



Dr ROHIT SINGH

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Address: Kanpur ,Uttar Pradesh,India - 208001

Expertise

Inorganic and Nuclear Chemistry

Hybrid Inorganic-organic chemistry, Supramolecular Chemistry, MOFs, Computational investigation, Coordination polymers, in-situ ligand transformation

Work experience

1. DAV Post Graduate College 2019 — Present

Assistant Professor
Kanpur

Education

1. Ph.D - 2017

Indian Institute of Technology Delhi

Honours and Awards

1. GATE in Chemistry - 2016
MHRD, GOI
2. NET in Chemical Sciences - 2012
CSIR-UGC
3. GATE in Chemistry - 2009
MHRD, GOI
4. JRF in Chemical Sciences - 2008
CSIR-UGC
5. Dr. R. N. Singh Memorial Award - 2008
BOM, R. B. S. College, Agra

Publication

1. A combined experimental and computational study of a supramolecular assembly based on cationic zinc(II)-ethanesulfonate
Shankar R.
Journal of Molecular Structure, Volume 1202, Year 2020
2. Three-dimensional hydrogen-bonded magnesium(II) supramolecular motifs based on in situ generated alkanesulfonate (Me/Et/nPrSO₃⁻) ligands: A combined experimental and computational study
Rohit Singh and Gabriele Kociok-Köhn and Amanpreet Kaur Jassal and Larisa Singh
Polyhedron, Volume 175, Year 2020, Pages 114200
3. Influence of ligand coordination, solvent, and non-covalent interaction on the structural outcomes in coordination polymers with direct Cd(II)-alkanesulfonate bonds: A combined experimental and computational study
Rohit Singh ., Gabriele Kociok-Köhn ., Kaman Singh ., Sarvesh Kumar Pandey ., Larisa Singh .,
Journal of Solid State Chemistry, Volume 280, Year 2019
4. A rational synthesis of ladder-like motif in zinc-methylphosphonate from a preformed coordination assembly
Shankar R.
Inorganica Chimica Acta, Volume 482, Year 2018, Pages 681-686

5. **A Computational Scrutiny on the Stability, Structure, and Electronic Features of Alkanesulfonate Based Zincate Salts with Varying Counteranions**

Singh, Rohit and Singh, Kaman and Pandey, Sarvesh Kumar
ChemistrySelect, Volume 3, Year 2018, Pages 13048-13056

6. **Synthesis and Structural Studies of Three-Dimensional Supramolecular Motifs Derived from Neutral and Cationic Zinc Alkanesulfonates**

Shankar, Ravi and Singh, Rohit and Mendiratta, Swati and Jassal, Amanpreet Kaur and Kociok-Köhn, Gabriele and Molloy, Kieran C.
European Journal of Inorganic Chemistry, Volume 2017, Year 2017, Pages 2081-2087

7. **Studies on the coordination behavior of methanesulfonate in zinc(II) based two and three dimensional supramolecular assemblies**

Shankar, Ravi; Singh, Rohit; Kociok-Köhn, Gabriele; Molloy, Kieran C.
Proceedings of the National Academy of Sciences India Section A - Physical Sciences, Volume 84, Year 2014, Pages 157-163