



CHRIST

COLLEGE (AUTONOMOUS)

IRINJALAKUDA, KERALA

Reaccredited by NAAC with 'A++' grade

CERTIFICATE COURSE ON

BASIC CHEMISTRY SOFTWARE'S

Department of Chemistry Self

**Fee
1000₹**

PROGRAM HIGHLIGHTS

- THEORY AND PRACTICAL SESSIONS
- LECTURE INCLUDE DOWNLOADING AND INSTALLATION OF SOFTWARES
- HANDS ON TRAINING
- CANDIDATE CAN USE OPEN-SOURCE SOFTWARE'S INDEPENDENTLY

*Certificate will be issued
to succesful candidate*

ELIGIBILITY

***BSc.Chemistry final year
students
& MSc Chemistry students***

FOR DETAILS CONTACT

Ms. Krishnapriya KM

(Course incharge) 8021643748

CERTIFICATE COURSE- STUDENTS LIST

SI.NO	REGISTER NUMBER	NAME
1	CCAXMCH017	AMITHAMITHAL DAS
2	CCAXMCH018	ANAGHA SUNIL
3	CCAXMCH019	ANGELENA WILSON
4	CCAXMCH020	ANVIN P STANLY
5	CCAXMCH021	AUGUSTINE JOYSON.K
6	CCAXMCH022	DENNA ELIZABETH D
7	CCAXMCH023	GOURI REJUKUMAR
8	CCAXMCH024	HANNA K
9	CCAXMCH025	JESNA WARSON
10	CCAXMCH026	SHAHANAZ FATHIMA M M
11	CCAXMCH027	SNEHA ANIL KUMAR
12	CCAXMCH028	SREELAKSHMI P B
13	CCAXMCH029	SREERAG SHANIL

Certificate course on Basic Chemistry Software's (30 Hours)

PG Department of Chemistry (Self)

Objectives

Post graduate department of chemistry Christ College, Irinjalakuda offers 30 hours Certificate course in basic chemistry software's. This course aimed at imparting skills on use of various open-source chemistry tools that are essential for any student or researcher with chemistry as a major subject. At the end of course, the participants will be able to use these softwares for drawing chemical structures, generation of their names, retrieve information about physical properties, calculations, three-dimensional molecular structure calculations, spectroscopic signatures, chemical reaction pathways prediction and other parameters efficiently.

Course Duration– 30 Hours

Eligibility– All B.Sc. final year students having chemistry as major subject and all M.Sc. Chemistry students are eligible

Evaluation Process– Assessment of candidates will be done through theoretical assignments, projects & practical examinations after completion of each module. All successful candidates will be awarded with certificates.

Contents for certificate course in basic chemistry software's

Module 1 (4 hours)

ACD ChemSketch software: – Introduction, download and installation process, Drawing various chemical structures, name generation from structures, conversion of name of molecule into its structure, calculation of physical properties such as density, molecular weight, molecular formula, refractive index from structural formula, bond angles, bond lengths, dihedral angles.

Learning outcomes: - After successful completion of this module candidate will be able to use ACD ChemSketch for generation and processing of simple and complex chemical structures.

Module 2 (8 hours)

ChemDraw Ultra software– Introduction, download and installation process, Drawing various chemical structures, calculation of physical properties ^1H , ^{13}C NMR prediction from molecular structure, drawing structure of bigger molecules such as proteins, carbohydrates, and RNA/DNA, bio arts, use of templates

Chem3D software: - Introduction, download and installation process, 3D structures of molecules, conversion of 2D structure into 3D structure, Dihedral angles, Energy minimization, calculation of surface properties, Calculation of dipole moments, MM2 calculations, Huckel calculations, Calculation of UV and IR spectra using MM2 calculations.

Learning outcomes: - After successful completion of this module candidate will be able to use ChemDraw Ultra for generation, processing and calculation of physical/chemical properties of simple and complex molecules.

Module 3 (5 hours)

Introduction to computational methods-Molecular mechanics and electronic structure methods-*ab initio* and semi empirical methods-basis set approximation. Introduction to Gaussian Programme- the structure of a Gaussian input file, types of key words. Specification of molecular geometry using Cartesian co-ordinates and internal co-ordinates(Z-Matrix). Geometry optimization of simple molecules, computation of normal modes of vibration of simple molecules, computation of MO coefficients of simple molecules, computation of NMR coupling constants, introduction and application of Gaussian as a software.

Learning outcomes: - After successful completion of this module candidate will be able to use Gaussian program and its various applications in chemistry.

Module 4 (5 hours)

Introduction to online chemical database search, Searching and downloading research papers using keywords in Science direct, Sci-Hub and google scholar, reaction search, product search, reactant search, structure search, Markush search using Sci-finder. Introduction to Mendeley reference manager and its applications.

Learning outcomes: - After successful completion of this module candidate will be able to use online research tools efficiently and will be able to search research papers related to their topics more efficiently.

Module 5 (8 hours)

SciDavis software - Introduction to SciDavis, basic features like Scientific graphing, drawing various 2D & 3D plots, Data analysis, statistics, signal processing, curve fitting, conversion of graph to various file format like JPEG, GIF, EPS.

Ouriginal software: - Introduction to Ouriginal software, how does Ouriginal work to prevent plagiarism? Document submission, Retrieval of sources, Analysis powered by sophisticated algorithms, Report creation and delivery

Learning outcomes: - After successful completion of this module candidate will be able to understand scientific graphing and data analysis and also utilise the software Ouriginal to avoid plagiarism in their project or research work.

Salient features of certificate course

- Theory and practical session as per curriculum
- Lectures include entire process of downloading and installation of these software's.
- Hands on training on all these software's.
- At end of course candidate will be able to use these open-source software's independently for their work.

A certificate will be issued to the successful candidates

Certificate course on Basic Chemistry Software's (30 Hours)

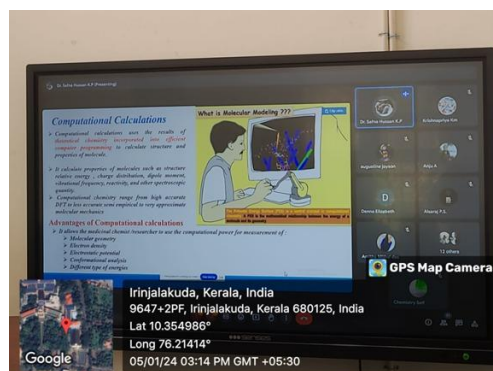
Couse code - CPCC57

PG Department of Chemistry (Self)

Teacher Coordinator Report

Number of students	13
Date of examination	12 th March, 2024
Total students who passed exam	13
Total course duration	30 hrs

The course started on 5th January 2024. There were 13 M.Sc. 1st year students participated in the program and all completed the course. The duration of the course was 30 hrs. The classes were taken as both practical and theory sessions.



Feedback analysis:

- Students enjoyed the practical session very much.
- Students became more interested in computational chemistry.
- downloading and installation of these software's help students to work on it as their wish.
- The resource persons were very helpful.

Course Coordinator: Krishnapriya.K.M

**CHRIST COLLEGE (AUTONOMOUS) IRINJALAKUDA
CERTIFICATE COURSE EXAMINATION**

**Certificate course on Basic Chemistry Software's
PG Department of Chemistry (Self)**

TIME: 2 Hours

MAX. MARKS: 50

Answer any ten questions. Each question carries 5 marks.

10x5 = 50

1. What is chemdraw used for?
2. List out 5 major uses of ACD Chems sketch.
3. Write gaussian input file for the geometry optimization at HF/6-311G* level of theory
4. Write the z-matrix of FORMALDEHYDE molecule.
5. Compare Ab initio and semiempirical methods.
6. Give a brief comparison of STO and GTO.
7. Draw the structure of NH₃ molecule using chemdraw software
8. Show the animations of vibrations of H₂O molecule.
9. Draw the structure of CO₂ molecule using gaussian software.
10. Find out the bond energy and bond order of N₂ molecule.
11. Draw the structure of BENZALDEHYDE molecule using chemsketch software.
12. Find out the dipole moment of NH₃ molecule

Computational Calculations

- Computational calculations uses the results of theoretical chemistry incorporated into efficient computer programming to calculate structure and properties of molecule.
- It calculate properties of molecules such as structure relative energy , charge distribution, dipole moment, vibrational frequency, reactivity, and other spectroscopic quantity.
- Computational chemistry range from high accurate DFT to less accurate semi empirical to very approximate molecular mechanics

Advantages of Computational calculations

- It allows the medicinal chemist/researcher to use the computational power for measurement of:
 - Molecular geometry
 - Electron density
 - Electrostatic potential
 - Conformational analysis
 - Different type of energies

What is Molecular Modeling ???



Dr. Safna Hussain K.P

Krishnapriya Kim

Augustina Joyson


Anja A

Denna Elizabeth

Abhraj P.S.

Anitha Sankar

12 others

 **GPS Map Camera**

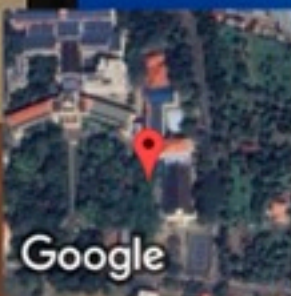
Irinjalakuda, Kerala, India

9647+2PF, Irinjalakuda, Kerala 680125, India

Lat 10.354986°

Long 76.21414°

05/01/24 03:14 PM GMT +05:30



Google



GPS Map Camera

Irinjalakuda, Kerala, India

9647+2PF, Irinjalakuda, Kerala 680125, India

Lat 10.354986°

Long 76.21414°

05/01/24 03:14 PM GMT +05:30



Google

**Certificate course on Basic Chemistry Software's
PG Department of Chemistry (Self)**

Summary Report 2024

The course started on 5th January 2024. There were 13 M.Sc. 1st year students participated in the program and all are completed the course. The duration of the course was 30 hrs. The classes were taken as both practical and theory session. The doubt clearing session was very interesting and informative for students.

Course Outcome:

- The students were satisfied with the class. Students were familiarized with chemistry software's like Chems sketch, Chemdraw, Avogadro, gaussian etc., and also the theoretical part of computational chemistry including z- matrix. from this course the students achieve the skills like drawing chemical structures, generation of their names, retrieve information about physical properties, calculations, three-dimensional molecular structure calculations, spectroscopic signatures, chemical reaction pathways prediction and other parameters efficiently. At end of course student can able to use these open-source software's independently for their work and applications.

Course Coordinator: Krishnapriya.K.M



CHRIST

COLLEGE (AUTONOMOUS)
IRINJALAKUDA, KERALA

Reaccredited by NAAC with Grade 'A++' & SAAC 'A+'

CERTIFICATE OF PARTICIPATION

Date : 30-08-2024

This is to certify that

Mr/Mrs *Amithamithal Das*

has successfully completed 30-hour course on "Basic Chemistry Software's Program"

with A grade, conducted by Department of Chemistry (Self),

Christ college (Autonomous) Irinjalakuda, Thrissur.

Ms. Krishnapriya K M
Course Coordinator

Ms. Greeni K I
HoD

Dr. Fr. Jolly Andrews CMI
Principal
CHRIST COLLEGE (AUTONOMOUS)