

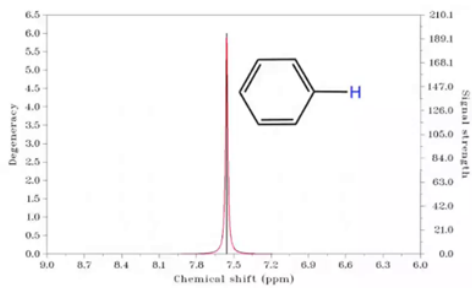


### ST. XAVIER'S COLLEGE, MAPUSA GOA

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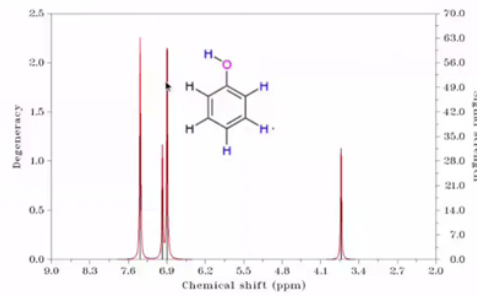
<b>Nature of Event</b> (Workshop, Guest Lecture, Addon Course, Seminar, etc.)	Webinar
<b>Name of Department</b>	Chemistry
<b>Faculty In-charge</b>	Dr. Johnross V. Albuquerque
<b>Stratum of Event</b> (College, State, Regional, National)	College
<b>Title of Event</b>	Computational Chemistry
<b>Date of Event</b>	15 <sup>th</sup> October 2022
<b>Venue</b>	Online platform (MS Teams)
<b>Resource Person details</b>	Mr. Vishnu Chari, Assistant Professor, School of Chemical Sciences, Goa University
<b>Objective/ Scope of Event</b>	To provide the participants an opportunity to learn about the subject of Computational Chemistry by introducing the topic, what it has to offer, and the theoretical basis required to venture into the field.
<b>Particulars of Event</b>	Mr. Vishnu spoke on how the subject of Quantum Chemistry came into being and the various aspects of the Schrodinger Equation, which is the heart of Quantum Mechanics. He also spoke on the basic postulates of Quantum Mechanics and ended the session with several examples on how Computational Chemistry was helpful for organic chemists.
<b>Outcome of Event</b>	Participants learnt about Computational Chemistry, different type of calculations and software available.
<b>Feedback</b>	Very informative and interesting session
<b>Total No. of Participants</b>	46 online participants

## Photographs



Protons attached to the aromatic ring in phenols show up near the aromatic region of an NMR spectrum (7-8 ppm). These peaks will have splitting typical for aromatic protons. The protons directly attached to the alcohol oxygen of phenols appear in the region of 3 to 8 ppm.

The benzene protons are highly deshielded. Their chemical shift is far downfield, in the range of 6.5–8.5 ppm.



KT Kapila Talwar	DA Dr. Afreen Abb...
	VC Vidhu Chel... (G...
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TH Tanuja Chakrab...	FF Fani Fernandes
AS Arshad	AS Arshad
S S. 25 7578 indid	JM Jani Mousa
S Srinika	GP Godam Raju P...
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