

Dr. U. P. Singh

Professor

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Photo

Academic Profile

- Ph.D. – Banaras Hindu University, 1988
- M.Sc. – Banaras Hindu University, 1984
- B.Sc. – Banaras Hindu University, 1982

Post Doctoral Experience

Alexander von Humboldt Fellow 2007 (Max-Planck-Institute for Bioinorganic Chemistry, Muelheim), 2006 (University of Stuttgart), 2005 (University of Freiburg), 2001 (Max-Planck-Institute for Strahlenchemie, Muelheim), 1991-1992 (University of Resensburg)

JSPS Visiting Scientists, 2003 (The Institute for Physical and Chemical Research, RIKEN, Saitama), 1999 (Tokyo Institute of Technology).

Science and Technology Agency Fellow, Japan, 1995-1996 (The Institute for Physical and Chemical Research, RIKEN, Saitama).

UNESCO Research Fellow at Tokyo Institute of Technology, Japan, 1989-1990

Research Interests

- Coordination Chemistry, Bio-inorganic Chemistry, Heme-Protein and Host-guest / Supramolecular.

Selected Research Publications (up to 10 from last 5 years)

1. Optically active pyrazolylborate: Synthesis, Characterization and uses in Enantioselective Cyclopropanation Reaction, **Udai P. Singh**, Preeti Babbar, B. Hassler, H. Nishiyama, H Brunner, J. Mol. Cat. A, Chem., 2002, 185, 33.
2. Synthesis, Molecular Structure and Emission Properties of Benzoato–Bridged Lanthanide Complexes with Hydrotris(pyrazolyl)borate, **Udai P. Singh**, S. Tyagi, C. L. Sharma, H. Görner, T. Weyhermüller, J. C. S., Dalton Transactions, 2002, 4464.
3. Cobalt Complexes Bridged with a (μ -X)(μ -Carboxylato) unit (X = OH, N₃): Synthesis and Structural Studies, **Udai P. Singh**, P. Babbar, A. K. Sharma, Inorg. Chim. Acta, 2005, 358, 271.
4. Mononuclear Manganese Carboxylate Complexes: Synthesis and Structural Studies, **Udai P. Singh**, A. K. Sharma, P. Tyagi, S. Upreti, Raj. K. Singh, Polyhedron, 2006,

25, 3628.

5. Design and synthesis of *de Novo* peptide for manganese binding, **Udai P. Singh**, Raj K. Singh, Y. Isogai, Y. Shiro, Int. J. of Peptide Research and Therapeutics, 2006, 12, 379
6. Synthesis, Structural, Photophysical and Thermal Studies of Benzoate bridged Sm (III) Complexes, **Udai P. Singh**, R. Kumar, S. Upreti, J. Mol. Structure, 2007, 831, 97.
7. Mononuclear Cobalt (II) Carboxylate Complexes: Synthesis, Molecular Structure and Selective Oxygenation Study, **Udai P. Singh**, V. Aggarwal, A. K. Sharma, Inorg. Chim. Acta, 2007, 360, 3226.
8. Manganese Complexes as model for Manganese-containing Pseudocatalase enzymes: Synthesis, Structural and Catalytic activity studies, Udai P. Singh, P. Tyagi. S. Upreti, Polyhedron, 2007, 26, 3625.
9. Preparation, Crystal Structure and Thermolysis of Phenylenediammonium Diperchlorate salts, I. P. S. Kapoor, P. Srivastava, G. Singh, **Udai P. Singh**, R. Frölich, J. Phys. Chem. A, 2008, 112, 652.
10. Nickel Pyrazolyl Borate Complexes: Synthesis, Structure and Analytical Application in Biological and Environmental Samples as Anion Selective Sensors, A. K. Singh, V. Aggarwal, **Udai P. Singh**, S. Mehtab, Talanta, 2008, 77, 718.

Projects/Awards/Honors

Completed:

1. Synthesis of Optically active Polypyrazolylborate Ligands for Enantioselective Cyclopropanation reaction, DST, New Delhi (under young scientists scheme).
2. Binuclear Manganese Complexes as Model for the Manganese-containing Ribonucleotide Reductase Enzymes, CSIR, New Delhi.
3. Synthesis of Model compounds for Zinc-containing Enzymes, UGC, New Delhi.
4. Fixation of Atmospheric Carbon dioxide by Mononuclear Hydroxo Complexes of Divalent Metals, AICTE, New Delhi.
5. Metal-Nucleic acid Base Pair Interaction – Solution and Antitumor Studies, UGC, New Delhi.
6. Dioxygen Complexes of Manganese and Cobalt: Synthesis, Molecular Structure and Reactivity Studies, CSIR, New Delhi.
7. Synthesis, Characterization and Reactivity Studies of Vanadium and Manganese Nitrido Complexes, DST, New Delhi.

In hands:

1. Synthesis and Characterization of Some Complexes as MRI (Magnetic Resonance

Imaging) Contrast agents, MHRD, Govt. of India, New Delhi.

2. Zn(II) and Cd(II) Hydroxo Complexes with Tris(pyrazolyl)borate (N3) and Tris(thioimidazolyl)borate (S3) ligands for Ester Hydrolysis, CSIR, New Delhi.

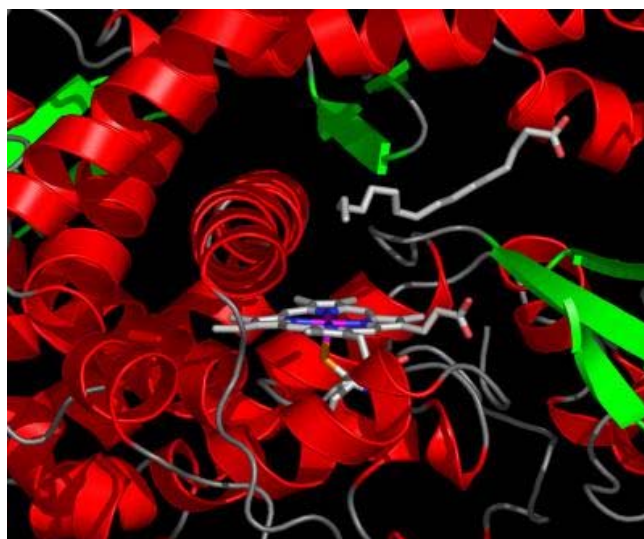
Awards/Honors

1. Dr. B. C. Haldar Memorial Award, 1987.
2. Recipient of Indian Science Congress Association Young Scientist Award, 1991.
3. Life Member: Indian Science Congress Association.
4. Life Member: Chemical Research Society of India.
5. Member: Society for Biological Inorganic Chemistry, USA
6. Life Member: Indian Council of Chemists

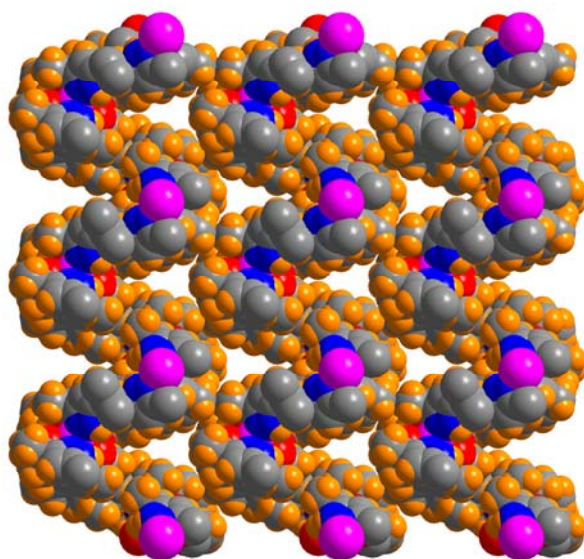
Courses Taught

- CY-101 Chemistry, CY-741, Analysis of Foods and Drugs, CY-752, Environmental Chemistry, CY-621, Inorganic Chemistry - I

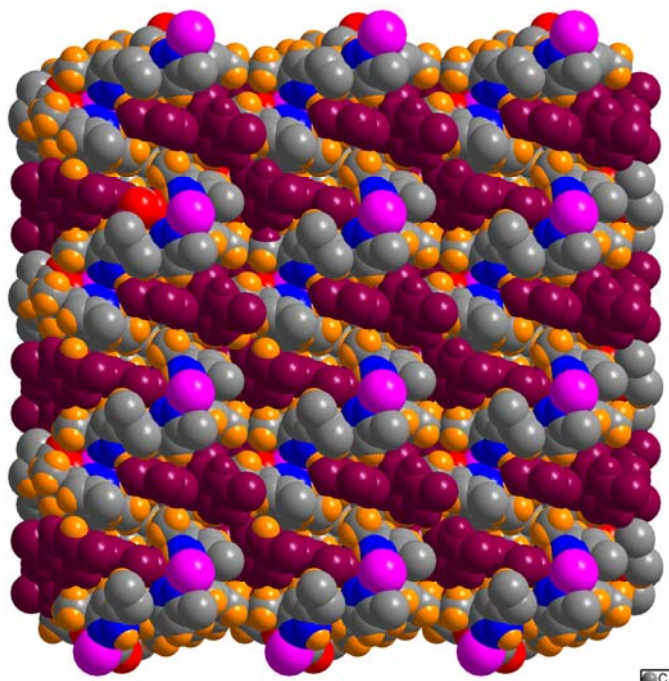
Some recently solved interesting X-ray structure by our groups are –



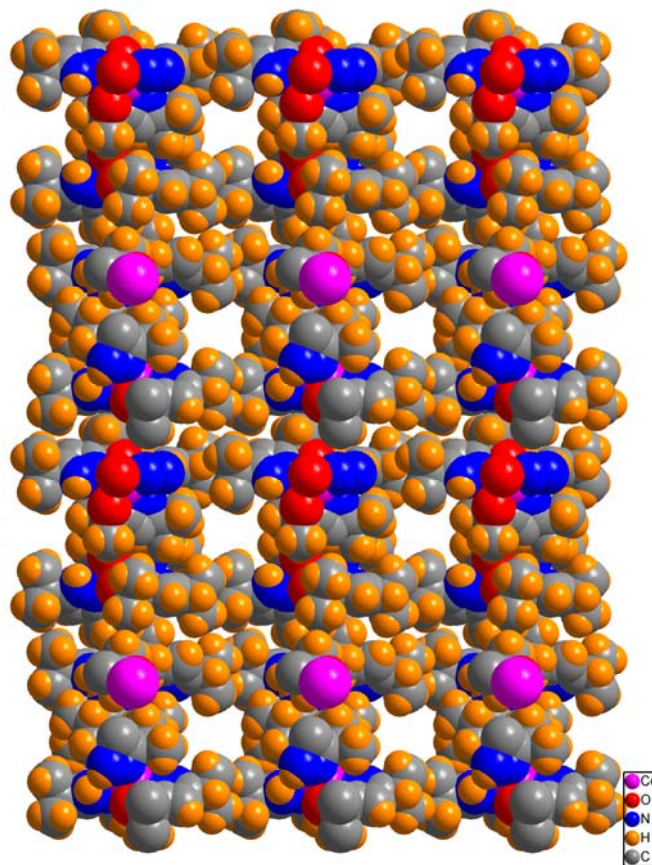
Active site of P450-BM3 with Palmitate bound to the heme face



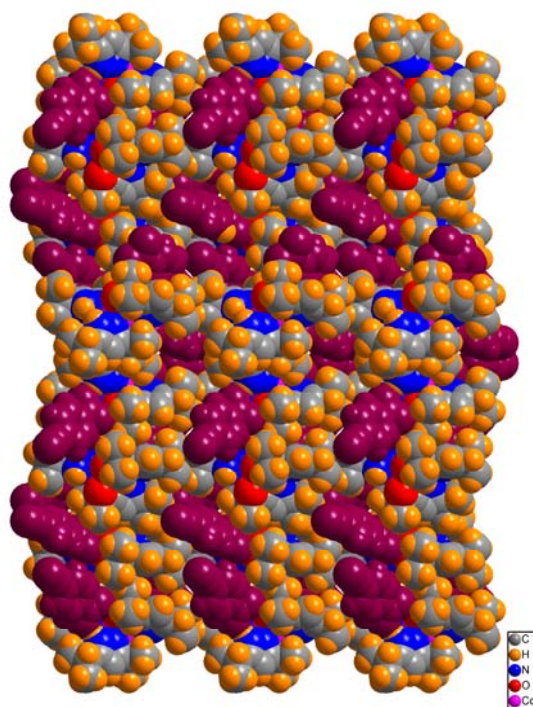
Three – dimensional packing of $[\text{Co}(3\text{-OCMe}_2\text{-5-}^{\text{Pri}}\text{pzH})_3]\cdot(\text{F-OBz})_2$ without guest molecules (fluorobenzoate)



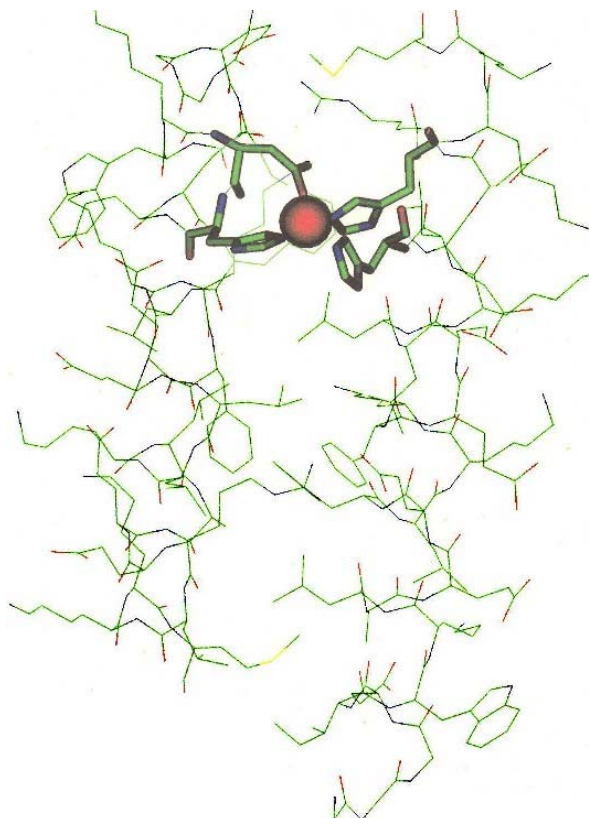
Three – dimensional packing of $[\text{Co}(3\text{-OCMe}_2\text{-5-}^{\text{Pri}}\text{pzH})_3]\cdot(\text{F-OBz})_2$ with guest molecules (fluorobenzoate)



Three - dimensional rectangular packing of the complex $[\text{Co}(3\text{-OCMe}_2\text{-5-Pri-pzH})_3] \cdot (\text{CN-OBz})_2$ without guest molecules. Guest molecules will be present in the triangular void space shown above.

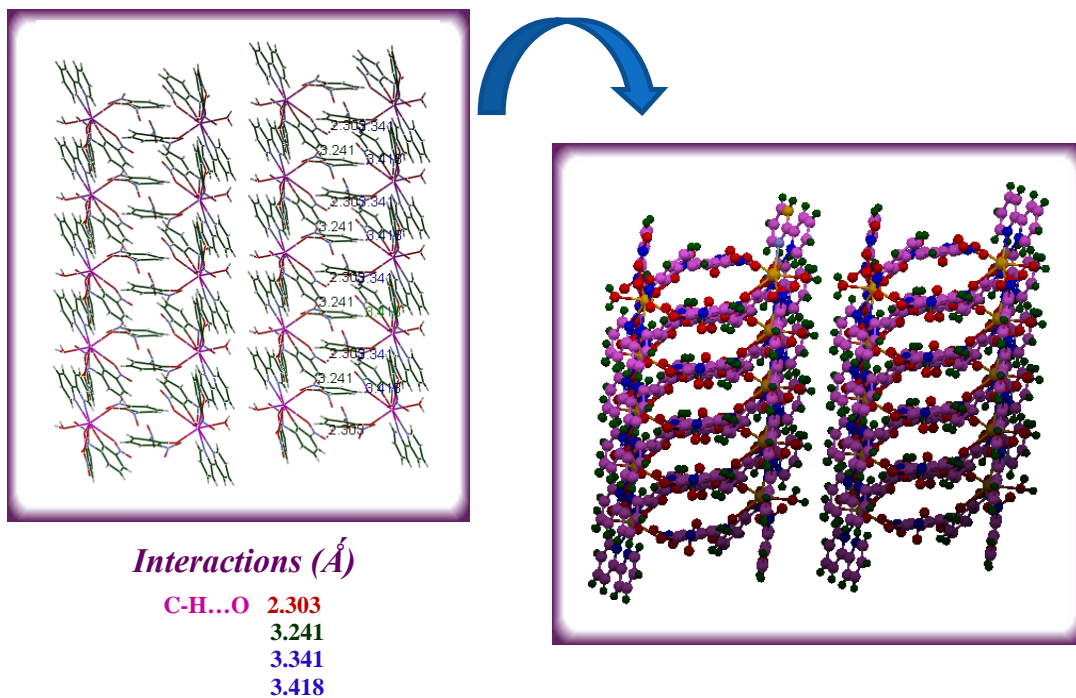


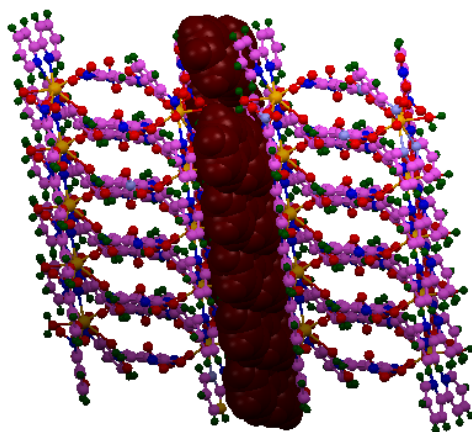
Three - dimensional rectangular packing of $[\text{Co}(3\text{-OCMe}_2\text{-5-Pri-pzH})_3] \cdot (\text{CN-OBz})_2$ without guest molecules. Guest molecules will be present in the triangular void space shown above.



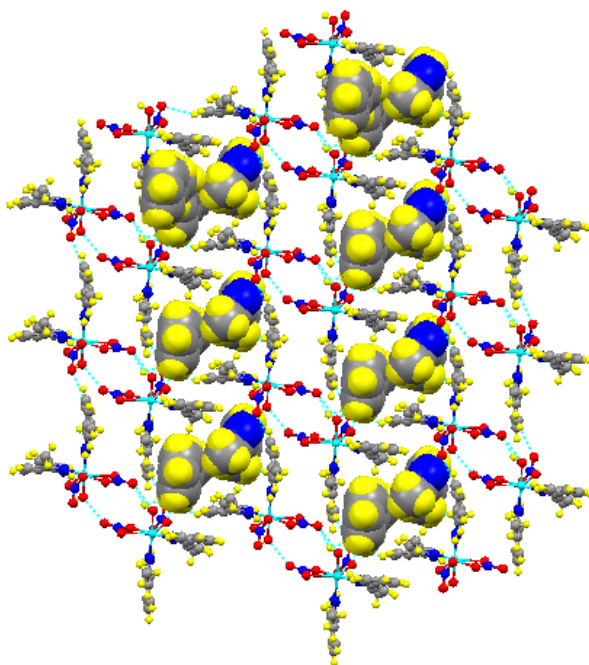
Model for manganese binding with designed MHB peptide

$\text{C-H}\cdots\text{O}$ interactions between one host to other give ladder like packing
Without guest molecule

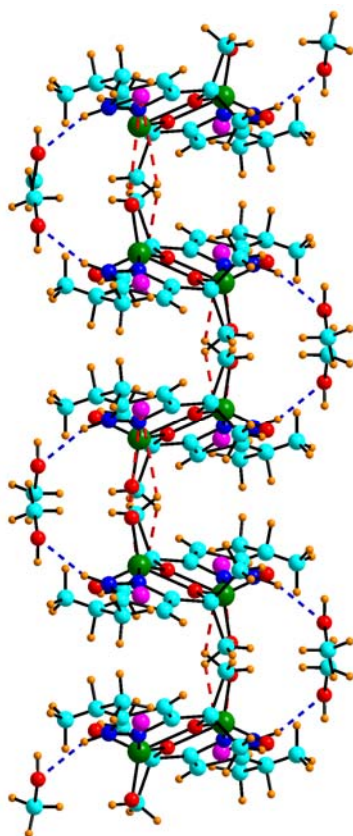




Ladder packing of the complex molecule with guest (2,2' bipyridine) molecule



Three Dimensional Packing of $2[\text{Cu}(\text{Pz}^{\text{Ph,MeH}})(\text{OH})(\text{NO}_3)_2] \cdot 2 \text{Pz}^{\text{Ph,MeH}} \cdot \text{CH}_3\text{CN}$



One Dimensional Spiral Snake Shaped Packing of complex $[V_2(\mu O)_2O_4(PzH^{iPr}).CH_3OH]$