SCHOOL OF CHEMICAL SCIENCES

MAHATMA GANDHI UNIVERSITY

Proposal for

Value Added Courses on

1. CSM22VA01 Spectroscopic Methods in Chemistry

2. CSM22VA02 Learning Computational Chemistry using Gaussian software

(Value Added Programme - Certificate Course(30 h, 3 credits))

Programme Poject Report

(a) **Programme's mission & objectives:**

Value-added courses are designed to enhance the standard of the students beyond those levels specified in the academic curriculum. The aim of the Value-Added Course on Spectroscopic Methods is to prepare students to become experts and develop skills for doctoral studies, and /or professional industrial careers in chemical analysis, and structural characterization of materials. This module will provide the student with an understanding of the theory, practices, and instrumentation associated with various spectroscopic techniques.

Value added course is not mandatory to qualify for any programme and the credits earned through this course shall be over and above the total credit requirement prescribed in the curriculum for the award of the degree.

(b) **Relevance of the program with HEI's mission and goals:**

The course focuses on state-of-the-art developments in their practices and instrumentation, as well as issues dealing with the identification of samples in complex matrices. This course places a strong emphasis on the professional development of the students. Such a qualification will enable and facilitate career progression for the students.

(c) **Nature of prospective target group of learners**:

Students with science backgrounds can join the programme. Students doing their Masters/Doctoral studies can join the program to strengthen their analytical skills.

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(c) **Appropriateness of programme to be conducted in Add mode to acquire specific skills and competence:**

This course places a strong emphasis on the professional development of the students. Such a qualification will enable and facilitate career progression for the students. Upon successful completion of this module, a student will be able to (i) Understand the principles, practices, and instrumentation associated with various spectroscopic techniques, (ii) Describe sample preparation and method development issues relating to the use of advanced techniques for analysis and identification, (iii) Competently operate and calibrate associated laboratory instrumentation, and (iv) Critically appraise the literature and identify future trends in this area.

(d) **Instructional design:**

The duration of the Value-added course is 30 hrs which includes theory (60%) and practicals (40%). Classes for a VAC are conducted beyond the regular class

hours. The value-added courses may be also conducted during weekends/vacation periods. A student will be permitted to register for only one Value Added Course ina Semester. The course can be offered only if there are at least 5 students optingfor it.

(e) **Procedure for admissions, curriculum transaction, and evaluation:**
Any student with minimum B.Sc. in chemistry, physics, and biology can apply. The student has to pay an amount for the programme which is decided by the School. For practicals, 20% will be virtual and remaining will be direct laboratory work. This course will have three types of graded activities that will be included in the overall course grade. These include: **Quizzes (20%), Open-ended Questions (30%), and Final project (50%).** At the end of the course, the candidate will be asked to complete a final project. The final project will be conducted in groups of 2 students. It will consist of a written report that focuses on the utilization of spectroscopic techniques for various applications. The final project will be graded and will contribute to 50% of the overall course grade

(f) **Requirement for the laboratory support and library resources:**
To handle the practical components in the syllabus, technicians, and consumables are required.

Syllabus

1. CSM22VA01 Spectroscopic Methods in Chemistry

Principles, instrumentation, and applications of the following spectroscopic techniques:

- Infrared (IR) spectroscopy
- UV/visible spectroscopy
- Fluorescence spectroscopy
- Raman spectroscopy
- X-ray absorption spectroscopy

2. CSM22VA02 Learning Computational Chemistry using Gaussian software

Unit I: Single point energy calculations

1. Calculation of the energy of the three stereoisomers of 1,2-dichloro-1,2-difluroroethane using density functional theory (DFT).
2. Computation of the isomerization energy between acetaldehyde and oxirane at STP using DFT.

Unit II: Geometry optimization and prediction of chemical properties

1. Optimization of the structure of formaldehyde molecule using DFT method and analysis of the molecular orbitals, atomic charges and IR spectrum.
2. Computation of the bond enthalpies for the hydrides of the atoms in the second row of the periodic table using Hartree-Fock (HF) and DFT methods.
3. Explore the effect of basis set on the bond length in the phosphorous monoxide.
4. Understand the regioselectivity of Diels-Alder reaction using DFT.