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CSIF

UNIVERSITY OF CALICUT

**Cloud-based Virtual Workshop:**

# Gaussian 16 & Gauss View 06
# ChemOffice Professional
# Mnova Suite + CASE

**Date: 03rd & 04th December, 2020 ~ Time: 10.00am onwards**

## Day 1 (03rd Dec 2020)

### Gaussian 16 & Gauss View 06

Module 1: (2 Hrs)

Introduction of Gaussian 16

What is Gaussian 16? , Background of Electronic Structure Theory, Independent Particle Models, Model Chemistry, Basis Sets, Standard Basis Sets, SCF Convergence and Stability, Using ONIOM, Solvation, Periodic Boundary Conditions.

Module 2: (2 Hrs)

DFT Geometry & Frequency

What is DFT? Various Functions in DFT & Raman & IR frequency calculations. Geometry Optimization, Frequency, IRC, Scan calculations.

Module 3: (2 Hrs)

Introduction to GaussView 06 & Practical Considerations

Basics of Running Gaussian Calculations, Output Files, Anatomy of a Gaussian Input File, Gaussian Utility Programs, Computational, DFT Geometries and Frequencies, Summary of Standard Methods.

## Day 2 (04th Dec 2020)

### Session 1: ChemOffice Professional

Module 1: ChemDraw Professional (1 Hr)

- Basic Drawings in ChemDraw
- Page Layout
- Shortcuts and HotKeys
- Drawing Monomer Sequences
- Advanced Drawing Tools
- Templates
- Preferences and Settings
- Drawing Biopolymers
- Structure=Name
- ChemExcel/CombiChem

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### Module 2: Chem3D (30 min)

Building a model and rotations, Generate bond length/angles/dihedral angles, Trans to Cis isomers, Steric energy of eclipsed and staggered conformers, Overlaying model to compare structural similarities, HOMO-LUMO visualization, visualizing partial charges/lone pair electrons/van der wall radius, Conformational Analysis, Molecular Dynamics, Steriochemistry.

### Module 3: Signals NoteBook (30 min)

Make notebook and experiments; share the experiments, chemical details, ChemDraw embedded notebook, working with MS Office in ELN and Reporting.

## Session 2: Mnova Suite + CASE

### Module 1: Mnova NMR (30 min)

- Basic Processing of 1D NMR
- Basic Processing of 2D NMR

### Module 2: Mnova MS (30 min)

Basic MS Processing: TIC, Mass Spectra, CoAdd Peaks/Background Subtraction, MS Browser, UV Traces, Elemental Composition, Molecular Matching, Peak Purity, Reporting.

### Module 3: Mnova Predict (15 min)

Prediction of 1H/13C/HSQC spectra from Structure and X Nuclei prediction

### Module 4: Mnova CASE (30 min)

1D and 2D spectral data importing, MCD, Structure constrain, Prediction of proposed structure

### Workshop Speakers:

- Mr. Charitra Gour
- Dr. Sourab Sinha

**Registration:**

Registration is open for 50 participants, Register here: https://forms.gle/JmyX7YQ6nSYv9T157 or Scan the QR Code

**Enquiries:**

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