

PROFILE OF THE TEACHERS

1. **Name:** Dr. Pradeep Kumar Rao
2. **Father's Name:** Shyam Dev
3. **Mother's Name:** Barsati Devi
4. **Department:** Chemistry
5. **Date of Joining the University:** 02 July, 2018



6. **Total Teaching Experience:** UG- 3 Year 9 Month PG- 3 Year 9 Month
7. **Total Research Experience:** 12 Year
8. **Area of specialization:** Physical Chemistry
9. **Academic Qualifications:**

B.Sc.	2007	St. Andrew's College, Gorakhpur	First
M.Sc.	2009	DDU Gorakhpur University, Gorakhpur	Second
Ph.D.	2014	DDU Gorakhpur University, Gorakhpur	Awarded
PDF	2015	Savitribai Phule Pune University, Pune	
Any Other			

10. International/National fellowship/financial support for advance studies/research

S. No.	Name of the fellowship/ financial support	Year of Award	National/International	Awarding Agency
1	DSA-BSR Fellowship	2010	National	UGC, New Delhi
2	RGNF	2011	National	UGC, New Delhi
3	DS Kothari Fellowship	2015	National	UGC, New Delhi

11. International/National award/recognition for academics

S. No.	Name of the award/recognition	Year of Award	Title of the innovation	National/Int ernational	Awarding Agency
1	Startup-Grant	2019	Computational Studies on Hydrofluoro- olefins	National	UGC, New Delhi

12. Extension activity participation

S. No.	Name of activity	Year

If any award/recognition received-

S. No.	Name of activity	Name of the award/recognition	Year of Award	National/International	Awarding Agency

13. Ph.D. supervised

S. No.	Name of the Ph.D. scholar	Title of the thesis	Year of registration of the scholar	Year of award of Ph.D.
1	Kamal Kant Rav	Computational Studies on Atmospheric Degradation of Olefins		

14. Research/Review Papers published

S. N.	Title of paper	Name of the author/s	Name of journal	Year of publication	ISSN number	Link to the recognition in UGC enlistment of the Journal		
						Link to website of the Journal	Link to article/paper /abstract of the article	Is it listed in UGC Care list/Scopus /Web of Science /other, mention
1.	Temperature Dependent Kinetic Study of the Gas Phase Reaction of Ozone with 1-penten-3-ol, cis-2-penten-1-ol and trans-3-hexen-1-ol: Experimental and Theoretical Data	C. Kalalian, G. El Dib, H. J. Singh, P. K. Rao , E. Roth, A. Chakir.	<i>Atmos. Environ</i>	2020		https://www.journals.elsevier.com/atmospheric-environment	Temperature dependent kinetic study of the gas phase reaction of ozone with 1-penten-3-ol, cis-2-penten-1-ol and trans-3-	YES

							hexen-1-ol: Experimental and theoretical data - ScienceDirect	
2.	Product Investigation of the Gas Phase Ozonolysis of 1-penten-3-ol, cis-2-penten-1-ol and trans-3-hexen-1-ol	C. Kalalian, E. Roth, G. El Dib, H. J. Singh, P. K. Rao , A. Chakir	<i>Atmos. Environ</i>	2020		https://www.journals.elsevier.com/atmospheric-environment	Product investigation of the gas phase ozonolysis of 1-penten-3-ol, cis-2-penten-1-ol and trans-3-hexen-1-ol - ScienceDirect	YES
3.	Synthesis and biological activity of imidazole based 1,4-naphthoquinones.	D. Choudhari, S. S. Gawalia, D. Chakravarty, S. Shaikh, D. N. Lande, S. P. Gejji, P. K. Rao , S. Satpute, V. G. Puranik, R. Gonnade.	<i>New. J. Chem</i>	2020		New Journal of Chemistry Home-A journal for new directions in chemistry (rsc.org)	Synthesis and biological activity of imidazole based 1,4-naphthoquinones - New Journal of Chemistry (RSC Publishing)	YES
4.	Understanding the Atmospheric Oxidation of HFE-7500 (C ₃ F ₇ CF(OC ₂ H ₅)CF(CF ₃) ₂) Initiated by Cl and NO ₃ Radical from	P. K. Rao , R. C. Deka, N. K. Gour and S. P. Gejji	<i>J. Phy. Chem. A</i> ,	2018		The Journal of Physical Chemistry A (acs.org)	Understanding the Atmospheric Oxidation of HFE-7500 (C₃F₇CF(YES

	Theory.						OC2H5)C F(CF3)2 Initiated by Cl Atom and NO3 Radical from Theory The Journal of Physical Chemistr y A (acs.org)	
5.	Reaction Pathways andRate Constants for Atmospheric Oxidation of HCFO-1233zd(E) Initiated by OHRadical, Cl Atom and O ₃ Molecule.	P. K. Rao and S. P. Gejji.	<i>J. Fluor. Chem.</i>	2018		Journal of Fluorine Chemistry ScienceDi rect.com by Elsevier	Atmosphe ric degradati on of HCFO- 1233zd(E) initiated by OH radical, Cl atom and O3 molecule: Kinetics, reaction mechanis ms and implicatio ns - ScienceDi rect	YES
6.	Kinetics andMechanistic Investigations of Atmospheric Oxidation of HFO-1345fz by OHRadical: Insights from Theory	P. K. Rao and S. P. Gejji	<i>J. Phys. Chem. A.</i>	2017		The Journal of Physical Chemistry A (acs.org)	Kinetics and Mechanis tic Investigat ions of Atmosphe ric Oxidation of HFO- 1345fz by	YES

							OH Radical: Insights from Theory The Journal of Physical Chemistry A (acs.org)	
7.	Molecular Insights for the HFO-1345fz + X (X=Cl, O ₃ or NO ₃ [□]) Reaction and Fate of Alkoxy Radicals Initiated by Cl: DFT Investigations.	P. K. Rao and S. P. Gejji.	<i>J. Fluor. Chem.</i>	2017		Journal of Fluorine Chemistry ScienceDirect.com by Elsevier	https://www.sciencedirect.com/science/article/abs/pii/S0022113917303512	YES
8.	Kinetics and Mechanism of Gas-phase Reaction of CF ₃ OCH ₂ CH ₃ (HFE-263) with the OH radical - A Theoretical Study	P. K. Rao and H. J. Singh	<i>Can. J. Chem.</i>	2015		https://cdnsciencepub.com/journal/cjc	https://cdnsciencepub.com/doi/abs/10.1139/cjc-2014-0400	YES
9.	Computational Study on the Kinetics of OH initiated Oxidation of Methyl Difluoroacetate (CF ₂ HCOOCH ₃).	H. J. Singh, L. Tiwari and P. K. Rao.	<i>Molecular Physics</i>	2014		https://www.tandfonline.com/journals/tmph20	https://www.tandfonline.com/doi/abs/10.1080/00268976.2013.868554	YES
10.	Computational Study on OH and Cl Initiated Oxidation of 2,2,2-Trifluoroethyl Trifluoroacetate (CF ₃ C(O)OCH ₂ C	H. J. Singh, L. Tiwari and P. K. Rao	<i>Bull. Korean Chem. Soc</i>	2014		https://www.koreascience.or.kr/journal/JCGMCS.page	https://www.koreascience.or.kr/article/JAKO201416760764773.page	YES

	F ₃).							
11.	Theoretical Studies on OH and Cl initiated Hydrogen Atom Abstraction of HFE-227pc (CF ₃ OCF ₂ CHF ₂).	H. J. Singh, P. K. Rao and L. Tiwari.	<i>J. Atmos. Chem</i>	2013		https://www.springer.com/journal/10874/	https://link.springer.com/article/10.1007/s10874-013-9266-5	YES
12.	Theoretical Investigation on the Kinetics and Branching Ratio of the Gas-phase Reaction of Sevofluorane with Cl atom	H. J. Singh, N. K. Gour, P. K. Rao and L. Tiwari.	<i>J. Mol. Model.</i>	2013		https://www.springer.com/journal/894/	https://link.springer.com/article/10.1007/s00894-013-1977-7	YES
13.	Computational Study on the Thermal Decomposition and Isomerization of the CH ₃ OCF ₂ ORadical.	H. J. Singh, B. K. Mishra and P. K. Rao	<i>Can. J. Chem</i>	2012		https://cdnsciencepub.com/journal/cjc	https://cdnsciencepub.com/doi/abs/10.1139/v2012-005	YES
14.	Hydrogen- Atom Abstraction Reaction of CF ₃ CH ₂ OCF ₃ by Hydroxyl Radical	H. J. Singh, B. K. Mishra and P. K. Rao	<i>Bull. Korean Chem. Soc.</i>	2010		https://www.koreascience.or.kr/journal/JCGMCS.page	https://www.koreascience.or.kr/article/JAKO201004140972736.page	YES

15. Books and chapters in edited volumes / books published

S No.	Title of the book	Title of the chapter	National / international	Year of publication	ISBN number	Affiliating Institute at the time of publication	Name of the publisher

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16. Papers in national/international conference-proceedings

S No.	Title of the proceedings of the conference	Name of the conference	National / international	Year of publication	ISBN/ISSN number of the proceeding	Affiliating Institute at the time of publication

17. Professional development Programmes, viz., Orientation Programme, Refresher Course, Short Term Course, Faculty Development Programmes

S. No.	Year	Title of the professional development Programme	Date and Duration (from – to)
1	2021	Refresher Course in Chemistry from Human Resource Development Centre, DDU Gorakhpur University	11 th -24 th September, 2021 (14 days)
2	2020	Orientation Course from Human Resource Development Centre, DDU Gorakhpur University	4 th -24 th January, 2020 (21 days)
3	201	Faculty Development Programme (FDP) on IPR awareness and commercial competences (IAACC)	May 10-15, 2021(6 days)
4	2020	Faculty Development Programme (FDP) on future scope of chemical sciences and research methodology (FSCSRM-2020)	September 21-25, 2020 (5 days)

18. Research projects sponsored by government agencies

S. No.	Name of the principal Investigator or	Name of the Research Project	Name of funding agency	Amount/Fund provided	Year of sanction	Duration of the project	Status (Completed/Ongoing)

19. Research projects sponsored by non-government sources such as industry, corporate houses, international bodies

S. No.	Name of the principal Investigator	Name of the Research Project	Name of funding agency	Amount/Fund provided	Year of sanction	Duration of the project	Status (Completed/Ongoing)

20. Patents filed/granted

S. No.	Name of the patent filed/granted	Patent Number	Year of filing/award/ publish of patent

21. Collaborative activities with other institutions/ research establishments/industry for research and academic development

Title of the collaborative activity	Name of the collaborating agency with contact details	Year of collaboration	Duration	Nature of the activity

22. Functional MoUs with institutions/ industries in India and abroad for internship, on-the-job training, project work, student / faculty exchange and collaborative research

Name of the Organisation/ Institution/ Industry with whom MoU is signed	Year of signing MoU	Duration of MoU	Actual activities under each MOU year wise

23. E-content is developed

i. For e-PG-Pathshala, ii. For CEC (Under Graduate), iii. For SWAYAM, iv. For other MOOCs platform, v. For NPTEL/NMEICT/any other Government Initiatives

Name of the module developed	Platform on which module is developed	Date of launching e content	Link to the relevant document and facility available in the institution	List of the e-content development facility available	Provide link to videos of the media centre and recording facility
Postulates of Quantum Mechanics	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Fundamentals of Quantum Mechanics-Part A	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Fundamentals of Quantum Mechanics-Part B	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Fundamentals of Quantum Mechanics-Part C	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Hohenberg Kohn Theorem	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Molecular Mechanics-Part A	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Molecular Mechanics-Part B	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Molecular Mechanics-Part C	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Molecular Mechanics-Part D	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Basis-sets Part A	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Basis-sets Part B	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		
Basis-sets Part C	E-Pathshala		http://182.18.165.51/epathshala_content.aspx		

24. Consultancy and corporate training-

Consultancy

Name of consultancy project	Consulting/Sponsoring agency with contact details	Year	Revenue generated (amount in rupees)

Corporate training

Title of the corporate training program	Agency seeking training with contact details	Year	Revenue generated (amount in rupees)	Number of trainees

25. Details of Conference/Seminar attended –

Year	Name of the conference/ workshop	International/National /State	Name of the professional body for which membership fee provided	Amount of support (in INR)
2020	Webinar on “ <i>Leveraging Science and Technology to Combat COVID-19</i> ”, organized by Faculty of Science, DDU Gorakhpur University, Gorakhpur, May 23-24, 2020	Naational		
2017	International seminar on “ <i>Biomolecules and Dynamics</i> ”. D.D.U. Gorakhpur University, Gorakhpur, January 27-28, 2017 .	National		
2014	National seminar on “ <i>Current Perspectives in Chemical Science Research</i> ”. D.D.U.	National		

	Gorakhpur University, Gorakhpur, March 26, 2014.			
2013	Symposium on “ <i>Modern trends in Inorganic Chemistry- XV (MTIC-XV)</i> ”. IIT Roorkee, December 13-16, 2013.	International		
2013	National Seminar on “ <i>Current Trends in Chemical Education</i> ”. D.D.U. Gorakhpur University, Gorakhpur. 2013.	National		
2012	National Symposium on “ <i>Current Trends in Computational Chemistry (CTCC- 2012)</i> ”. NEHU, Shillong, March 16- 17, 2012.	National		
2012	National seminar on “ <i>Advance in Chemical Sciences</i> ”. UdaiPratap Autonomous	National		

	College, Varanasi, September 08, 2012 .			
2011	National Conference on “ <i>Computational Chemistry - Current Perspectives</i> ”. D.D.U. Gorakhpur University, Gorakhpur. March 14-15, 2011 .	National		
2010	ICTS school on “ <i>Understanding Molecular Simulations: Theory and Applications (UMS-2010)</i> ”. IIT Kanpur, November 04-13, 2010 .	National		