R O M Â N I A
MINISTERUL EDUCAȚIEI ȘI CERCETĂRII
Universitatea din Craiova
FACULTATEA DE ȘTIINȚE/ DEPARTAMENTUL DE CHIMIE
Craiova, Str. Calea București, nr. 107I
Tel/ fax: 0251597048, e-mail: chimie@ucv.ro

Subject Description

1. Program information

1.1. Institution	University of Craiova
1.2. Faculty	Science
1.3. Department	Chemistry
1.4. Study field	Chemistry
1.5. Study level	Master
1.6. Type of education	full-time
1.7. Study program	Advanced Chemistry

2. Subject information

2.1. Subject			**Assessing and modelling of inorganic species**				
2.2. Course coordinator			Prof. dr. Paul CHIRIȚĂ				
2.3. Application coordinator			Prof. dr. Paul CHIRIȚĂ				
2.4. Year of study	I	2.5. Semester	2	2.6. Type of evaluation	E	2.7. Subject type	DS/DOB

3. Total estimated tipe (hours/semester)

3.1. Number of hours per week	4	from which: 3.2 course	2	3.3. seminar/lab	2
3.4. Total hours in curriculum	56	from which: 3.5 course	28	3.6. seminar/lab	28
Time allocation – hours/week					
Study using textbooks, course materials, bibliographies, and notes					35
Additional documentation in the library, on specialized electronic platforms, and in the field					15
Preparation of seminars/labs, assignments, reports, portfolios, and essays					10
Tutoring					5
Examinations					4
Other activities.....					
3.7. Total hours of individual study					69
3.8. Total hours per semester					125
3.9. Number of ECTS					5

4. Preconditions (if the case)

4.1. of curriculum	•
4.2. of competences	•

5. Conditions (if the case)

5.1. for course	• Lecture hall equipped with computer, video projection system, and internet connection
5.2. for labs	• Laboratory equipped with the materials, equipment, and reagents necessary to carry out experimental work

6. Course objectives - expected learning outcomes achieved by completing and passing the course

Knowledge	1. Graduates define, understand, explain, and apply advanced knowledge of chemistry from specialized literature in practice. 2. Graduates select and use appropriate experimental and theoretical methodologies to investigate complex scientific problems, assessing their impact on the environment and society. 3. Graduates write analysis and scientific reports, presenting the results of their research and experiments, in line with professional ethics and standards. 4. The graduate describes and integrates interdisciplinary knowledge into the implementation of research projects.
Skills	1. Graduates apply major concepts in analytical, inorganic, organic, and physical chemistry to chemical practice. 2. Graduates evaluate and analyze experimental techniques to conduct and design experiments, analyze and test (qualitatively and quantitatively) chemical elements and substances; design, coordinate, and conduct chemical experiments. 3. Graduates apply critical thinking, following the structure and principles of scientific writing to develop and present scientific reports. 4. Graduates apply interdisciplinary methods to solve complex theoretical and practical chemical problems in their professional and research activities.
Responsibility and authonomy	1. Graduates are able to adapt major scientific concepts in the field of chemistry to conduct research, improve or develop new concepts, knowledge, theories, and operational methods, products, and services in order to apply them in specific activities for product and process quality control. 2. Graduates use classical laboratory instruments/techniques and modern equipment independently, design experiments, and interpret and analyze the obtained results accurately. They design learning situations focused on developing experimental techniques and methods specific to chemical laboratories. 3. Graduates prepare and present scientific reports in line with ethical standards for collecting and interpreting results. 4. Graduates assume responsibility for managing interdisciplinary collaborations and coordinating activities within work and research teams.

7. Table of contents

7.1. COURSE	Mode of operation	Teaching methods	Allocated time (hours)
1. General concepts related to inorganic speciation: definition of inorganic speciation, oxidation state, ligand association, physical form	On site (weeks 1-2)	Lecture, explanation and interactive presentation, heuristic conversation, problem solving	4
2. Assessment of inorganic speciation within adsorption/desorption reactions. Assessment of inorganic speciation within ion exchange reactions. Assessment of inorganic speciation within precipitation/dissolution reactions	On site (weeks 3-4)	Lecture, explanation and interactive presentation, heuristic conversation, problem solving	4
3. Assessment of inorganic speciation within acid-base reactions (proton exchange reactions). Speciation in inorganic acid-base buffer systems	On site (weeks 5-6)	Lecture, explanation and interactive presentation, heuristic conversation, problem solving	4
4. Assessment of inorganic speciation within redox (reduction-oxidation) reactions. Graphical representation of redox equilibria in aqueous media,	On site (weeks 7-8)	Lecture, explanation and interactive presentation, heuristic conversation, problem solving	4

logC_i/pE diagrams and E-pH (Pourbaix) diagrams. Speciation in inorganic redox buffer systems			
5. Control of inorganic speciation in redox couples through competitive equilibria of the type: acid-base reactions, precipitation reactions and complexation reactions. Geological and biological factors controlling inorganic speciation	On site (weeks 9-10)	Lecture, explanation and interactive presentation, heuristic conversation, problem solving	4
6. Methods for assessing inorganic speciation: - Chemical separation methods: selective chemical extractions, liquid-liquid extraction, precipitation/filtration, etc. - Measurement techniques: volumetric analysis, spectrophotometric methods, electrochemical procedures, AAS, ICP-MS, etc. - Computational modeling: thermodynamic and geochemical models, quantum chemical methods, etc.	On site (weeks 11-12)	Lecture, explanation and interactive presentation, heuristic conversation, problem solving	4
7. The relationship between speciation, mobility, dispersivity and bioavailability. Speciation and toxicity of the elements: arsenic, mercury, chromium, cadmium, lead, etc.	On site (weeks 13-14)	Lecture, explanation and interactive presentation, heuristic conversation, problem solving	4

References:

1. C.G. Constantinescu, M. Negoiu, C. Constantinescu, Chimie Anorganică (Vol. I). Editura Tehnică, 1986.
2. S. Ahrland, Inorganic chemistry of the ocean. In K. J. Irgolic & A. E. Martell (Eds.), Environmental Inorganic Chemistry. VCH Publishers, Inc, 1985.
3. W. Salomons, Environmental impact of metals derived from mining activities: Processes, predictions, prevention. Journal of Geochemical Exploration 52 (1995) 5-23.
4. G. Hanrahan, Modelling of Pollutants in Complex Environmental Systems. Volume II. Edited by ILM Publications. First edition, 2010.
5. D.C. Adriano, (Editor), Biogeochemistry of trace metals. Boca Raton, CRC Press, 1992.
6. Lecture notes, 2025

7.2. Lab	Mode of operation	Teaching methods	Allocated time (hours)
1. Safety rules in *Assessment and modelling of inorganic species* lab	On site (week 1)	Experiment, explanation, discussion, debate, and questioning	4
2. Determining the effect of speciation on Hg(II) reduction	On site (week 3)	Experiment, explanation, discussion, debate, and questioning	4
3. Determination of magnesium and calcium	On site (week 5)	Experiment, explanation, discussion, debate, and	4

species in water		questioning	
4. Characterization of immobile Fe(III) species. Precipitation of iron(III) hydroxide	On site (week 7)	Experiment, explanation, discussion, debate, and questioning	4
5. Characterization of immobile Pb(II) species. Precipitation of $PbCO_3$	On site (week 9)	Experiment, explanation, discussion, debate, and questioning	4
6. Assessing element speciation with programs such as PHREEQC or The Geochemist's Workbench. Chromium speciation as a function of E and pH	On site (week 11)	Experiment, explanation, discussion, debate, and questioning	4
7. Lab Verification	On site (week 13)	Experiment, explanation, discussion, debate, and questioning	4

References:

1. G. Brauer, Handbook of preparative inorganic chemistry (Vol. I), Academic Press, New York-London, 1963.
2. G. Brauer, Handbook of preparative inorganic chemistry (Vol. II), Academic Press, New York-London, 1965.
3. Lab work presentations, 2025.

8. Corrrelation of the discipline content with the expectations of representatives of the epistemic community, professional associations, and representative employers in the field related to the program

The content of the course contributes to the understanding of issues of national and international interest, such as environmental contamination with inorganic species that can have a toxic effect on living beings and the implementation of technologies to prevent environmental contamination with such toxic species.

9. Evaluation

Activity	9.1. Evaluation criteria	9.2. Evaluation method	9.3. Contribution to final score
9.4. Course	- Assimilation of the theoretical concepts of inorganic speciation - Critical analysis of models related to inorganic speciation	Written Exam	70%
9.5. Lab	- The ability to process and interpret the results obtained in experiments - Practical skills	Portofolio	30%
9.6. Minimum performance standard			
• Knowledge of chemical and other processes that control inorganic speciation. • Understanding the factors that control inorganic speciation. • Using interdisciplinary knowledge to analyze the complexity of inorganic speciation.			

Date
22.09.2025

Course coordinator,
Prof. dr. Paul CHIRIȚĂ

……

Date of approval
25.09.2025

Head of Department,
Conf. dr. Nicoleta Cioateră