

## **Title: Solution State Topological Dichotomy in Multifaceted Heteroannulenes**

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Aromaticity is one important single parameter that controls stability, structure, reactivity and material applicability of various molecular species. In this respect, the conformational flexibility of expanded heteroannulenes and aromaticity in many cases become specular images of one another. Thus, there always remains challenge in designing or finding a suitable preorganized precursor (s) that can probe the serious exploratory problems owing to usually larger conformational mobility while maintaining aromaticity for expanded porphyrins with full potential as efficient NIR dyes. The first part of my talk will highlight the induced correspondence of local  $\pi$ -aromatic sextet onto the macrocyclic  $\pi$ -conjugation pathways leading to different topologies with aromaticity switching. I would discuss the very first report of an unconventional tripyrrane moiety that has been obtained from regioselective  $\beta$ -benzoylated pyrrole. The unconventional 3, 4-linkages of N-methyl pyrrole unit has admirably served as incentive to two different types of highly stable metal free [20] Möbius aromatic heteroannulenes. Most importantly, the presence of the “local” aromatic unit (N-methyl pyrrole considering 3, 4-linkages) in the macrocycle core didn't necessarily quench the macrocyclic diatropic ring current effect (*Chem. Asian. J.* **2016**, *11* (7), 986-990). On the other hand, attempt to include local  $\pi$ -aromatic sextets viz the N-methyl pyrrole rings through  $\beta$ ,  $\beta$ -linkages and  $\alpha$ ,  $\beta$ -linkages has led to the isolation of first ever heteroannulenes cross conjugated at four points and two points respectively within the macrocycles and hence the loss of aromaticity in these macrocycles (*Chem. Eur. J.* **2016**, *22*, 5504-5508). In the second part of my talk, the induced correspondence of fused heterocycles in to the macrocyclic  $\pi$ -conjugation pathways leading to NIR absorption and emission (*Chem. Eur. J.* **2016**, chem.201600917). The impact of such topology switching has led to dynamic aromaticity switching. Excellent agreement between the theoretically determined and experimentally spectroscopic measurement are key to the evidence of such aromaticity switching.

### **Biography**

Harapriya Rath has completed her PhD in 2006 from Indian Institute of Technology, Kanpur and JSPS postdoctoral studies from Kyoto University, Japan followed by Royal Society Newton International Postdoctoral studies from Manchester University. She has been awarded the Ramanujan fellowship by Department of Science and Technology, India. She currently holds the position of Assistant Professor in the Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, Kolkata, India. Her major research area includes highly conjugated topologically controlled Aromaticity, molecular spintronics, NIR absorptive and emissive dyes.