Basic Software tools for Molecular Modeling and Graphics

an

Add-On Course

Session: 2022-2023

(March, 23 to May, 23)

Offered

By

Department of Chemistry

Mahatma Gandhi College, Lalpur

Daldali, Purulia

To

The Principal
Mahatma Gandhi College
Lalpur, Purulia

Through
IQAC, M. G. College

Subject: Application for Offering Add on course for the session:- 2022-23

Sir,

With due respect I, Kalyan Senapati, Department of Chemistry want to inform you that, our department is willing to offer an add on course entitled '**Basic Software tools for Molecular Modeling and Graphics**' for the ongoing session. The details of the course and evaluation procedure are attached herewith.

Kindly do the needful in our favor so that we could run the program successfully.

Thanking you

Yours faithfully

Kalyan Senapati

14.3.2023

Approved

14.3.23

MAHATMA GANDHI COLLEGE
ESTD: 1981
LALPUR, PURULIA

COURSE DETAILS

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MODULE-I: (Theory + Practical) 10 hrs

1. Installation of ChemDraw Software
2. Usage of tools present in the ChemDraw
   Lasso, Marquee, Structure perspective, Solid bond, Erasor, Multiple bond, Text, Dashed Bond, Pen Tools, Hashed Bond, Different types of arrow tools, Bold bond, Drawing tools, Wedged bond, Bracket tools, Hollow wedged Bond, Chemical symbol tools, Wavy bond, Query tools, Sequence tools, Advance tools, Acyclic chain, Templates etc.
3. Drawing of Chemical molecules, Chemical equation with Chem Draw
4. Drawing of chiral centered molecules.
5. Practicing the drawing of different types of molecules and chemical equations.

MODULE-II: (Theory + Practical) 10 hr

1. Convert the IUPAC name into structure and structure to IUPAC name
2. Find the stereochemistry of molecules
3. How to make colored structure for better understanding.
4. Use of apply objecting setting from.
5. Usage of tools that is Group, ungroup, sent back, Bring forward, flip horizontal, flip vertical, Rotate the molecule horizontally and vertically.
6. Find the analysis report of different molecules that is Name of compound, Chemical Formula, Exact Mass, Molecular Weight, m/z value, Elemental Analysis.
7. Predict the ^{1}H NMR spectra and chemical shift values
8. Predict the ^{13}C NMR spectra and chemical shift values
9. Predict the melting point, boiling point values
10. Practicing session

MODULE-III: (Theory + Practical) 5 hrs

1. Convert the 2D structure into 3D structure
2. Find the energy minimized structure of different molecule.
3. Find the bond lengths and bond angles
4. Save the molecules in different formats
5. Save molecular structures into MS word and PPTs.
6. Convert the 3D structure into ball and stick model, change the color of the model.
7. Convert the 3D structure into wire and cloud model; change the color of the model.
8. Practice session.

MODULE-IV: (Theory + Practical) 5 hrs

1. Drawing the orbital picture of different molecules.
2. Drawing the intermediate orbital structure of different reaction (Pericyclic reactions)
3. Convert the 3D structure into mesh model
4. Find the electronic surface of the molecule
5. Application of internet to draw the chemical molecules. (About scifinder)
6. Standard parameters for drawing molecules.
7. Summary of ChemDraw

Total Course Duration: 30 Hrs. (Excluding Examination)

Course objectives: One can use the chemical structure drawing program that is ChemDraw to draw different structures of organic compounds. Programs like these are used to draw not only chemical structure but also orbital picture and tentative chemical and physical property could be predicted.The course is regarding training about how to operate ChemDraw. This also gives an idea about the 3D-stereochemistry of known and unknown organic compounds.

Course outcome:-This course gives enough knowledge to the student regarding preparation of ppt for their different kind of dissertations, research work presentation for securing jobs or higher education.

Evaluation Procedure

1.	Practical performance per class -2 marks.	
	For 30 classes 2 x 30 -	60 marks.
2.	End exam and viva -	40 Marks
	Total	100 Marks

Grading

	Marks obtained	Grade
1.	80-100	**A**
2.	60-79	**B**
3.	40-59	**C**
4.	Below 40	**F** (fail)

Faculty Members:

1. Prof. KalyanSenapati, Assistant Professor & Course Co-ordinator

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NOTIFICATION TO THE STUDENTS FOR ENROLMENT

Date: 14.03.2023

Notice

It is notified for all Students of Mahatma gandhi college that Department of Chemistry, Mahatma Gandhi College, Lalpur, Purulia is going to offer an 'Add-On Course' on "**Basic Software tools for Molecular Modeling and Graphics**" Interested students are asked to enroll their name in the Dept. of Chemistry.Course fee –Nil.

(Maximum intake for this course is 20)

The Last Date of Enrolment: 29.03.2023 Time: - 2.00 PM

Venue: - Chemistry Department, M. G. College.

The Course will be started from: 31.03.2023

Venue: Computer Lab, (1st floor Administrative building) M. G. College, Purulia

Date and Time are mentioned in Course Routine

Note:

1. Successful candidates will be issued certificates by the College
2. Enrollment will be on the basisof first cum first serve.

Kalyan Senapati
Course Co-ordinator
14.3.23

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Registration sheet of Add on Course in Basic Software tools for Molecular Modeling and Graphics

Date:- 29.03.2023. **Time:-** 2:00 P.M.

SL	Roll No.	Name	Signature	Semester
1.	437	APURBA MANDAL	Apurba Mandal	IV
2.	442	SUSHANTA SEN	Sushanta Sen	IV
3.	440	RAHUL DUTTA	Rahul Dutta	IV
4.	1772	RUMPA MAHATO	Rumpa Mahato	IV
5.	07	MOUPIYA KAITY	Moupiya Kaity	VI
6.	083	Ujjwal Mandal	Ujjwal Mandal	VI
7.	11	PURNIMA KARMAKAR	Purnima Karmakar	VI
8.	447	Abhi Mukherjee	Abhi Mukherjee	IV
9.				
10.				

29.03.23

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Class Schedule

Basic Software tools for Molecular Modeling and Graphics

An ADD-ON COURSE

SL	Date	Day	Time	Hours	Respective Teacher
1	31.03.23	Friday	12 'O' clock – 3:00 PM	3 Hrs	KS
2	01.04.23	Saturday	11.30 PM – 1.30 PM	2 Hrs	KS
3	04.04.23	Tuesday	1.00PM – 4:00 PM	3Hrs	KS
4	05.04.23	Wednesday	2.00- 4.00 PM	2 Hrs	KS
5	06.04.23	Thursday	2.00- 4.00 PM	2 Hrs	KS
6	11.04.23	Tuesday	2.00- 4.00 PM	2 Hrs	KS
7	02.05.23	Tuesday	2.00- 4.00 PM	2 Hrs	KS
8	03.05.23	Wednesday	2.00- 4.00 PM	2 Hrs	KS
9	04.05.23	Thursday	2.00- 4.00 PM	2 Hrs	KS
10	10.05.23	Wednesday	2.00- 4.00 PM	2 Hrs	KS
11	11.05.23	Thursday	2.00- 4.00 PM	2 Hrs	KS
12	12.05.23	Friday	2.00- 4.00 PM	2 Hrs	KS
13	16.05.23	Tuesday	2.00- 4.00 PM	2 Hrs	KS
14	17.05.23	Wednesday	2.00- 4.00 PM	2 Hrs	KS
15	20.05.23	Saturday (Examination)	2.00- 4.00 PM	2 Hrs	In-Charge SK

Kalyan Senapati

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ok

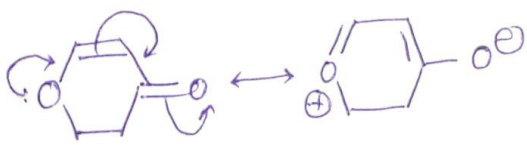
Attendance sheet of Add on Course in Basic Software tools for Molecular Modeling and Graphics

Date:- 31.3.23 Time = 12.00 to 3.00 PM.

SL	Roll No.	Name	Signature	SEM
1.	07	Moupiya Kaity	Moupiya Kaity	VI
2.	11	PURNIMA KARMAKAR	Purnima Karmakar	VI
3.	1772	RUMPA MAHATO	Rumpa Mahato	IV
4.	03	Ujjwal Mandal	Ujjwal Mandal	VI
5.	437	Apurba Mandal	Apurba Mandal	IV
6.	447	Abhi Mukherjee	Abhi Mukherjee	(IV)
7.	442	Sushanta Sen	Sushanta Sen	(IV)
8.	440	Rahul Dutta	Rahul Dutta	(IV)
9.				
10.				
11.				
12.				
13.				
14.				
15.				
16.				
17.				

lecture on

Introductory of chem draw Soft ware and Step by Step details of the software was delivered. Students practiced the ~~following~~ drawing of following Structures using chemdraw Soft ware.



Kalyan Sengupta
31.3.23

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NOTIFICATION OF EXAMINATIONS

The examination of add-on course entitled "Basic Software tools for Molecular Modeling and Graphics" will be held on 20.5.2023 in the Computer lab at 2:00 P.M. Students are requested to be present 15 minute in advance in the exam venue.

Course Title: -'Basic Software tools for Molecular Modeling and Graphics'
Full Mark: - 40
Date: - 20.5.2023
Time: - 2.00- 4.00P.M.

Kalyan Senapati.
Course Co-ordinator
16.05.2023.

Mahatma Gandhi College, Lalpur

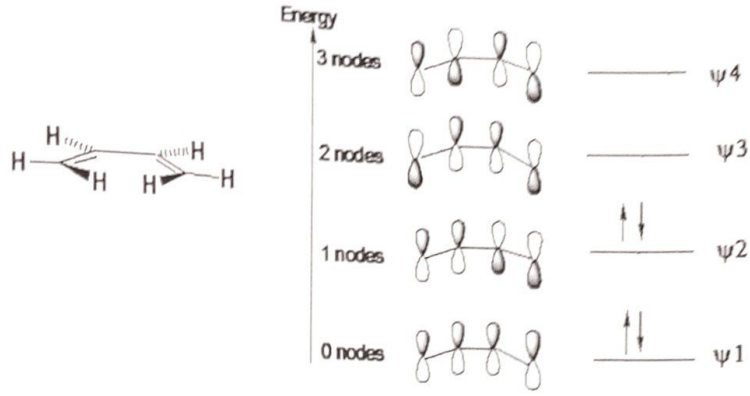
Add-on Course Examination, 2022-23

Course Title - Basic Software tools for Molecular Modeling and Graphics

F.M.-40 Time 2 hrs

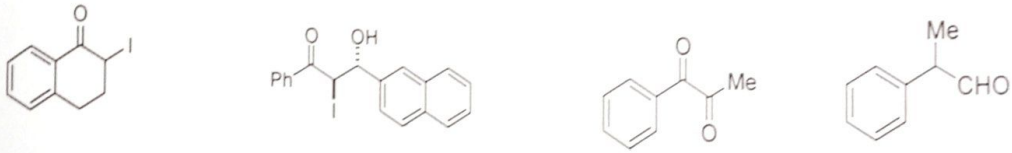
All questions are compulsory

1. Draw the orbital picture 20

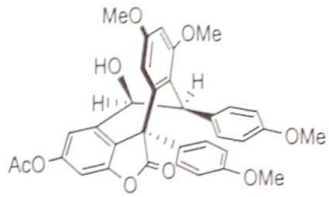


2. Draw the structure of the compounds and find out the Exact mass formula and ^{1}H NMR Spectrum.

2.5x4=10



3. Draw the structure 10



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LALPUR, PURULIA

Attendance sheet for examination of Add on Course in "Basic Software tools for Molecular Modeling and Graphics"

Date:- 20.05.2023 **Time:-** 2.00 - 4.00 PM

SL	Roll No.	Name	Signature	Semester
1.	442	SUSHANTA SEN	Sushanta Sen	IV
2.	437	APURBA MANDAL	Apurba Mandal	IV
3.	440	RAHUL DUTTA	Rahul Dutta	IV
4.	1772	RUMPA MAHATO	Rumpa Mahato	IV
5.	07	MOUPIYA KAITY	Moupiya kaity	VI
6.	083	Ujjwal Mandal	Ujjwal Mandal	VI
7.	447	Abhi Mukherjee	Abhi Mukherjee	IV
8.	11	PURNIMA KARMAKAR	Purnima Karmakar,	VI
9.				
10.				

20.05.23.

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Score Sheet with Grade

Sl	Name	Full marks	Marks obtained			Grade
			Daily work	Final exam	Total	
1.	Apurba Mandal	100	60	36	96	A
2.	Susanta Sen	100	60	35	95	A
3.	Rahul Dutta	100	60	35	95	A
4.	Rumpa Mahato	100	60	37	97	A
5.	Moupiya Kaity	100	60	38	98	A
6.	Ujjal Mandal	100	58	34	92	A
7.	Purnima Karmakar	100	60	36	96	A
8.	Abhi Mukherjee	100	60	32	92	A
9.						
10.						

Kalyan Senapati

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ESTD: 1981
LALPUR, PURULIA

MAHATMA GANDHI COLLEGE, LALPUR

Daldali , Purulia PIN 723130

mahatmagandhicollegelalpur.ac.in

NAAC Accredited, Grade 'B+' w.e.f. 16.09.201

Certificate

This is to certify that ..... fied student

of Sem ..... of Mahatma Gandhi Collea ... Purulia has

successfully completed the Add-on Course on "...Basic...Softwar...ols for.....

Molecular...Modeling and Graphics....." organi... ...partment of

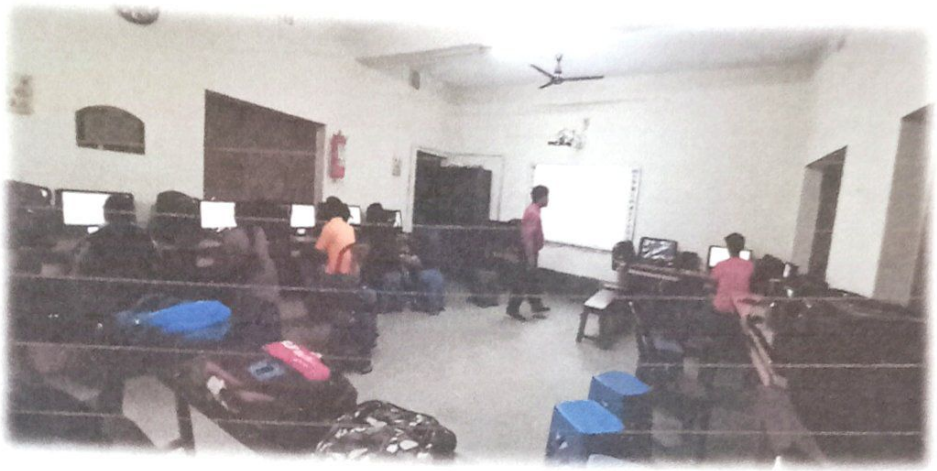
Chemistry.....from March,2023.....to ...May, 2023 ...and he

/ she has obtained A/B/C grade.

Principal

Course C...

PICTURES



Add-on class taken by Prof. Kalyan Senapati

Valedictory session