



Dr. Dibyajit Dash

Designation: Assistant Professor, (Guest Faculty)

Qualification: M.Sc, M. Phil., PhD

Date of Birth: 11.06.1991

Date of Joining: 01.07.2024

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Area of Interest

Inorganic Chemistry, Theoretical chemistry, Nano Science

Courses taught

Organic Chemistry, Inorganic Chemistry, Physical Chemistry, Analytical Chemistry, Polymer Chemistry, Green Chemistry.

Career

Assistant Professor,(Guest) (2024-present): Rama Devi Women's University, Bhubaneswar

Teaching Experience

2 years

Research Experience

8 years

Administrative/Executive Experience

Nil

Publications

Journal publications (Give the entire list of publication in Scopus/SCI-WoS/UGC care only)

1. Dash, D., Baral, M., & Kanungo, B. K. (2020). Synthesis of a new tetradentate chelator with 1-Hydroxy-2(1H)-pyridinone (HOPO) as chelating unit: Interaction with Fe (III), solution thermodynamics and DFT studies. *Journal of Molecular Structure*, 128796. doi:10.1016/j.molstruc.2020.128796 .
2. D. Dash, M. Baral, B.K. Kanungo, Development of a Flexible Tripodal

Hydroxypyridinone Ligand with Cyclohexane Framework: Complexation, Solution Thermodynamics, Spectroscopic and DFT Studies, *ChemistrySelect*. 6 (2021) 12165–12181. <https://doi.org/10.1002/slct.202102962>.

3. Dash, D., Singh, S., Baral, M. et al. *TMACH-1,2-HOPO, a versatile tripodal metal chelator: complexation, solution thermodynamics, spectroscopic and DFT studies*. *J Incl Phenom Macrocycl Chem* (2024). <https://doi.org/10.1007/s10847-024-01221-9>.
4. V.K. Choudhary, A.K. Bhatt, D. Dash, N. Sharma, *DFT calculations on molecular structures, HOMO–LUMO study, reactivity descriptors and spectral analyses of newly synthesized diorganotin(IV) 2-chloridophenylacetohydroxamate complexes*, *J. Comput. Chem.* 40 (2019) 2354–2363. <https://doi.org/10.1002/jcc.26012>.
5. V.K. Choudhary, A.K. Bhatt, D. Dash, N. Sharma, *Synthesis, characterization, thermal, computational and biological activity studies of new potential bioactive diorganotin (IV) nitrosubstitutedhydroxamates-A comparative study*, *Appl. Organomet. Chem.* 34 (2020) 1–18. <https://doi.org/10.1002/aoc.5360>.
6. S. Sharma, M. Baral, D. Dash, B.K. Kanungo, *Synthesis, solution studies and DFT investigation of a tripodal ligand with 3-hydroxypyran-4-one scaffold*, *J. Incl. Phenom. Macrocycl. Chem.* 101 (2021) 275–289. <https://doi.org/10.1007/s10847-021-01088-0>.
7. [Vineet Kumar Choudhary](#), [Kanika Mandhan](#), [Dibyajit Dash](#), [Sachin Bhardwaj](#), [Meena Kumari](#), [Neeraj Sharma](#), *Density functional theory studies on molecular geometry, spectroscopy, HOMO–LUMO and reactivity descriptors of titanium(IV) and oxidozirconium(IV) complexes of phenylacetohydroxamic acid*, *J. Comput. Chem.* 43 (2022) 2060–2071. <https://doi.org/10.1002/jcc.27004>.

Participation in Conferences & Seminars (as invited/plenary/chair)

- 1- Participated in MMT-2018 (One Day National Conference on Molecules and Materials Technology) at NIT Kurukshetra, Haryana. “Synthesis and Studies on Binding Properties of a Multifunctional Chelator Containing two 1-Hydroxy-2(1H)-pyridinones as Chelating units with Trivalent Iron”.
- 2- National Science Week -2018 as Research scholar Day. Sant Longowal Inst. Of Engg. & Tech. (Deemed University, Under MHRD, Govt. of India) Longowal, Sangrur - 148106 (Punjab), India. “Molecular Modeling of a New Multifunctional Chelator Containing two 1-Hydroxy-2(1H)-pyridinones Chelating Units and its Iron Complexes.”
- 3- Participated in UGC Sponsored National Seminar, Feb. 6 & 7, 2018 in Municipal College, Rourkela entitled as Recent Advances on Molecules of Chemical and Biological Importance (RAMCBI) and presented a research paper entitled Molecular Modeling of a New Multifunctional Chelator Containing two 1-Hydroxy-2(1H)-pyridinones Chelating Units and its Iron Complexes.

4- Participated and presented in National Conference entitled "Emerging Research Trends in Chemical, Physical and Life Sciences for Entrepreneurial Skill Development" held on 26-27 Dec. 2018 at Department of Biotechnology, H. P. University Shimla.

Theoretical Investigation at DFT Level of a New Multifunctional Chelator Having two 1-Hydroxy-2(1H)-pyridinones Chelating Units and its Iron Complexes.

5- - National Science Week -2019 as Research scholar Day held on 28th Feb. at Sant Longowal Inst. Of Engg. & Tech. (Deemed University, Under MHRD, Govt. of India) Longowal, Sangrur -148106 (Punjab), India. "Experimental and Theoretical Study of New Tripodal Polydentate Chelators Containing three 1-Hydroxy-2(1H)-Pyridinone Chelating Units"