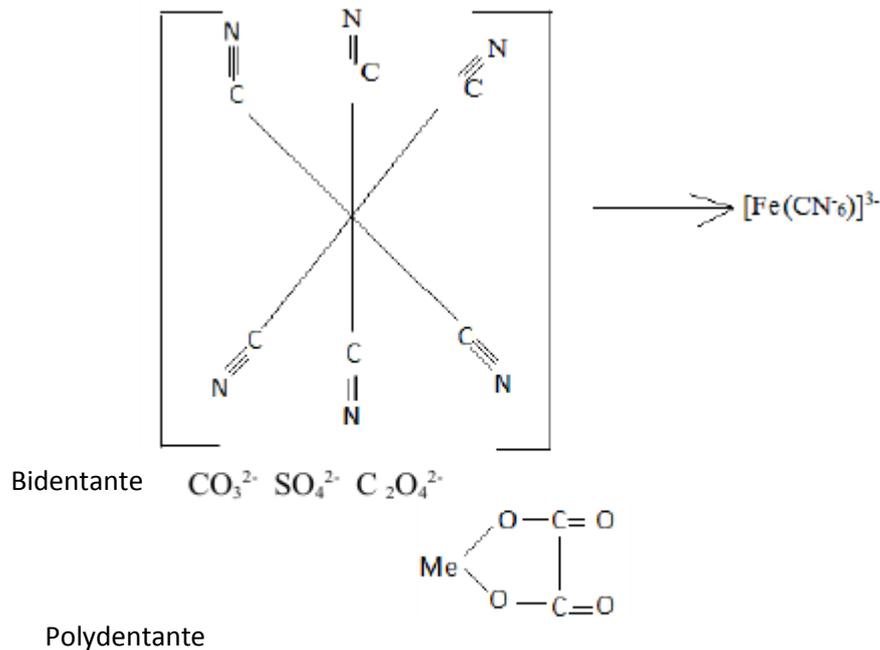
The value of coordination number depends on the nature complexing Fe^{2+}

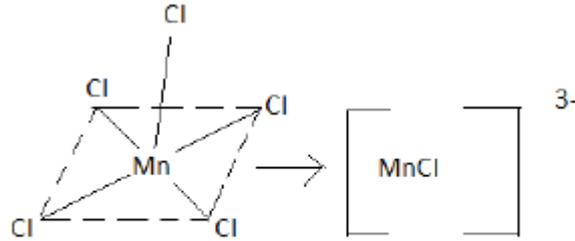
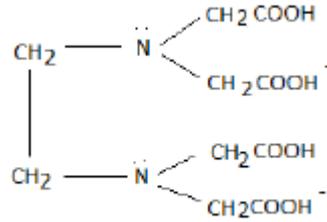


Ligand from complexing forms the inner sphere complex compound. Ions that are not included in the domestic sphere, form outer sphere. The charge computer. Jonah determined by simple algebraic amounts of charges ions it contains.

A significant contribution to the development of the theory of coordination made Chuhayev, Kurnikov, Yatsymirskyy.

An important feature of the ligands is their capacity or coordination denticity, which is determined by the number of places that occupy ligands internal coordination sphere of the complex. There monodentate ligands F^- Cl^- NH_3 H_2O CN^-





a square pyramid

Outdoor areas more ions are ions of alkali and alkaline – Land metals. The compounds have outdoor areas. Nomenclature cationic complex: In the first coordination sphere called ligands - acid anions, then ligands are neutral molecules on the central atom. Coordinated ligands - acid anions kept its name attached to the end of "O" fluoro, sulfo carbonate. OH - hydroxyl. H - Hydride. O- Oxo. Ligands - neutral molecules retain their usual name

$C_2H_5NH_2$ - ethylamine

N_2H_4 - hydrazine

But ammonia - amine, aqua water. If several identical ligands - two, three, four names of neutral molecules followed by the name of complexing. The central atom retains Ukrainian name and oxidation Roman indicated in parentheses.

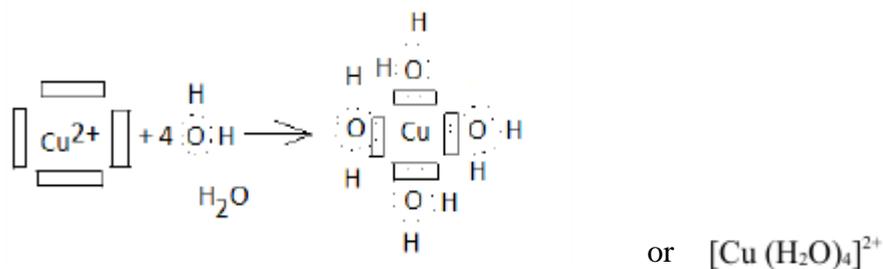
$[Ag(NH_3)_2]Cl$ - diamino silver (I) chloride.

The name of the complex compound complex ion - anion is as follows: first in the nominative case record title complex, anion and more in the genitive case - out spherical cation. The title complex. Anion first name listed ligand, then – title complexing with the end of BP and its degree of oxidation. Title cation and anion record separately $K_3[Co(NO_2)_6]$ – hexanitrocobalt (III) potassium. Nature Communications. The underlying idea of quantum mechanics. Now using three theories:

- Valence bond theory;
- Crystal field theory;
- The method of molecular orbit lei.

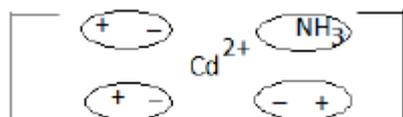
Valence bond theory in the basic assumption that the chemical bonds always have two electronic communication.

Only computer compounds increasing role played by the donor – acceptor indivisible interaction of electron pairs and free ligand orbit lei complexing. The mechanism is called a donor - acceptor. This covalent bond is called coordination bond.



Here two electrons cloud of oxygen atoms of copper ion donor is accepted (Acceptor) and becomes universal.

The advantage of this method is surveillance, but not always two electrons ties, explains the optical properties of the absorption spectrum. So find more use of crystal field theory, which provides the relationships between ligands and complexing ion or ion - dipole, which arise due to electrostatic attraction.

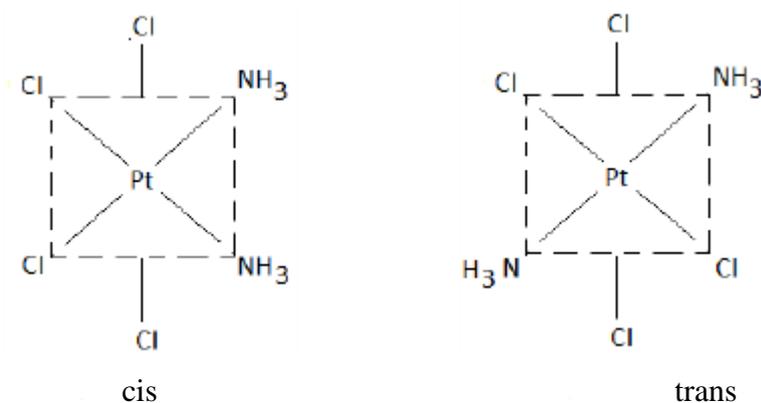


The method of molecular orbit lei considers as one of taking into account the structure and complexing ligands.

The properties of complex mathematical result set settlement systems, which consist of nuclei and electrons. Electrons located on binding and loosening orbit poses can. Method approximations calculation for simple molecules. In simple cases establishing qualitative side of the issue are three theories.

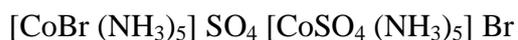
5. Isomerism: distinguish the geometric hydration, ionization, optical, coordination, communication and others isomerism.

Geometric - cis - trans isomers due to various provisions ligands relative to each other $[\text{Pt}(\text{NH}_3)_2\text{Cl}_2]$



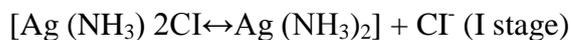
Hydrogen isomers due to uneven distribution of water molecules between internal and external areas of the computer compounds. $[\text{Cr}(\text{H}_2\text{O})_6]\text{Cl}_3$ $[\text{CrCl}_2(\text{H}_2\text{O})_4]\text{Cl} \cdot 2\text{H}_2\text{O}$

Ionization isomers - unequal location acid residues ions between inner and outer worlds.



The stability of complex compounds:

When dissociation:



It takes a minor degree. The constant instability

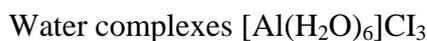
$$K_{\text{неуст}} = \frac{[\text{Ag}^+] \cdot [\text{NH}_3]^2}{[\text{Ag}(\text{NH}_3)_2]^+} = 6,8 \cdot 10^{-8}$$

$$K_{\text{ст}} = \frac{1}{K_{\text{неуст}}} = \frac{[\text{Ag}(\text{NH}_3)_2]^+}{[\text{Ag}^+] \cdot [\text{NH}_3]^2} = \frac{1}{6,8 \cdot 10^{-8}}$$

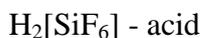
The higher stability constant, the greater the resistance complex compounds. On impact resistance sets ligand nature, the nature of metals. Alkaline metals <alkaline earth <Mg²⁺ <transition metals.

Classification

- By nature, ligands:



- By belonging to acids, bases, salts

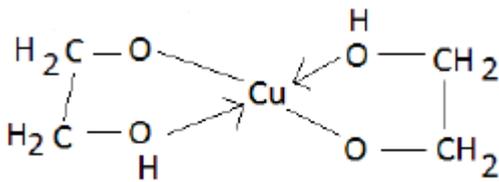
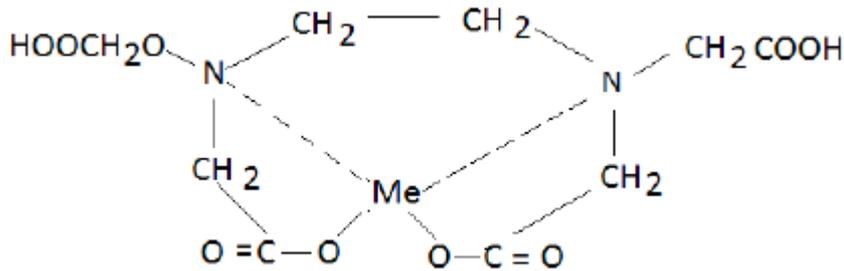
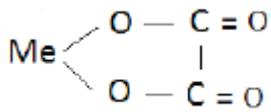


OH - bridged group

Compounds in which metal atom is placed between two organic molecules cyclic structure called sandwich complexes.

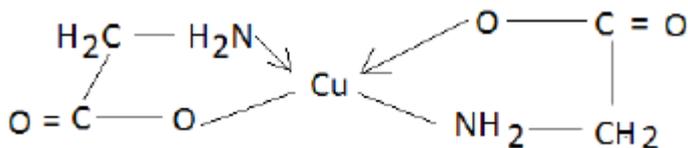
A special type of computer compounds is clathrates (inclusion compounds). They are formed by the inclusion of some molecules (guests) in oral lattice other (host). Especially important biological importance is ionofoms - natural compounds which are capable of form complexes with cations of alkali and alkaline earth metals. They are built from amino acid residues that can carry through membrane. Cryptands – macrocyclic ligands, which form chelate compounds with metal cations.

- Cyclical or chelates

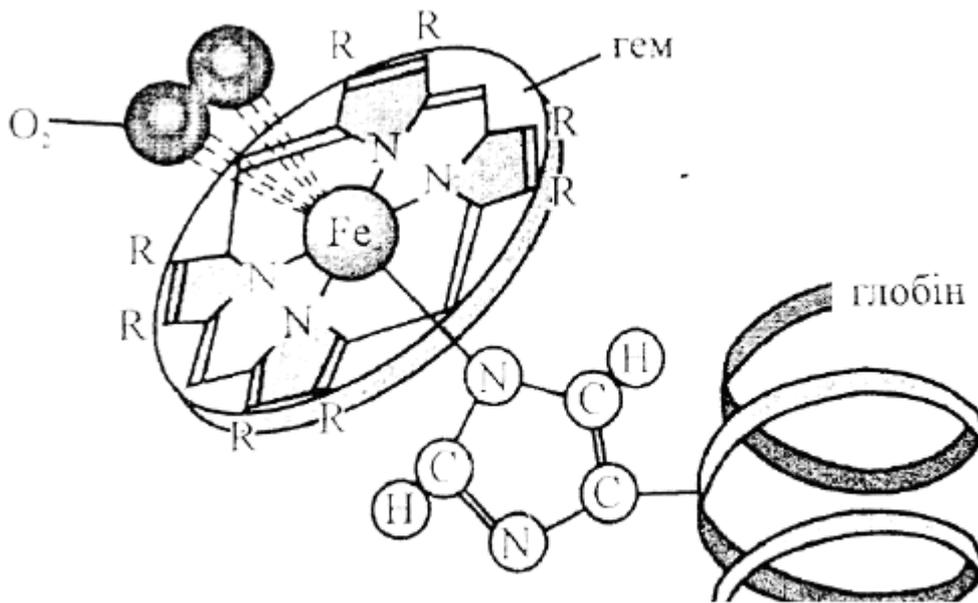
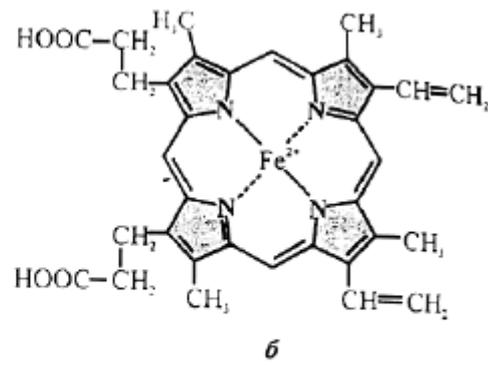
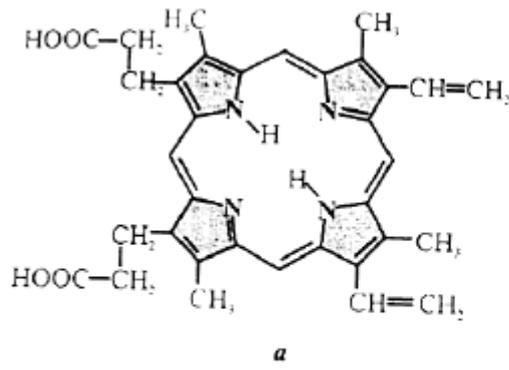
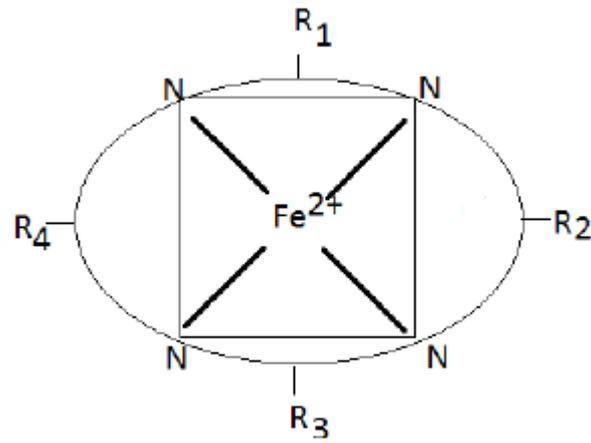


Ethylenicolyat copper (II) Qualitative reaction on polyhydric alcohol.

Prominent among in the middle of the complex take chelate compounds in which the central atom is part of the cycle. Complexes of this type characteristic of amino acids. Amino acetic acid forms a chelate complexes such structure:

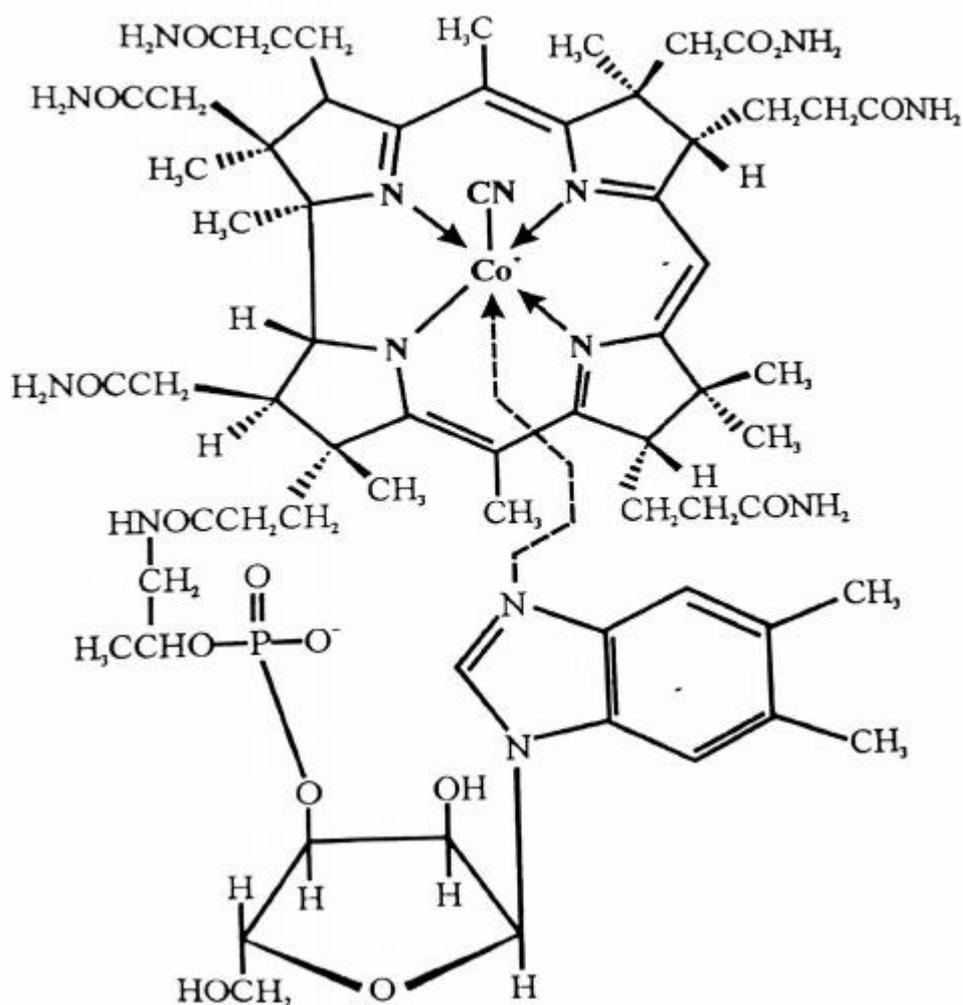


Ligands of this type are called COMPLEXONES complexation (using in analytical chemistry). Most of the chemical elements contained in the organs and tissues form complex compounds with proteins and other biopolymers. It proteins, amino acids, nucleic acids, peptides, fatty acids, carbohydrates, vitamins, hormones, enzymes. Complexing ability can explain biolihandiv the presence in their molecules of several functional groups - COOH, NH₂ - nitrogen primary, secondary are able to coordinate ions metals. Examples include porphyrin system. It etradentate macromolecule. Schematically, are as follows:



Nitrogen atoms are located on the corners of the square, hard coordinated in space, which means the same type carbon arc chains that connect donor nitrogen atoms in a vicious cycle. R – Various radicals. Therefore, porphyrins form stable complex compounds with metal. Thus, as the central atom can act Mg^{2+} Fe^{2+} form active center of chlorophyll, hemoglobin. The protein molecule of 400 globin polypeptide chains forms. Each one is connected heme. In the iron atoms 6 coordination bonds. 4 Hold it in plane of the porphyrin core and 2 are directed perpendicular to this plane. One of them is the relationship with oxygen. 10,000 atoms form hemoglobin $S3082O870N760S8Fe4$. There are other BIOCOMPLEXES metals (Cu, Al, Si, Mn). Some invention used in medical practice as medical drugs.

Feramid - a complex of ferric chloride with the amide of nicotinic acid $[Fe(C_6H_5CONH_2)]Cl_2$ Cobalt complex is part of vitamin B12, which plays an important role in the development and formation of red blood cells, its shortage leads to pernicious anemia.



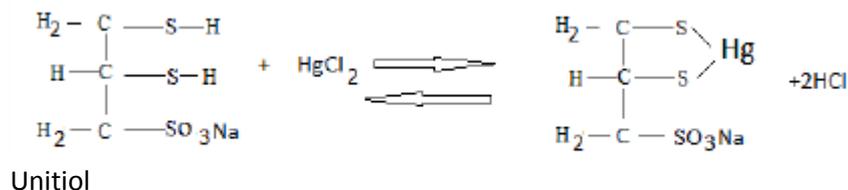
Integrated zinc compounds used in dermatology as antibiotics and iron carbonyls (ferrosteron) belongs to

Ferrum deficit drugs for the treatment of anemia. The purpose lokompleksni gem properties manifested by the action of toxic substances like CO (carbon monoxide) and HCN - cyanides, salts of hydrocyanic acid. When inhaled CO ratified metal-compound - carbonyl hemoglobin $NbSO_4$ constants the stability of which 200 times more than NbO_2 . As a result of access to oxygen of decreases appear signs of hypoxia.

A similar mechanism of cyanide, but their toxicity is higher. High toxicity due to a large resistance due $\text{Fe} = \text{CN}^-$, which causes more stability cyanide. The toxicity of copper due that copper ions interact with thiol - SH groups (binding) and amino - NH_2 (blocking) proteins.

Toxic effects due to silver compounds that interact with silver ions thiol sulfur and nitrogen containing proteins (nucleic acids).

Similarly, compounds are gold. Toxicity increases with atomic number. Property ions Metal ratified strong ties with sulfur ligands used in the selection of drugs that are used in poisoning. These drugs are called - antidotes. Thus, using unithiol which is composed of sulfhydryl groups



Complexons used as antidotes.

Metal ligand homeostasis is a form of general homeostatic system. The body has a clear self-regulating system homeostasis, which trace elements play a role in the compounds of bio ligand. Their level blood, tissue homeostasis is maintained regulatory mechanisms: the processes of absorption, secretions, water, and electrolytes non-electrolytes, stability constant chelates. Poor absorption heavy metal is the result of the formation of soluble complexes.

Often abnormal digestive processes are the cause of abuse homeostasis. There are many ways of regulation of homeostasis metal ligands. So, for Cu, Co, Fe, Zn- main way is to change the level of adsorption of cadmium and iodine urinary excretion of metal complexes.

Hazardous substances are excreted through bio ligands that bind them in complexes (chelation therapy).

Many chemical elements with positive impact on bio ligand immunogenesis (Protective reaction), increase the formation of antitoxins. Trilon B is use in complexometry. For Yatsymirskyy words "complexing is organized life."