FACULTAD DE CIENCIAS QUÍMICAS

APPLIED COMPUTER CHEMISTRY

COURSE GUIDE

BSc Chemistry

Academic Year 2023-2024

UNIVERSIDAD COMPLUTENSE MADRID

I.- IDENTIFICATION

COURSE NAME:	**Applied Computer Chemistry**
CREDITS (ECTS):	**6**
CHARACTER:	**Mandatory**
SUBJECT:	**Applied Computer Chemistry**
MODULE:	**Basic**
DEGREE:	**Bachelor in Chemistry**
SEMESTRE/TERM:	**Second semester (first course)**
DEPARTAMENTS:	**Analytical Chemistry; Physical Chemistry; Inorganic Chemistry, Organic Chemistry**

LECTURERS:

Coordinator	**Lecturer:**	RODRIGO GONZÁLEZ PRIETO
	Department:	Inorganic Chemistry
	Office:	QA-216, 2nd floor A building
	e-mail:	rodgonza@ucm.es

Group A		
Seminars and Tutorials	**Lecturer:**	FRANCISCO ORTEGA GÓMEZ
	Department:	Physical Chemistry
	Office:	QB-212B, 2nd floor B building
	e-mail:	fortega@ucm.es
Group B		
Seminars and Tutorials	**Lecturer:**	VALENTÍN GARCÍA BAONZA
	Department:	Physical Chemistry
	Office:	QA-254, 2nd floor A building
	e-mail:	vgbaonza@ucm.es
Group C		
Seminars and Tutorials	**Lecturer:**	JORGE OMAR CÁCERES GIANNI
	Departament:	Analytical Chemistry
	Office:	QB-342G, 3rd floor, B building
	e-mail:	jcaceres@ucm.es
Group D		
Seminars and Tutorials	**Lecturer:**	SILVIA ORTEGA GUTIÉRREZ
	Departament:	Organic Chemsitry
	Office:	QB-401, 4rd floor, B building
	e-mail:	siortega@ucm.es

Group E		
Seminars and Tutorials	**Lecturer:** **Department:** **Office:** **e-mail:**	SARA CEMBELLÍN SANTOS Organic Chemistry QA-332A, 3rd floor, A building scembellin@ucm.es
Group F		
Seminars and Tutorials	**Lecturer:** **Department:** **Office:** **e-mail:**	RODRIGO GONZÁLEZ PRIETO Inorganic Chemistry QA-216, 2nd floor A building rodgonza@ucm.es
Group G		
Seminars and Tutorials	**Lecturer:** **Department:** **Office:** **e-mail:**	VALENTÍN GARCÍA BAONZA Physical Chemistry QA-254, 2nd floor A building vgbaonza@ucm.es

Laboratory

Group	Sem.	Lecturer	E-mail	Office	Depart.
A1	2º	Isabel Coloma Manjón-Cabeza	iscoloma@ucm.es	QA-213	QI
A2	2º	Diana Vilela García	divilela@ucm.es	QB-439	QA
A3	2º	Jesús Fernández Castillo	jfernand@ucm.es	QA-241	QF
B1	2º	Miguel Tinoco Rivas	mitinoco@ucm.es	QA-109-A	QI
B2	2º	Esther Sánchez Tirado	esther.sanchez@ucm.es	QA-405	QA
B3	2º	Reynier Suardiaz del Río	reysuard@ucm.es	QA-511	QF
B4	2º	Santiago Romano Martín	sromano@ucm.es	QA-332A	QO
C1	2º	Miguel Cortijo Montes	miguelcortijomontes@ucm.es	QA-210	QI
C2	2º	María Raquel Mateos Briz	marmat07@ucm.es	QA-402	QA
C3	2º	Eduardo Sanz García	esa01@ucm.es	QB-256	QF
C4	2º	Santiago Romano Martín	sromano@ucm.es	QA-332A	QO
D1	2º	Miguel Cortijo Montes	miguelcortijomontes@ucm.es	QA-210	QI
D2	2º	Verónica Serafin González-Carrato	veronicaserafin@ucm.es	QB-435	QA
D3	2º	Eduardo Sanz García	esa01@ucm.es	QB-256	QF
D4	2º	María Josefa Rodríguez Yunta	mjryun@ucm.es	QA-329D	QO

E2	2º	Juan José Rodríguez Bencomo	juanjr10@ucm.es	QA-321A	QA
E3	2º	Jesús Fernández Castillo	jfernand@ucm.es	QA-241	QF
E4	2º	Ana Belén Descalzo López	abdescal@ucm.es	QB-348A	QO
F1	2º	Rodrigo González Prieto	rodgonza@ucm.es	QA-216	QI
F2	2º	Esther Sánchez Tirado	esther.sanchez@ucm.es	QA-405	QA
F3	2º	Francisco Gámez Márquez	frgamez@ucm.es	QA-503	QF
F4	2º	Santiago Romano Martín	sromano@ucm.es	QA-332A	QO
DG1	2º	Paula Kayser González	pakayser@ucm.es	QA-118	QI
DG2	2º	Silvia Ortega Gutiérrez	siortega@ucm.es	QB-401	QO

II.- OBJETIVES

■ GENERAL OBJECTIVE

The main objective of this subject is to provide students with enough skills to handle different computer software that allows them to solve problems in the field of Chemistry, related to common calculations and statistical analyses, creation and management of chemistry databases and with the visualization of molecules, crystals and their symmetry.

■ SPECIFIC OBJECTIVES

- Use of basic applications such as word processors, spreadsheets editors, scientific graphing and statistical packages that allow curve fittings and statistical analyses related to chemistry, as well as the writing of professional scientific reports.
- Use of office document applications, such as Microsoft EXCEL, to create simple databases.
- Learn how to manage more complex online databases to obtain specific chemical information (information on chemical substances, structures, properties, etc.) and bibliography.
- Management of crystal and molecular modelling programs to create and visualize chemical structures and their symmetry.

III.- PREVIOUS KNOWLEDGE AND RECOMMENDATIONS

■ PREVIOUS KNOWLEDGE:

Nomenclature and chemical formulation (both inorganic and organic). Balancing simple chemical equations. Usual units for measuring physical and chemical quantities.

■ RECOMMENDATIONS:

Only basic computer skills are required (Windows at user level).

IV.- CONTENTS

BRIEF DESCRIPTION:

Introduction to scientific computing. Use of databases. Creation of databases containing specific information. Drawing molecules and crystals. Geometry-properties relationship. Numerical differentiation: application to titrations. Fitting data using different functions: application to electrochemical measurements. Linear regression: kinetic applications. Statistics. Replicate measurements.

Practical sessions in the laboratory will cover a wide variety of fundamental aspects of chemistry (vapour pressure measurements, reaction kinetics, electrolysis, thermodynamics, titrations, etc.). The calculations and treatment of the data generated in the practical sessions will be carried out in the computer rooms. Simultaneously, in the seminar sessions, the students will learn and manage different packages frequently used in the field of Chemistry, related to general calculations and statistics, creation and management of databases and the visualization of molecules and crystals.

SYLLABUS:

LABORATORY

Practical sessions in the laboratory

1. Graphing and data analysis. Borax solubility. Determination of thermodynamic magnitudes.
2. Graphing and numerical analysis with non-linear functions. Monitorization of slow kinetic reactions and determination of partial orders and kinetic coefficients.
3. Graphing and numerical analysis of derivatives. Acid–base titration curves with a pH-meter.
4. Solving systems of linear equations. Determination of the stoichiometry of coordination complexes.
5. Graphing and data fitting. Water electrolysis and Faraday constant determination.
6. Graphing and data analysis, least-squares fit to a straight line and linearizing functions. Measurement of the vapour pressure of a pure liquid.

Practical sessions in the computer room

1. Numerical solution of algebraic equations. Monoprotic and polyprotic aqueous acid–base equilibria.
2. Drawing chemical structures and reactions schema. Getting started with the software ACD/ChemSketch.

THEORY (SEMINARS)

1. **Working with Microsoft Excel**.

   The concept of worksheet. Basic operations in a worksheet. Excel formulas and functions. Making charts. Data fitting: Linear regression and curve fitting. Methods for solving equations with one unknown. Practical examples.

2. **Working with Origin**.

Basic information on the Origin workspace. Main components of an Origin project, workbooks, worksheets and columns and graphing. Tools for numerical analysis in Chemistry. Curve fitting: Linear and Polynomial Fit. Statistics. Examples.

3. **Creating databases with Microsoft Excel**.

   Introduction to a database: utilities. Use of Excel worksheets as simple databases. Sorting lists, multiple data filtering and auto filtering in Excel worksheets. Examples.

4. **Useful databases in chemistry**.

   Management and utilities of the NIST Chemistry webbook. Access to the abstract and citation index databases in the *Web of Science*..

5. **Computer resources for molecular symmetry**.

   Visualization of the symmetry elements and their operations in molecules. Introduction to molecular modelling packages.

6. **Statistical analyses of the results obtained in the practical sessions**.

   Global average values and deviations of the results obtained by the students in the practical sessions. Average values by practice and group. Comparative charts between groups.

V.- COMPETENCES

GENERAL:

- **CG2:** To recognize the importance of Chemistry in different contexts and relate it with other areas of knowledge.
- **CG3:** To carry on their studies in specialized areas of chemistry or in multidisciplinary areas.
- **CG4:** To rigorously express the chemical knowledge acquired so that it is well understood in multidisciplinary areas.
- **CG6:** To analyse and solve qualitative and quantitative problems.
- **CG8:** To evaluate, interpret and synthetize data and chemical information.
- **CG12:** To interpret data from observations and measurements performed in the laboratory in terms of their significance and the theories that support them.
- **CG13:** To develop good scientific practices for measurement and experimentation.

SPECIFIC:

- **CE38-IAQ1:** To manage different databases.
- **CE38-IAQ2:** To interpret the data extracted from a database.

- **CE39-IAQ1:** To handle, at the user level, commonly used software packages for data graphing and drawing molecules and crystals.
- **CE40-IAQ1:** To fit data with simple functions.
- **CE40-IAQ2:** To handle basic statistic tools.

■ **GENERIC:**

- **CT3:** To demonstrate critical thinking and self-criticism.
- **CT4:** Adaptability to new situations.
- **CT5:** To manage quality chemical information, bibliography, specialized databases and accessible resources from the Internet.
- **CT7:** To use tools and computer packages for the treatment of experimental results.
- **CT11:** To develop self-learning capacity.

VI. – LEARNING OUTCOMES

After the course, in relation to the knowledge acquired in the seminars, the student should be able to:

Unit 1

1. Use a spreadsheet software, for instance Microsoft Excel, for simple mathematical calculations.
2. Perform mathematical operations that involve formulas predefined by the software.
3. Represent experimental data and perform linear or polynomic fittings.

Unit 2

1. Use the Origin software for data calculation and graphing.
2. Fit experimental data with linear or polynomic functions.
3. Derive and integrate experimental data.

Unit 3

1. Create databases in Excel or similar computer programs that facilitate the control and management of the laboratory.
2. Employ ordering and filtering procedures to facilitate the search of information in the databases.

Unit 4

1. Search for basic chemical information (molecular formula, structure, thermodynamic data, etc.) of chemical substances.

2. Use the information extracted from the NIST database to solve simple chemistry problems, in which thermodynamic aspects are considered.
3. Get scientific and bibliographic information through the Web of Science (previously known as Web of Knowledge**)** online citation indexing service.

Unit 5

1. Identify and differentiate the point symmetry elements in basic molecules.
2. Draw molecules in two and three dimensions through molecular editor and visualizer platforms or molecular modelling programs.

Unit 6

1. Establish the basic statistical parameters (mean, median, mode, standard deviation, etc.) of a series of experimental measures, through the use of programs such as Microsoft Excel or Origin.
2. Calculate the statistical confidence limits of series of experimental measurements.
3. Determine the confidence limits of chemical variables calculated from regression models.

And with regard to the practical sessions, once completed, the student must be able to:

- Plot titration curves by using their own experimental data, and then perform their derivatives to establish the titration final point.
- Determine physicochemical parameters such as the Faraday constant, based on experimental data fitted to mathematical models.
- Calculate the variation of both the standard enthalpy and entropy of a reaction from equilibrium constants obtained at different temperatures.
- Analyse the experimental data obtained during a slow kinetic reaction and determine the order of the reaction and its rate constant.
- Establish the stoichiometry of coloured complexes by measurements of radiation absorption and graphic resolution of linear systems.
- Use a simple vacuum line to measure the vapour pressure of pure liquids as a function of the temperature. Calculate the vaporization enthalpy of the liquid by means of least-squares fitting of the data.
- Use spreadsheets to perform simulations and calculations related to acid-base equilibria.
- Draw molecular structures using the ACD/ChemSketch package.

VII. – WORKING HOURS DISTRIBUTED BY ACTIVITY

Activity	Attendance (hours)	Self-study (hours)	Credits
Lectures			
Seminars	25	25	2
Tutorials/ Guided work	3	4,5	0,3
Labs	30	45	3
Realization and presentation of individual exercises and exams	6	11,5	0,7
Total	**64**	**86**	**6**

VIII.- METHODOLOGY

The teaching practice will follow a mixed methodology based on cooperative learning, collaborative learning and self-learning. The training activities will be carried out through seminar classes (2 credits), computer room work (0.3 credits) and data collection in the laboratory (3 credits). During the seminar sessions, the most common applications of different software packages will be explained and in the computer room they will work with specific examples that, in some cases, may have been previously obtained in the laboratory. The elaboration of tutored works, reports and taking exams will suppose a total of 0,7 credits.
Each student will undertake one weekly practical session, in a time slot different from their seminar sessions. In total, there will be six experimental sessions in the laboratory and two more in the computer room. After every two experimental sessions, the analysis of data will be performed in the computer room the day after the second one, except for the students of the group G (double bachelor's degree "Chemistry-Biochemistry") who will perform the analysis of data just after the laboratory session. This session will take place in the computer rooms and its duration will be two hours (one hour in the case of group G). Once an experimental session has been carried out, each group of students and their instructor will proceed to perform the following experimental session and the calculations corresponding to these two experimental sessions in that week. The cyclic process will be repeated until all students have completed the six laboratory practical sessions and two in the computer room.

In parallel to the practical sessions, and in a schedule that does not interfere with these, a lecturer will give 14 **seminar sessions** (of 110 min of duration) in the computer room. In these sessions the student will be introduced to the management and the main applications of different programs useful to solve problems in chemistry.

The **Virtual Campus** will be used to allow a fluid communication between lecturers and students and as an instrument to make available to students the material that will be used in the practical sessions and seminars.

IX.- BIBLIOGRAPHY

BASIC:

- Laboratory practical guide Ed. 2024.
- S.R. Crouch; F. James Holler: "*Application of Microsoft Excel in Analytical Chemistry*", Thomson Ed., Belmont, CA (USA) 2004.

COMPLEMENTARY:

- Excel and Origin video tutorials (Available in the Virtual Campus)
- Origin video tutorials.
  http://www.originlab.com/index.aspx?go=SUPPORT/VideoTutorials

If necessary, in addition to this material, the students will be informed about the specific bibliography for each laboratory session.

X.- ASSESSMENT PROCEDURE

In order to access to the final evaluation, the student must have participated in at least 70% of all the face-to-face activities (seminars, tutorials, practical lab and computer sessions). Group changes due to the incompatibility with the activities of other courses or the recovery of unrealized practical sessions will not be allowed, regardless of the causes for the absence. Absence from a practical session will be marked with a zero. Absence from a data processing session will therefore imply that both practical sessions covered in that session will be marked also with a zero. In very exceptional cases, and by appropriate justification, the absence could be considered justified, but never more than one practical or data processing session.
The evaluation and the final mark of the course will be made according to the following concepts and weighting coefficients. All marking scales have a score over 10 points, in agreement with the scale established in RD 1125/2003. It will be necessary to reach 5 points among all the activities to pass the course. This criterion will be maintained in all calls.

The marks of the practical sessions and tutorials/workshops will be communicated to the students with enough time, before the call of the final exam, so that they can properly plan the study of the course. In any case, the minimum period of seven days between the publication of the marks and the date of the final exam will be respected.

PRACTICAL SESSIONS: 20%

It's 20% of the final mark. To pass the subject in the ordinary call, the students may not have failed more than 3 practices neither get less than 5 points in the average score of them. The absence to a practical session or to a data processing session implies a zero score in this practice or corresponding practices and the non-admission of the corresponding report.

Evaluated competences: GC4, GC6, GC8, GC12, GC13, SC39-ACC1, SC40-ACC1, SC40-ACC2, TC3.

PERSONAL WORK: 20%

It's 20% of the final mark and consists in the preparation of reports. The student must present a report corresponding to each practical session, that must be written in electronic format using the appropriate office tools with deadline according to a pre-established calendar. The presentation of the report after the deadline of without the established format will result in a penalty with a reduction of the qualification of the practical session. Failure to present such report will be equivalent to an absence to the practical session, so the global mark of the practice will be ZERO.

Associated competences: GC6, GC8, GC12, SC38-AAC1, SC38-AAC2, SC39-AAC1, SC40-AAC1, SC40-AAC2, TC3, TC5, TC7, TC11.

At the end of the practical sessions and after the presentation of the reports, the lecturer will publish a mark for each practice, with a score between 1 and 10 points. The mark must reflect the work in the laboratory, considering the operations carried out during each session as well as the results obtained, the student's willingness to learn, the correct presentation of the reports and the understanding of the theoretical-practical aspects.

For those students who have not passed the minimum number of practices or do not get the minimum score of 5 in the average mark of the practical sessions, a theoretical-practical exam will be carried out in the extraordinary call, which will consist of the performance of one of the practices previously carried out during the course and to answer in writing a series of questions on aspects related to the practical sessions and the seminars.

TUTORIALS/ GUIDED ACTIVITIES (SEMINARS): 10%

In the seminar classes, problems and practical examples will be proposed to the students, that must have them solved and delivered before the deadline indicated by the seminar lecturer for each of the cases. The mark obtained in this activity will represent 10 % of the final mark and it will be compulsory to reach a **minimum mark of 3 points** to pass the subject in the ordinary call.

Associated competences: GC6, GC8, GC12, SC38-AAC1, SC38-AAC2, SC39-AAC1, SC40-AAC1, SC40-AAC2, TC3, TC5, TC7, TC11.

FINAL EXAM: 50%

Only the students who have attended 70% of the face-to-face activities and have passed the practical sessions (5 points) and tutorials/workshop (3 points) may access to the final evaluation. The students who did not fulfill any of these requirements will be classified as FAIL in the ordinary call record and their numeric mark will be ZERO.
The final exam will take place at the end of the second semester at the date, time and place previously established by the academic authorities of the centre. In this exam, no longer than three hours, the students must demonstrate the knowledge acquired in the practical and seminar sessions by answering a series of theoretical questions related to

all aspects of the work carried out both in the laboratory and in the computer room. The qualification of this exam will suppose 50% of the final mark, being necessary, for weighting purposes with the other qualifications, that the student obtains at least a **mark of 4 points**.

Those students who failed the subject in the ordinary call because they do not fulfill the requirements to access the final evaluation, or whose mark, once the weightings have been applied, does not reach the minimum score of 5 points, must attend the extraordinary call. This exam will be only theoretical for those students who, even though they failed the course in the ordinary call, have passed the practical session (minimum average score of 5 and with 3 or less practices failed). For those students who failed the subject in the ordinary call for having failed more than 3 practices, or for not having passed the average score of 5 points in the set of practices, they will pass a theoretical-practical exam in the extraordinary call, having both parts an equal weight. The final mark of this extraordinary exam will be obtained from the average between both parts, being necessary a score equal to or greater than 4 points out of 10 in each part. Those students who have not achieved a minimum mark of 3 points in the guided activities must deliver, before the extraordinary call, a set of activities similar to those carried out throughout the course and get a minimum mark of 3 points.

Associated competences: GC6, GC13, TC3, TC4, TC11.

ACTIVITY SCHEDULE

SEMINARS and TUTORIALS

UNIT	ACTIVITY	HOURS	START	END
1.- Working with Microsoft Excel	Seminar	7	1th week	4th week
	Tutorial	1	4th week	
2.- Working with Origin	Seminar	7	5th week	8th week
	Tutorial	1	8th week	
3.- Creating databases with Microsoft Excel	Seminar	2	9th week	
4.- Useful databases in chemistry	Seminar	2	10th week	
5.- Computer resources for molecular symmetry	Seminar	5	11th week	13th week
6.- Statistical analyses of the results obtained in the practical sessions	Seminar	2	13th week	14th week
	Tutorial	1	14th week	

Seminars and tutorials schedules
(all weeks of the semester)

Group	Schedule	Room
A	Thursday (9:30 –11:20)	QC26
B	Tuesday (15:30 –17:20)	QC26
C	Friday (8:30 –10:20)	QC26
D	Monday (14:30 –16:20)	QC26
E	Thursday (11:30 –13:20)	QC26
F	Wednesday (15:30 –17:20)	QC26
G	Thursday (14:30 – 16:20)	QB68

PRACTICAL SESSIONS SCHEDULE

Group	Schedule	Place
A	Monday (15:30 -18:30)	General Chemistry Laboratory
	Tuesday (15:30 -17:30)	Computer Room
B	Monday (9:30 - 12:30)	General Chemistry Laboratory
	Tuesday (9:30 - 11:30)	Computer Room
C	Tuesday (15:30 -18:30)	General Chemistry Laboratory
	Wednesday (15:30 -17:30)	Computer Room
D	Tuesday (9:30 - 12:30)	General Chemistry Laboratory
	Wednesday (9:30 - 11:30)	Computer Room
E	Wednesday (15:30 -18:30)	General Chemistry Laboratory
	Thursday (15:30 -17:30)	Computer Room
F	Wednesday (9:30 - 12:30)	General Chemistry Laboratory
	Thursday (9:30 - 11:30)	Computer Room
G	Friday (9:30 - 12:30)	General Chemistry Laboratory
	Friday (12:45 - 13:45)	Computer Room

SUMMARY OF ACTIVITIES (in hours)

Teaching activity	Associated competences	Lecturer activity	Student activity	Learning assessment	P	NP	Total	C
Seminars	GC2, GC3, GC4, GC12, GC13, SC38-ACC1, SC38-ACC2, SC39-ACC1, SC40-ACC1, SC40-ACC2, TC4, TC5, TC7.	Explanation of relevant aspects for the development of the practical sessions. Preparation for the discussion of data and results. Presentation of the theoretical knowledge necessary to solve the practical problems.	Attendance and active participation. Note-taking. Formulation of questions and doubts.	Qualification of the written answers (approach and result) for the resolution of practical exercises and numerical problems	25	25	50	10%
Tutorials		Direction and supervision of the student's study and activities. Asking questions. Resolution of doubts or queries.	Consult the lecturer about the conceptual and methodological difficulties encountered when studying the subject. Approach of questions and response to the proposals made by the lecturer.		3	4,5	7,5	
Laboratory	GC4, GC6, GC8, GC12, GC13, SC39-ACC1, SC40-ACC1, SC40-ACC2, TC3.	Supervision and advice on the appropriate procedure for the work during the practical sessions. Explanation of the most relevant theoretical issues of each session.	Attendance and completion of the tasks proposed by the instructor. Collection and interpretation of measured or calculated data.	Evaluation of the experimental work and the procedures employed.	30	45	75	20%
Individual work	GC6, GC8, GC12, SC38-ACC1, SC38-ACC2, SC39-ACC1, SC40-ACC1, SC40-ACC2, TC3, TC5, TC7, TC11.	Support the students in the resolution of problems that may arise in the preparation of the laboratory notebook or the required reports. Guide the students in the handling of the computer programs.	Preparation of the laboratory notebook and reports requested by the instructor in each practical session.	Review of the laboratory notebooks and reports.		11,5	11,5	20%
Exams	GC6, GC13, TC3, TC4, TC11.	Proposal, monitoring and correction of exams. Students grading.	Preparation and realization of exams and/or test	Evaluation of the practical and written works	6		6	50%
P: In-class; NP: Self-study; C: Evaluation								