

DEPARTMENT OF CHEMISTRY SELF
CHRIST COLLEGE (AUTONOMOUS)
IRINJALAKUDA



*Certificate course
on*

Basic Chemistry Software's

Program Highlights

- Theory and practical sessions
- Lectures include downloading and installation of software's.
- Hands on training
- Candidate can use open-source software's independently.

*Course Fee:
1000/-*

*certificate will be issued to
the successful candidates*

Eligibility-

B.Sc. Chemistry final year students & M.Sc.
Chemistry students are eligible.

For details contact

Ms. Athira E (Co-ordinator) 8281190582

Certificate course on Basic Chemistry Software's
PG Department of Chemistry (Self)
Course Code: CPCC44
Summary Report 2023

The course started on 25th January 2023. There were 14 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:

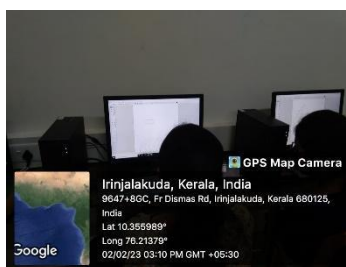
- The students were satisfied with the class. Students were familiarized with chemistry software's like Chems sketch, Chemdraw, Avogadro, gaussian etc., and also the theoretical part of computational chemistry including z- matrix. from this course the students achieve the skills like drawing chemical 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

Certificate course on Basic Chemistry Software's (30 Hours)
PG Department of Chemistry (Self)
Course Code: CPCC44
Teacher Coordinator Report

Number of students	14
Date of examination	20 th March, 2023
Total students who passed exam	14
Total course duration	30 hrs

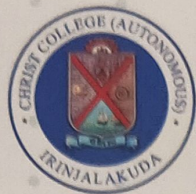
The course started on 25th January 2023. There were 14 M.Sc. 1st year students participated in the program and all completed the course. The duration of the course was 30 hrs. The classes were taken as both practical and theory sessions.



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, KERALA

DEPARTMENT OF CHEMISTRY (SELF)

**CERTIFICATE
OF PARTICIPATION**

Date: 31-03-2023

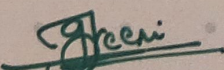
This is to certify that

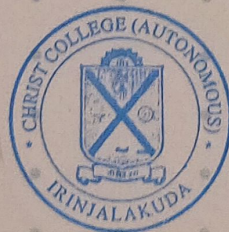
Mr/Mr's Akshaya Ramachandran

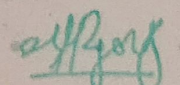
has successfully completed 30-hour course on "Basic Chemistry Software's "

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

Christ college (Autonomous) Irinjalakuda, Thrissur.


Ms. Greeni K I
Program Coordinator




Rev. Fr. Dr. Jolly Andrews CMI
Principal

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

Certificate course on Basic Chemistry Software's

PG Department of Chemistry (Self)

Course Code: CPCC44

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 ammonia molecule.
5. Compare Ab initio and semiempirical methods.
6. Give a brief comparison of STO and GTO.
7. Draw the structure of CO₂ molecule using chemdraw software
8. Show the animations of vibrations of H₂O molecule.
9. Draw the structure of water molecule using gaussian software.
10. Find out the bond energy and bond order of N₂ molecule.
11. Draw the structure of acetanilide molecule using chemsketch software.
12. Find out the dipole moment of NH₃ molecule

Certificate course on Basic Chemistry Software's

PG Department of Chemistry (Self)

Course Code: CPCC44

Assessment Procedure

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.

Assessment of candidates will be done through theoretical assignments, theoretical and practical based examinations after completion of each module. At the end of the course an exam will be conducted on the basis of syllabus. All successful candidates will be awarded with certificates.

Some sample questions are

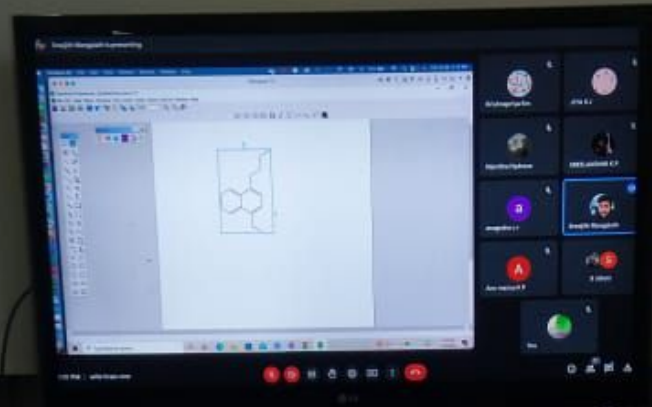
Assignment :


- draw the structures of some aromatic compounds.
- Draw the structure and show the animations of vibrations of H₂O molecule.
- Draw the structure of ammonia molecule using gaussian program. Etc.,

Examination questions:

- Write the z-matrix of CO₂ molecule.
- What are the applications of chemsketch software.
- Distinguish between GTO and STO. Etc.,

Course Coordinator: Krishnapriya.K.M



 **GPS Map Camera**



Irinjalakuda, Kerala, India

**9647+8GC, Fr Dismas Rd, Irinjalakuda, Kerala 680125,
India**

Lat 10.355989°

Long 76.21379°

02/02/23 03:10 PM GMT +05:30



GPS Map Camera

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