

AVOGADRO CHE.C.23.1

ALL SAINTS' COLLEGE THIRUVANANTHAPURAM Affiliated to University of Kerala spoken-tutorial Re-accredited with A+ Grade by NAAC wered by n Resources and Certificate Course conducted by The Department of Chemistry, All Saints' College, Thiruvananthapuram in Association with Spoken Tutorial Programme IIT Bombay for the academic year 2023-24 On Avogadro

Duration – 4 weeks

Registration starts on 01/04/24 and ends on 07/04/24 Event Date: 10/04/24 to 08/05/24

Jessy Velusamy **Training Manager** Spoken Tutorial - IIT Bombay

Event coordinator Dr. Nimmy Mohan

HOD Dr. Sunita Kurur

Principal Prof. Dr. Reshmi R Prasad



NCIPAL All Saint's College Thiruvananthapuran-

ALL SAINTS' COLLEGE



Thiruvananthapuram-695007, Kerala, India Phone: 0471-2501153

E-mail: allsaintscolegeasc@gmail.com

2023-2024

Name of Course	Certificate on Course on "Avogadro"	
Department offering the Course	Department of Chemistry	
Course Duration	30 Hours	
Start date	10/04/2024	
End date	08/05/2024	
Faculty In Charge	Dr. Nimmy Mohan	

SYLLABUS

Avogadro is a free and open source, advanced molecule editor and visualizer designed for crossplatform use in computational chemistry, molecular modelling, material science, bioinformatics, etc.

Avogadro has features for high quality rendering, interactive tools, commands and powerful plugin architecture. The features also include easy import of chemical files from Open Babel, multiple computational packages, crystals and biomolecules.

The Spoken Tutorial Effort for Avogadro has being contributed by Madhuri Ganapathi and Dr. Snehalatha Kaliappan

Basic Level

1. Overview of Avogadro

- About Avogadro software
- · Download and installation of Avogadro in Windows OS
- Download and installation of Avogadro in Mac OSX
- Download and installation of Avogadro in Ubuntu Linux
- Open documentation page
- About Avogadro interface and menus
- Explain the benefits of Avogadro
- Play the video clippings of the tutorial series on the Spoken Tutorial website

2. Build Molecules

- Import Molecules from chemical database
- Rotate the molecules
- · Zoom in and zoom out the structures
- Build molecules on the Panel using Draw tool
- Set up force field and optimize the geometry using optimization tool
- Measure bond lengths, bond angles and dihedral angles
- Show fragment library
- Build DNA/RNA molecules and peptides



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3. Edit Molecules

- Add and delete atoms
- Add and delete bonds
- Rotate bonds and change length of the bond
- Change hydrogen to methyl group
- Copy, paste and join structures.

4. Create Surfaces

- View properties of the molecule
- Label the atoms with partial charge
- Create Van der waals surface
- Color the surface according to the electrostatic potential energies.

5. Hydrogen Bonding

- How to configure Avogadro
- Show Intermolecular hydrogen bonding
- Show Intramolecular hydrogen bonding
- Measure length of hydrogen bonds
- Show Force display type in water molecules
- Show dipole moments in molecules

Intermediate Level

1. General Features in Avogadro

- Proton transfer in compounds by changing pH values
- · Load crystal structures from Crystal library
- Explain about Miller indices and planes
- Show various Miller planes in crystal systems
- Build super cell in three dimensions
- Show geometries in coordination compounds
- Build carbon nano tubes

2. Stereoisomerism

- Define stereoisomerism
- Define conformational isomerism
- Show conformations of 1,2-dichloroethane
- Show conformations of cyclohexane
- Define geometrical isomerism
- Demonstrate geomertical isomerism
- Explain R S configuration priority rules
- Demonstrate R-S configurations with examples

Advance Level

File Extensions

- Prepare input files for computational chemistry programmes such as: GAMESS, Gaussian, MOPAC, NWChem etc.
- View Molecular orbitals and calculated IR spectrum using output files generated from GAMESS and Gaussian software.



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Course outcome:

Upon completion of the course the student will be able to

- Create and visualize chemical structures in 3D.
- Render secondary structures of proteins and nucleic acids.
- Can show hydrogen bonding in various structures.
- Display structures in various display formats such as ball-and-s/ck, CPK, sticks etc.
- Change the thickness of bonds, colour of atoms and bonds.
- Rotate and view the molecule from various angles.
- View R and S configurations
- Show geometries of coordination compounds like trigonal bipyramidal, octahedral, pentagonal bipyramidal.
- Use images in PDFs and publications
- Load crystal structures and show miller indices
- Build carbon nano tubes

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2023-2024

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Department offering the Course	Certificate on Course on "Avogadro"	
Course Duration	Department of Chemistry	
	30 Hours	
Start date 10/04/2024		
End date	08/05/2024	
Faculty In Charge	Dr. Nimmy Mohan	

Course summary

The certificate course "**Avogadro**" has been organized by the Department of Chemistry, All Saints' College, Thiruvananthapuram, coordinated by Dr. Nimmy Mohan, Assistant Professor in the Department of Chemistry. The course was conducted in association with IIT Bombay, Spoken Tutorial Program, powered by MoE, Govt. of India. 37 students enrolled for the program. The course registration started on 01/04/2024 and ended on 07/04/2024. The event started on 10/04/2024 and ended on 08/05/2024. After completion of the course the students appeared for the online exam by IIT Bombay, Spoken Tutorial on 17/05/24. All students passed in the examination and obtained Participation certificate and Course completion certificate.





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Students attending the course



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All Saint's College

Sample Certificates of "Avogadro"





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Certificate of Participation

This is to certify that Sreethu 2003 has participated in Student Training Programme from 2024-04-10 to 2024-05-08 on Avogadro organized by All Saints College, TVM with course material provided by Spoken Tutorial Project, IIT Bombay.

This training is offered by the Spoken Tutorial Project, IIT Bombay.

Prof. Kannan M IIT Bombay

Credits for the Spoken Tutorial courses are based on our estimates of the work required to complete them. Recipient institutions are required to apply due diligence and get them ratified/modified by their own duly formed academic/assessment body. Spoken Tutorial is a project at IIT Bombay, started with funding from the National Mission on Education through ICT, Ministry of Education (previously MHRD), Govt. of India.



Certificate for Completion of Training

This is to certify that **Sreethu 2003** successfully passed a **Avogadro** test, remotely conducted by the Spoken Tutorial project, IIT Bombay, under an honour invigilation system. Self learning through Spoken Tutorials and passing an online test completes the training programme.

Credits: 1 Score: 72.50%

May 8th 2024

Prof. Kannan M N IIT Bombay

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Credits: 1 Score: 75.00%

May 8th 2024

Prof. Kannan M M UT Bom bay

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ANDRUM

All Saint's College Thiruvananthapuram



Certificate of Participation

This is to certify that **Devika R saji** has participated in **Student Training Programme** from **2024-04-10** to **2024-05-08** on **Avogadro** organized by **All Saints College, TVM** with course material provided by Spoken Tutorial Project, IIT Bombay.

This training is offered by the Spoken Tutorial Project, IIT Bombay.

IIT Bombay

Credits for the Spoken Tutorial courses are based on our estimates of the work required to complete them. Recipient institutions are required to apply due diligence and get them ralified/modified by their own duly formed academic/assessment body. Spoken Tutorial is a project at IIT Bombay, started with funding from the National Mission on Education through ICT, Ministry of Education (previously MHRD), Govt. of India.



Certificate for Completion of Training

This is to certify that **Devika R saji** successfully passed a **Avogadro** test, remotely conducted by the Spoken Tutorial project, IIT Bombay, under an honour invigilation system. Self learning through Spoken Tutorials and passing an online test completes the training programme.

Credits: 1 Score: 45.00%

May 8th 2024

> Hondys Prof. K galys IIT Bombay

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All Saint's College Thiruvananthapurar



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Indian Institute of Technology Bombay

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CERTIFICATE OF SPOKEN TUTORIAL (ST) TRAINING

Ref. No. STIITB/2024/3739

4th June 2024

To, **The Principal** All Saints' College Thiruvananthapuram, Kerala-695007

We are delighted to provide your Institute with the Letter of Certification depicting the Training you undertook for students. All Saints' College, Thiruvananthapuram, Kerala engaged many learners right in taking the - ST-IIT Bombay courses and acquiring powerful IT knowledge. This is under the partnership agreement between All Saints' College and ST (Spoken Tutorial) Program- IIT Bombay-powered by the National Mission on Education through ICT, MoE, Govt. of India.

The Student Development Program (SDP) on **Avogadro** was appreciated by the students of your Institute. The training was done between 10th April 2024 & 8th May 2024 and covered 37 students. Again, in deep acknowledgement of your stellar efforts. We wish to collaborate many more times in this manner with you.

Details of Participants	enrolled in the Softwa	re Training Workshops	under Spoken Tutorial, III
Bombay:			

Sombay:		Sr no.	Name	Sr no.	Name
Sr no.	Name		Sreenandha BS	25	Asiya SS
1	Sumayya Safrin S	13			
2	Kavya PR	14	Gopika Baiju	26	Fousiya S
3	Amritha S	15	Anjana Cletus	27	Fathima Siddique
4	Megha Ramakrishnan	16	Nabeesathul Misiriya m.s	28	Anna Gifty
5	Gowri JR	17	Lekshmi Sushanth	29	Adithya R. S
6	Avani A.S	18	Sanusha M	30	Vincy V G
7	Devika R saji	19	Saniya Sulaiman	31	Sreethu
8	Anjali. S	20	Athena Bigi joe	32	Sanviya Paulson
9	Gayathri. L.S	21	Rudra Suresh	33	Glinda G. S
10	Devika RS	22	Aswani A S	34	Ashna R
10	Shahma N	23	Lisha Joy LS	35	Parvathy S Kumar
12	Aswini M	24	Irfana. s	36	Noura Fathima
				37	Abira Krishna B R

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For and On behalf of Spoken Tutorials, Indian Institute of Technology, Bombay

Akanksha Saini

Mrs. Akanksha Saini National Coordinator Spoken Tutorial Project, IIT Bombayy

PRINCIPAL All Saint's College Thirevananthapuram



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Letter of Association

Ref. No. STIITB/2024/3738

4th June 2024

To. The Principal All Saints' College Thiruvananthapuram, Kerala-695007

We are happy to announce the ASSOCIATION of Knowledge Partner Spoken Tutorial Program, IIT Bombay with All Saints' College, Thiruvananthapuram, Kerala. Your College is officially now an Academic Center-ILM for initiating Spoken Tutorial Training. The Program is a part of the National Mission on Education through ICT, MOE, Govt. of India, to spread IT Literacy all over India. We are promoting the learning and usage of Free & Open-Source Software (FOSS), through an Audio-Video teaching tool, viz, 'Spoken Tutorial'.

We support and motivate colleges to train students in Basic Computer Skills, Software, and IT. The course and the training are offered for Rs.236/student/course and Rs. 590/faculty/course including GST to the College. Your association is highly appreciated. The college has trained 37 learners (in Avogadro).

Looking forward to many enrolments and covering more departments in the College. You are making an outstanding contribution to using ICT-based teaching and learning methodology for students of your College.

For and On behalf of Spoken Tutorials, Indian Institute of Technology, Bombay

Akanksha Saini

Mrs. Akanksha Saini **National Coordinator** Spoken Tutorial Project, IIT Bombay



All Saint's College Thiruvananthapuram

List of students who have participated in the "Avogadro" certificate course organized by Department of Chemistry from 10/04/2024 to 08/05/ 2024

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34 23522100035 BIRLETHIC A S 35 23522100035 FATHIMA SIDDIQUE 36 23522100036 RUDRA SURESH	32	23522100032	SREENANDHA B S	
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36 23522100036 RUDRA SURESH 27 23522100036 RUDRA SURESH	34	23522100034	ANNA GIFTY JOSEPH	
23522100030 KODKA SUKESH	35	23522100035	FATHIMA SIDDIQUE	
37 23522100037 SANVIYA PAULSON	36	23522100036	RUDRA SURESH	
	37	23522100037	SANVIYA PAULSON	



estari PRINCIPAL

All Saint's College Thiruvananthapuram Mark List of students who have passed the National Level test for completion of Avogadro Certificate Course conducted by Spoken tutorial, IIT Bombay on 8th May 2024

SI. No	Candidate code	Name	Percentage marks
1	23522100001	Abira Krishna B.R	40%
2	23522100002	Adithya R.S	62.50%
3	23522100003	Amritha. S	60%
4	23522100004	Aswani A S	87.50%
5	23522100005	Aswini. M	87.50%
6	23522100006	Athena bigi joe	42.50%
7	23522100007	Devika RS	60%
8	23522100008	Fousiya S	75%
9	23522100009	Glinda G.S	57.50%
10	23522100010	Gopika Baiju	70.00%
11	23522100011	Lekshmi Sushanth	47.50%
12	23522100012	Lisha Joy LS	55%
13	23522100013	Megha Ramakrishnan	40%
14	23522100014	Noura Fathima R	72.50%
15	23522100015	Sanusha M	85%
16	23522100016	Shahma.N	75%
17	23522100017	Sumayya Safrin S	75%
18	23522100018	Vincy V G	70%
19	23522100019	Anjali.S	55%
20	23522100020	Anjana Cletus	85%
21	23522100021	Ashna.R	72.50%
22	23522100022	Asiya SS	52.50%
23	23522100023	Avani A.S	75%
24	23522100024	Devika R Saji	45%
25	23522100025	Gayathri LS	65%
26	23522100026	Gowri.JR	62.50%
27	23522100027	Irfana.s	47.51%
28	23522100028	Kavya PR	65%
29	23522100029	Nabeesathul Misiriya MS	72.50%
30	23522100030	Parvathy S Kumar	65%
31	23522100031	Saniya Sulaiman	40.00%
32	23522100032	Sreenandha BS	65%
33	23522100033	Sreethu AS	72.50%
34	23522100034	Anna Gifty Joseph	52.5
35	23522100035	Fathima Siddique	72.50%
36	23522100036	Rudra suresh	45%
37	23522100037	Sanviya Paulson	50%

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PRINCIPAL

All Saint's College Thiruvananthapuram