

Crystal Engineering and Supramolecular Synthons Approach for the Assembly of Hydrogen Bonded Metal Complexes

PI, Dr. Kafeel Ahmad Siddiqui,

Project Cost: Rs. 17.88 Lacs, Funded By SERB-DST

The work done during this project is summarized as below-

(i) PI has recognized C-H...M hydrogen bond and {...HCNM}₂ **synthons which was not reported earlier. (Chemical Communication, 2013, 49,8501).**

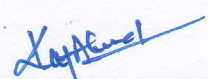
(ii) PI have identified the different types of hydrogen bonding patterns in lattice water molecules that **was not reported earlier in the scientific community. (Journal of Structural Chemistry, 2018,59(1),106).**

(iii) We have synthesized **first supramolecular orotic acid and Isonicotinic acid-based Zn-complex** [Zn(HOr)(Hiso)·3H₂O]·H₂O] that have future applications in metalo-drug chemistry. **(Journal of Structural Chemistry, 2018,59(1),166).**

(iv) In this project, we have successfully synthesized and characterized a series of metal-ototato coordination compounds of different architecture using crystal engineering principle involving N-H...O/ N-H...N and O-H...O/ O-H...N synthons as connecting tools. DFT calculation is used to rationalize the magnetic behaviour of reported complexes. These calculations underline the pathway of magnetic exchange interactions through N-H...O/ N-H...N and O-H...O/ O-H...N supramolecular synthons and confirm that the magnetic interactions propagate through such contacts. Due to N-H...O/ N-H...N and O-H...O/ O-H...N there is a varieties of structure we obtained with different magnetic properties. Such study will enriched the metal-organic structural chemistry and help the researchers to find a platform to design and synthesis of similar molecules.

(v) We have established a **“Crystal Engineering Laboratory”** for design and hydrothermal synthesis of *Single Crystal* of Porous Hydrogen Bonded Metal Complexes, Coordination Polymers and MOF materials for diverse applications like Magnetic, Photoluminescence, Sensor, Sorption etc. Hydrothermal synthesis is a special type of synthesis of material at high temperature, in programmable *Hydrothermal Oven*.

Department of Chemistry


Dr. Kafeel Ahmad Siddiqui, PI