SSD: CHIM/03 Academic year: 2017/18 Faculty: Department of Chemistry Study courses: MODELS OF CHEMICAL SYSTEMS Study plans/Curricula: Chemical Sciences Second degree (1st Level Master degree) Type: Affine and Integrative activity Total Credits: 4 Didactic Methods: Lectures and exercises Language of the course: Italian Didactic Period: 1° year - 2° semester (March – June) Exam type: Written (with open questions)/Oral Professor in charge: FABIO ARNESANO

Training objectives: 1) to deepen knowledge in the field of chemistry of coordination compounds (metallic complexes, clusters, and bioinorganic systems), with models of chemical bonding and reactivity; 2) to rationalize the electronic structure, magnetic properties, and reactivity of *d*-metal complexes and biological metal sites through theoretical models and experiments; 3) to interpret the electronic spectra of *d*-metal complexes.

Prerequisites: Basic concepts of inorganic chemistry of bachelor degree

Didactic Methods: Chalk and blackboard teaching with power point presentation

Course programme

COORDINATION COMPOUNDS. The *d*-Block Elements: Periodic Properties. Coordination compounds: definition. Coordinate bond. Coordination Numbers and Geometry. Valence bond theory. Crystal-field theory (octahedral, tetrahedral, square-planar geometry). Jahn-Teller effect. Ligand-field theory. Electronic states and spectroscopic terms. Correlation diagrams. Electronic spectra and magnetic properties of metallic complexes. Luminescence. Metal-metal bonded compounds and clusters.

REACTIVITY OF COORDINATION COMPOUNDS. Labile and inert complexes. Mechanisms of ligand substitution reactions (in octahedral and square-plane complexes). Mechanisms of redox reactions. The Marcus equation. Photochemical reactions.

BIOINORGANIC CHEMISTRY. Metal ions in biological systems. Metalloproteins and Metalloenzymes (Zn, Fe, Cu, Co, Mo). Chelating agents and metal-based drugs.

Reference Texts: Peter William Atkins, Tina Overton, Jonathan Rourke, Mark Weller, Fraser Armstrong. Inorganic Chemistry (Fifth Edition), W. H. Freeman and Company - New York (2010). Handouts and lecture notes.