NATIONAL UNIVERSITY OF DISTANCE EDUCATION

Compuestos Inorgánicos de Estructura Compleja

Idioma: EN

EXAM STATEMENT:

No general instructions specified in the form, but there are 5 questions in the exam.

Question 1: Structure and bonding of silicates

Question 2: What is a borane? Classification of boranes

Question 3: Give examples of the use of inorganic heterocycles in the synthesis of the corresponding polymers

Question 4: Crystalline defects

Question 5: Explain the polymerization of vanadates, VO43- as a function of concentration and pH

Question 1

Structure and bonding of silicates

STUDENT RESPONSE:

Silicates are the most abundant group of minerals in the Earth’s crust and are characterized by the presence of the silicate tetrahedron (SiO4)4- as the fundamental building block. This tetrahedron consists of one silicon atom covalently bonded to four oxygen atoms in a tetrahedral arrangement. The silicon atom possesses sp3 hybridization, and the oxygen atoms are arranged in a manner that maximizes electrostatic interactions with the positively charged silicon atoms of neighboring tetrahedra.

The bonding in silicates is primarily covalent, arising from the strong Si-O bonds. However, significant ionic character is also present due to the charge imbalance within the silicate tetrahedron. The overall charge of the silicate framework is neutral, achieved through a complex network of interconnected tetrahedra.

Silicates are classified based on their structural arrangement:

* **Nesosilicates:** Individual tetrahedra are linked through cations (e.g., Mg2+, Fe2+), forming a framework structure. Examples include olivine and garnet.

* **Sorosilicates:** Two tetrahedra share an oxygen atom, forming a double tetrahedron (Si2O7)6- structure. Examples include epidote.

* **Cyclosilicates:** Tetrahedra are linked in rings. Examples include beryl and tourmaline.

* **Inosilicates:** Chains or sheets of tetrahedra are formed. Chains can be single-chain (e.g., pyroxene) or double-chain (e.g., amphibole). Sheets can be two-dimensional (e.g., mica) or three-dimensional (e.g., serpentine).

* **Phyllosilicates:** Tetrahedra are linked in sheets, resulting in a layered structure with weak Van der Waals forces between the layers. Examples include micas and talc.

* **Tectosilicates:** Individual tetrahedra are not linked, but rather arranged in a three-dimensional network. Examples include quartz and feldspar.

The type of silicate structure significantly influences the physical properties of the mineral, such as hardness, cleavage, and density.

Question 2

What is a borane? Classification of boranes

STUDENT RESPONSE:

A borane is a chemical compound containing a boron atom bonded to three or more other atoms, typically hydrogen. The general formula is BH3n, where n ≥ 3. Boranes are Lewis acids due to the electron deficiency of boron.

Boranes are classified into several categories based on their structure and bonding:

* **Isolated Boranes:** These consist of a single boron atom bonded to three hydrogen atoms. Examples include BH3, B2H6, and HD.

* **Terminal Boranes:** These have a hydrogen atom directly bonded to the boron atom. They are generally more acidic than internal boranes. Examples include BH3 and B2H6.

* **Internal Boranes:** These have hydrogen atoms bonded to other boron atoms. Examples include B2H6, Mc2B6H12, and HB(CN)6.

* **Polyborenes:** These are cyclic or polymeric boranes containing multiple boron and hydrogen atoms. Examples include BxHy.

* **Boron Clusters:** These are aggregates of boron atoms held together by covalent bonds. Examples include carboranes (e.g., β-carborane).

Question 3

Give examples of the use of inorganic heterocycles in the synthesis of the corresponding polymers

STUDENT RESPONSE:

Polifosfacenos are utilized in the synthesis of polymers. Politiazilos are employed in the creation of conducting polymers. Silicon-containing heterocycles, specifically polysiloxanes and polysilanes, serve as monomers for the production of silicone polymers. These heterocycles contribute specific properties to the resulting polymers, such as thermal stability, flexibility, and conductivity, depending on the specific structure and polymerization method.

Question 4

Crystalline defects

STUDENT RESPONSE:

Crystalline defects are deviations from the perfect periodicity of a crystalline lattice. They can be classified into two main categories: point defects and extended defects.

Point Defects:

* Vacancy: An empty lattice site.
* Interstitial defect: An atom occupying a position not normally found in the lattice.
* Substitutional defect: An atom of a different element occupying a lattice site.
* Frenkel defect: A vacancy-interstitial pair within the same crystal.
* Schottky defect: An equal number of vacancies and interstitials in an ionic crystal.

Extended Defects:

* Dislocations: Linear defects involving a misaligned portion of the lattice.
* Edge dislocation: A line defect characterized by an increase in the density of atoms on one side of the dislocation and a decrease on the other.
* Screw dislocation: A line defect characterized by a spiral nature.
* Grain boundaries: Interfaces between differently oriented crystal grains in a polycrystalline material.
* Twin boundaries: Interfaces where the crystal structure is mirrored.
* Stacking faults: Imperfections in the stacking sequence of atomic planes.

The presence of crystalline defects significantly influences the physical and chemical properties of crystalline materials, such as their mechanical strength, electrical conductivity, and optical properties.

Question 5

Explain the polymerization of vanadates, VO43- as a function of concentration and pH

STUDENT RESPONSE:

The polymerization of vanadates, specifically VO43-, is a complex process strongly influenced by both concentration and pH. It proceeds through a series of steps, ultimately leading to the formation of polymeric structures with varying compositions and topologies.

At low vanadium concentrations and neutral pH, VO43- exists as monomeric units. As the concentration increases, polymerization initiates, forming oligomeric chains. These chains are predominantly composed of VO43- units linked through hydrogen bonding interactions between the oxygen atoms. The initial stages involve the formation of dinuclear vanadium units (VO2(VO4)2), which then aggregate to form larger oligomers.

The pH plays a crucial role in directing the polymerization pathway. At higher pH values (typically above 7), the vanadate ion undergoes hydrolysis, forming hydrated vanadium species such as V(OH)42- and V2(OH)6. These hydrated species are more reactive and facilitate the formation of polymeric chains with a greater degree of hydration. The degree of hydration significantly impacts the stability and structure of the resulting polymers.

At very high vanadium concentrations and elevated pH, the polymerization proceeds to form complex, three-dimensional networks. These networks are characterized by a highly interconnected structure and can exhibit gel-like behavior. The specific topology of the network depends on the precise conditions, including the vanadium concentration, pH, and temperature.

The resulting polymers are not static structures; they exhibit dynamic behavior due to the reversible nature of the hydrogen bonding and hydration interactions. The polymerization process is equilibrium-driven, and the composition and structure of the polymer can be tuned by adjusting the vanadium concentration and pH. Furthermore, the presence of other ions in solution can also influence the polymerization process and the final polymeric structure. The resulting polymers can range from simple linear chains to complex, branched, or network structures.