

# DIVITA GUPTA

Experience in infrared, microwave and laser spectroscopy for studies of gas-phase molecules/complexes and reaction kinetics. Looking for opportunities to explore astro-physically relevant species spectroscopically and investigate their reactions under low temperature conditions.



## CONTACT

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## SKILLS

### Programming

Python Fortran95  
C LaTex  
LabVIEW

### Software & Tools

#### Data handling/analysis

Igor Pro, Origin, numpy, scipy

#### Computational

Gaussian09, MESMER, AIM2000, PGO-PHER

#### Technical/Experimental

Vacuum systems, Pulsed lasers (excimer & dye), Cryogenics, FTIR spectroscopy, Chirped-pulse microwave spectroscopy

#### Visualisation

gnuplot, Inkscape, Adobe photoshop, GIMP

### Languages

English ●●●●●  
Hindi ●●●●●  
Punjabi ●●●●●  
French ●●●●●

## RESEARCH EXPERIENCE

📅 Sep'18 - present (Expected graduation: Sep'21) | **Ph.D.**

**Prof. Ian Sims** | University of Rennes 1, France

Integrating the CRESU technique with chirped-pulse microwave spectroscopy to study branching ratios for low-temperature astrochemically relevant reactions

Rotational Spectroscopy CRESU Laser-Induced Fluorescence Chemical Kinetics

📅 Aug'17 - May'18 | **Masters thesis**

**Prof. K.S. Viswanathan** | IISER Mohali, India

Ethylene glycol-water interactions using Matrix Isolation FT-IR Spectroscopy & *ab-initio* calculations

FT-Infrared Spectroscopy Matrix-Isolation Gaussian09 Quantum Calculations

### RESEARCH VISITS

📅 Mar'20 | **Prof. Dwayne Heard** | University of Leeds, U.K.

Understanding MESMER to calculate multi-channel reaction rates

MESMER Reaction Rate Calculations Stochastic Energy Grained Master Equation

📅 Dec'17 | **Dr. Bhalamurugan Sivaraman** | NSRRC, Taiwan

VUV and photolysis experiments on astrochemically relevant ices

Molecular Spectroscopy Synchrotron Electronic Spectroscopy Astrochemistry

### SUMMER INTERNSHIPS

📅 May'17 - Jul'17 | **Prof. Ian Sims** | University of Rennes 1, France

Using the CRESU technique to study rotational energy transfer during inelastic collisions

CRESU Lasers Gas phase Low-temperature Kinetics Molecular Spectroscopy

📅 Jun - Jul'16 | **Dr. Bhala Sivaraman** | Physical Research Laboratory, India

Ethylene glycol-water interactions on ISM cold dust analogs

Molecular Spectroscopy FT-Infrared Spectroscopy Ices Astrochemistry

📅 May - Jul'15 | **Prof. J. Chengalur, Dr. N. Ramanujam** | NCRA-TIFR, India

Spectral line commissioning of a 15m radio dish & HI mapping of the galactic plane

Radio Astronomy Observational Astronomy Programming Python

## ACHIEVEMENTS, AWARDS & GRANTS

🏆 IAU travel grant | Apr'19

Travel grant to present posters on Masters' and PhD projects at IAUS 350

🏆 CSIR-JRF Fellow | All India Rank: 48 | Jun'18

A competitive exam organized by the Council of Scientific & Industrial Research (CSIR), India, a premier national R&D organisation

🏆 S N Kaul Award | May'18

Awarded by the President of India for the best all-round performance, academic and extra-curricular, in the graduating class of 2018, IISER Mohali

🏆 Certificate of Excellence | Aug'13-May'18

Awarded for scoring the highest GPA among the graduating class of 2018 in Chemical Sciences, IISER Mohali

🏆 KVPY Scholar | Aug'13-Jul'18

National Program of Fellowship in Basic Sciences, initiated and funded by the Department of Science and Technology, Government of India

🏆 Lindau Nobel Laureate Meeting | Jul'17

Funded by DFG, Germany & DST, India. Dedicated to Chemistry; chosen among top 420 young scientists across the world to attend the meeting


🏆 Certificate of Academic Excellence, CNR Rao Scholarship | Aug'17, '15 & '14

Ranked first in the class (of 40 students in Chemistry) in semester 2016-17 and ranked first in the class (of 140 students) in 2014-15 & 2013-14

## PUBLICATIONS


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### Low Temperature Kinetics of the Reaction Between Methanol and the CN Radical

 **D. Gupta**, S. Cheikh Sid Ely, I. R. Cooke, T. Guillaume, O. Khedaoui, T. S. Hearne, B. M Hays, I. R. Sims


 2019  The Journal of Physical Chemistry A, 123(46), 9995-10003  DOI




### Rate Constants of the CN + Toluene Reaction from 15 – 294 K and Interstellar Implications

 J. P. Messinger, **D. Gupta**, I. R. Cooke, M. Okumura, I. R. Sims

 2020  The Journal of Physical Chemistry A., 124(39), 7950–7958  DOI

### Benzonitrile as a Proxy for Benzene in the Cold ISM: Low-Temperature Rate Coefficients for CN + C<sub>6</sub>H<sub>6</sub>

 I. R. Cooke, **D. Gupta**, J. P. Messinger, I. R. Sims

 2020  The Astrophysical Journal Letters, 891(2), L41  DOI, arXiv


### Design and performance of an E-band chirped pulse spectrometer for kinetics applications: OCS – He pressure broadening

 B. M Hays, T. Guillaume, T. S. Hearne, I. R. Cooke, **D. Gupta**, O. Khedaoui, S. Le Picard, I. R. Sims

 2020  Journal of Quantitative Spectroscopy and Radiative Transfer 2020, 250, 107001  DOI

## Submitted/Under preparation



### Vacuum ultraviolet photoabsorption spectra of an in-situ synthesized peptide precursor – hydroxylamine on a cold astrochemical dust analogue

 R. Thombre, **D. Gupta**, S. Pavithraa, J. -I. Lo, S. -L. Chen, Y. -J. Wu, K. K. Rahul, B. -M. Cheng, H. Hill, A. Bhardwaj, B. N. Raja Sekhar, N. J. Mason, B. Sivaraman


 In revision


### N-Graphene and Quantum Dots Synthesized in Astrochemical Ices

 K. K. Rahul, M. Ambresh, D. Sahu, J. K. Meka, S. -L. Chou, Y. -J. Wu, **D. Gupta**, A. Das, J. -I. Lo, B. -M. Cheng, B. N. Raja Sekhar, A. Bhardwaj, N. J. Mason, B. Sivaraman

 In revision  arXiv


### Measuring the Difference in Collisional Interaction of HCN and HNC with He at Low Temperatures

 B. M Hays, T. Guillaume, **D. Gupta**, O. Khedaoui, F. Thibault, F. Lique, F. Dumouchel, I. R. Sims

 Under preparation

### Quantitative Detection of Bimolecular Reaction Products in Continuous Low-Temperature Uniform Supersonic Flows by Chirped Pulse Millimeter-Wave Spectroscopy

 T. Guillaume, **D. Gupta**, ..., I. R. Sims

 Under preparation

## TEACHING EXPERIENCE

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<b>Instructor (Partial)</b>	Dec'20 - Jan'21 & Oct'19-Nov'19, Univ. Rennes 1   <b>Scientific and Technical Communication in English</b> (Masters level)
<b>Teaching Assistant</b>	Jan'21 - present Univ. Rennes 1   <b>Molecular Spectroscopy- introductory course</b> (Masters level)
<b>Teaching Assistant</b>	Oct'19 - Nov'19, Univ. Rennes 1   <b>Data Analysis</b> (Masters/Ph.D. level)
<b>Teaching Assistant</b>	Jan'18 - Apr'18, IISER Mohali   <b>Analytical Chemistry Laboratory course</b> (Masters level)
<b>Teaching Assistant</b>	Aug'17 - Nov'17, IISER Mohali   <b>Physical Chemistry Laboratory course</b> (Masters level)
<b>Tutor</b>	Aug'17 - Nov'17, IISER Mohali   <b>Chemistry of elements and chemical transformations</b> (First year undergraduate chemistry course)

## LEADERSHIP/MENTORING ROLES

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<b>Summer intern supervisor</b>	<b>May'19-Jun'19</b>   Supervised a summer intern on setting up & calibrating a UV-Vis spectrometer
<b>Co-organiser</b>	<b>May'20</b>   Co-organiser of "Women in Astrochemistry" session organised under Astrochem Discussions
<b>Head Coordinator</b>	<b>Oct'17</b>   Main coordinator for a science outreach event for school children
<b>Cultural Secretary</b>	<b>Sep'15- Aug'16</b>   Leading all the institute clubs and organizing various cultural events
<b>Co-convener, Astronomy Club</b>	<b>Sep'14- Aug'15</b>   Coordinating multiple activities/talks relevant to astronomy

## EDUCATION

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📅 Aug'13-May'18

Indian Institute of Science Education and Research,  
Mohali, India

Dual BS-MS in Chemistry

CPI: 9.4/10

## CONFERENCES/ OUTREACH TALKS

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- Oral Contribution**      *Rescheduled* Mar'21 | **Faraday joint interest group conference**  
Exploring product-specific reaction kinetics in uniform supersonic flow
- Oral Contribution**      Aug'20 | **Astrochemistry Discussions (online)**  
Laboratory Measurements of Gas-Phase Reaction Kinetics with CN radical at Low Temperatures
- Oral Contribution**      Jul'20 | **PCMI biennial conference (online due to COVID)**  
Laboratory measurements of gas-phase reactions between aromatic species and the CN radical at low temperatures
- Invited outreach talk**      July 31, 2020 | **Sacred Heart College, Tirupattur, India (online)**  
How Rocket Science proved Arrhenius (Partially) Wrong: Measuring Reaction Kinetics using Laser-Induced Fluorescence Spectroscopy
- Oral Contribution**      Oct'17 | **Astrochemistry in THz meeting, Chennai, India**  
Matrix Isolation-FTIR and *Ab-Initio* Studies of Ethylene Glycol and Ethylene Glycol:Water complexes
- Poster**      Apr'19 | **IAU Symposium on Laboratory Astrophysics, IAUS 350, Cambridge, U.K.**  
Kinetics of the reaction between the CN radical and methanol at low temperatures using the CRESU technique
- Poster**      Apr'19 | **IAU Symposium on Laboratory Astrophysics, IAUS 350, Cambridge, U.K.**  
Vacuum Ultraviolet photoabsorption of molecules with astrochemical and astrobiological relevance: Benzonitrile and Hydroxylamine

## REFEREES

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**Prof. Ian R. Sims** | Senior Professor  
Institut de Physique de Rennes  
Université de Rennes 1  
ian.sims@univ-rennes1.fr

**Dr. Bhalamurugan Sivaraman** |  
Associate Professor  
Atomic Molecular and Optical  
Physics Division  
Physical Research Laboratory, India  
bhala@prl.res.in

**Prof. K.S. Viswanathan** | Senior  
Professor (Retired), IISER Mohali  
Currently: Visiting Professor  
KREA University, India  
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