UNIVERSITY of BRADFORD

Module Descriptor

Module Details	
Module Title:	Practical Chemistry 1 for Computational Chemistry
Module Code:	CFS4027-D
Academic Year:	2019-20
Credit Rating:	40
School:	School of Chemistry and Biosciences
Subject Area:	Chemistry
FHEQ Level:	FHEQ Level 4
Pre-requisites:	
Co-requisites:	

Contact Hours	
Type	**Hours**
Supervised time in studio/workshop	60
Laboratory	168
Directed Study	172

Availability	
Occurrence	**Location / Period**
BDA	University of Bradford / Academic Year (Sept - May)

Module Aims

This module will introduce the fundamental techniques required to work safely and efficiently in the laboratory. You will develop your skills in the safe handling of chemicals, in making accurate qualitative observations, quantitatively analysing compounds prepared in the laboratory, and in reporting and interpreting experimental results. You will learn about spectroscopic techniques and use these methods in the analysis of what you synthesise in the lab. You will use measurements of physical parameters to investigate aspects of physical chemistry.
Through preparing laboratory reports you will be introduced to the standard formats and drawing packages used by professional chemists to share their results. The principles of Green Chemistry will be introduced, and you will learn how to assess the environmental impact of your laboratory work.
You will be introduced to numerical programming with the language python and the design and

implementation of simple programs to solve chemical problems.

Outline Syllabus

Chemical hazards and risk assessments, sources of safety data, on-line databases, definitions and safety terms, exposure limits, legislation, CHIP, COSHH, REACH.
The application of statistical methods for data manipulation, reporting, validation, interpretation and presentation of experimental results. Identification of errors and calibration of instruments. Precision, accuracy & sensitivity, linear regression, units.
Green chemistry - Definitions & metrics used, the tools used to assess the environmental impact of chemical processes.
Purification of single & mixed substances. Separation & identification of mixtures by thin layer chromatography. Solvent extraction from solids & liquids. Experiments to illustrate thermodynamic equilibria and the variation of equilibrium position with temperature.
Measurements of physical properties of states of matter; refractive index, boiling point & vapour pressure. Measurement of heats of reaction by calorimetry. Measurement of enthalpies of solution & partition coefficients. Experiments illustrating classical methods of inorganic analysis.
Laboratory techniques in separating organic mixtures: Elementary organic synthesis.
Spectroscopic characterisation of organic & inorganic compounds.
Professional Development: Presenting information effectively, monitoring & evaluating results, drawing conclusions, chemical reports, chemical structure drawing.
Programming: syntax and semantics of the python programming language, common algorithms and data structures. Design of programs to solve numerical problems in chemistry.

Learning Outcomes

1	Describe types of chemical hazards.
10	Identify and quantify experimental errors.
11	Measure physical and chemical properties of some compounds & interpret analytical data.
12	Purify and prepare some organic and inorganic compounds for spectroscopic analysis.
13	Create molecular structure diagrams and mechanistic reaction sequences using structure drawing software.
14	Tabulate results and present charts from manipulation of data in a spreadsheet.
15	Interpret infrared, ultraviolet, 1H NMR and mass spectra of simple compounds & combine the information gained from these spectra to deduce structures.
16	Quantify and report errors in numerical data-report writing & data handling skills; operate effectively as part of a group.
17	Use IT to prepare professional chemical documentation.
18	Use a range of information to analyse data & solve problems.
19	Prepare simple programs to solve numerical chemical problems.
2	State how to minimise risks in using hazardous substances; explain, with examples, how practical work reinforces theoretical studies; identify roles in group situations.
3	Describe principles and methods, and carry out experiments in, organic purification and organic and main group synthesis.

4	Carry out measurement of thermodynamic and kinetic properties.
5	Quantify and describe the environmental impact of experiments using Green Chemistry metrics.
6	Present laboratory reports in the appropriate format.
7	Perform basic chemical operations & carry out some measurements in practical organic, inorganic & physical chemistry.
8	Record experimental lab work in the appropriate format.
9	Carry out COSHH assessments.

Learning, Teaching and Assessment Strategy

Laboratory-based work will include staff-led demonstration of practical and manipulative skills at the bench and supervision of students' experimental work. Pre-laboratory workshops will be provided for each experiment to familiarise students with the concepts and procedures, the post lab workshops will allow students to reflect on the results and their significance. Teaching of health and safety and laboratory skills will be delivered in workshops. Laboratory skills will be taught and practised in laboratory sessions. Students will receive feedback in the form of marked laboratory reports; review of laboratory records and orally in seminars. Data analysis and programming will be taught and practised through problem-based learning and workshops. Workshops and seminars will be used to teach the fundamental spectroscopic techniques used in the lab, and to give instruction in the use of specialist software for the preparation of laboratory reports. Students will be directed to further develop programming and computational skills out with the timetabled sessions through directed exercises.

The experimental component will be continuously assessed by weekly revision of laboratory books, submission of lab reports and pre-lab assessments. This component assesses LOs: 1-18. Computational component will be assessed by two end of semester programming exercises on a previously unseen problem. Weekly formative feedback will develop the necessary skills to undertake the relevant exercises. This component will assess LOs: 16 - 19.

Mode of Assessment

Type	Method	Description	Length	Weighting
Summative	Coursework	Programming exercise - Semester 1.	-1000 words	20%
Summative	Coursework	Continuous Summative Assessment of practical work and reports		60%
Formative	Coursework	Feedback on weekly programming exercises		%
Summative	Coursework	Programming exercise - Semester 2.	-1000 words	20%

Reading List

To access the reading list for this module, please visit https://bradford.rl.talis.com/index.html.

Please note:

This module descriptor has been published in advance of the academic year to which it applies. Every effort has been made to ensure that the information is accurate at the time of publication, but minor changes may occur given the interval between publishing and commencement of teaching. Upon commencement of the module, students will receive a handbook with further detail about the module and any changes will be discussed and/or communicated at this point.