

Curriculum Vitae

Dr. Davuluri Yogeswara Rao

Department of Chemistry, Krishnaveni Degree and PG College,
Narasaraopet, Guntur - 522 601, Andhra Pradesh, INDIA.

Mobile: 9609783384, 8500723385

E-mails: yogi373@chem.iitkgp.ac.in , yogi373@gmail.com

Education

- Ph.D. in Computational Chemistry : **2019**
Department of Chemistry, Indian Institute of Technology Kharagpur, India
Supervisor: Prof. Anoop Ayyappan, Date of Viva-Voce: **09-11-2019**
- Master of Science in Chemistry (66%) : **2011**
T. J. P. S. PG College, Acharya Nagarajuna University, Andhra Pradesh, India
- Bachelor of Science in Chemistry (70%) : **2009**
Krishnaveni Degree College, Acharya Nagarajuna University, Andhra Pradesh, India

Awards and Fellowships

- Sponsered project Fellowship from SRIC-IITKgp: Jan-Mar, **2019**
- Teaching Assistantship from IIT Kharagpur : Jan-Dec, **2018**
- Senior Research Fellow(SRF): Jan-2015 to Dec-**2017**
- Junior Research Fellow(JRF) : Dec-2012 to Dec-**2014**
- CSIR-UGC National Eligibility Test (NET) Qualified : Jun-**2012**
- CSIR-UGC National Eligibility Test (NET) Qualified for Lecturership : Dec-**2011**
- Acharya Nagarajuna University Entrance Test to M.Sc. (ANUPGCET) : **2009**

Conferences and Workshops Attended / Poster Presented

- Poster presentation at the “8th edition of Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC 8)”, IIT Bombay, India, December, **2017**.
- Oral presentation at the “ 6th RESEARCH SCHOLARS DAY(RSD 2017)”, Department of Chemistry, IIT Kharagpur, India, December, **2017**.
- Poster presentation at the “Theoretical Chemistry Symposium (TCS)”, University of Hyderabad, India, December, **2016**.
- Poster presentation at the “Theoretical Chemistry Symposium (TCS)”, NCL Pune and IISER Pune, India, December, **2014**.
- DST-SERB sponsored Winter School on “Modeling Chemical and Biological (Re)Activity” IIIT Hyderabad, India, January, **2014**.

Computational program(s) executed

- Python program
- Turbomole, Gaussian, Chemshell, MultiWfn, and NBO

Details of professional and Research experience

Period	Position held	Professional Training and Research Experience
Jan 2013 to Jan 2019	PhD Student, Department of Chemistry, IIT Kharagpur	<p>Gave tutorial and laboratory classes in Chemistry, to Undergraduate Science/Engineering Chemistry students of IIT Kharagpur</p> <p><u>Doctoral Research:</u> Computational Study of Intramolecular Heck Reactions: Active Catalyst Formation, Regioselectivity, and Conformational Flexibility for the synthesis of poly-carbocyclic compounds which are experimentally observed. In addition to that, I had gained basic knowledge and experience in computational chemistry.</p>

List of significant publications (with details):

Publications in journals

1. "Density Functional Theory Study on the Formation of the Active Catalysts in Palladium Catalysed Reaction" **D. Y. Rao**, A. Anoop, *J. Ind. Chem. Soc.* **2019** (Just accepted).
2. "Pd-catalyzed intramolecular sequential Heck cyclization and oxidation reactions: a facile pathway for the synthesis of substituted cycloheptenone evaluated using computational studies" J. K. Ray, S. Paul, P. Ray, R. Singha, **D. Y. Rao**, S. Nandi, A. Anoop, *New. J. Chem.* **2017**, *41*, 278–284.
3. "Palladium-catalyzed expedient Heck annulations in 1-bromo-1,5-dien-3-ols: Exceptional formation of fused bicycles" J. K. Ray, R. Singha, D. Ray, P. Ray, **D. Y. Rao**, A. Anoop, *Tetrahedron Letters* **2019**, *60*, 931–935.
4. "Computational Study of tandem C-C Coupling and C-H Activation Reaction of a Flexible Substrate" **D. Y. Rao**, A. Anoop, (Manuscript Submitted).
5. "The pyrrole ring η^2 hapticity bridged binuclear tricarbonyl Mo(0) and W(0) complexes: catalysis of regioselective hydroamination reactions and DFT calculations" V. K. Jha; G. Mani; **D. Y. Rao**; A. Anoop, *Dalton Trans.* **2017**, *46*, 1840–1847.

Field of major scientific interest

Our research work is mainly focused on the computational study of transition metal catalyzed reactions for C-C and C-X bond formation. The main research activity is focused on density functional theory (DFT) studies for Palladium catalyzed reactions for C-C bond formations through C-C coupling and C-H activations.

Teaching experience

- **2014 - 2016** : Teaching Assistant in IIT Kharagpur.
- **Aug, 2019-** : Lecturer in Chemistry, Krishnaveni Degree College, Narasaraopet.

Reference

Dr. Anoop Ayyappan

Associate Professor

Department of Chemistry

Indian Institute of Technology Kharagpur

Kharagpur, West Bengal, INDIA - 721 302

Email: anoop@chem.iitkgp.ac.in

Phone: +91 3222 283 316.

Dr. Sabyashachi Mishra

Associate Professor

Department of Chemistry

Indian Institute of Technology Kharagpur

Kharagpur, West Bengal, INDIA - 721 302

Email: mishra@chem.iitkgp.ac.in

Phone: +91 3222 282 328.

Personal profile

- **Name:** Dr. Davuluri Yogeswara Rao
- **Mother and Father:** Seethamma and Govinda Rajulu
- **Mailing Address:** Department of Chemistry,
Krishnaveni Degree and PG College,
Narasaraopet, Guntur - 522 601,
Andhra Pradesh.
- **Permanent Address:** Gopuvari Palem(V),
Ipur(Md), Guntur(Dt) -522 658,
Andhra Pradesh.
- **Date of birth :** 27th July, 1989
- **Sex:** Male
- **Marital status:** Married

Date:

Place: