PREFACE

The journey of aromaticity from Kekulés definition of benzene has been extensive and the recent developments in this field provide a considerable better insight into the concept. The first chapter thereby provides a crisp discussion about the advancement in the field of aromaticity since its inception days to its recent developments. Any single property based index is unable to wholly describe the event of aromaticity, thereby rendering it to be multidimensional, so a plethora of indices exist to define aromaticity and to ascertain stability of molecules. These various theoretical constructs are discussed in chapter 2 including the reactivity parameters. On the basis of available literature, various criteria have been employed over the years for quantification of aromaticity, but magnetic criteria played an instrumental role in defining the concept of aromaticity. So, a mini review discussing aromaticity in the light of magnetic criteria is done in chapter 3. Although the concept of aromaticity has long been primarily confined to organic chemistry, but the recent advancements in the field of aromaticity made it an important unifying concept to ascertain the bonding and stability in many chemical species such as inorganic radicals, anions, cations and clusters surpassing the domain of organic chemistry. This encouraged us to widen the boundaries of the already existent concept of aromaticity in the fourth chapter where we explored a novel area of exo-cyclic aromaticity in newly designed $C_2B_2F_4$ molecule. Here, we extend beyond the limit of conventional aromatic molecules where the molecule gains the magic number of six π-electrons through an unusual electronic contribution from *exo*-cyclic atoms. This original concept is further manifested in chapter 5 where it is extended to novel three membered heterocyclic moieties. Among different all metal aromatic clusters, research on Be_3^{2-} cluster is prominent due to its structural variety and bond stretch isomerism. Be_3^{2-} is a comprehensively studied system due to the presence of few electrons and accordingly different sophisticated computations are possible. In chapter 6, we illuminate the underlying rationale behind the occurrence of bond stretch isomerism in Be_3^{2-}. Conceptual density functional theory involving the global and local reactivity parameters to elucidate the process of methylation of aromatic nucleobase cytosine and its subsequent oxidation to its derivatives is explored in the seventh chapter. In the final chapter, the essence of preceding chapters and the importance of the present study are surmised. In spite of abundant cultivation of the topic "aromaticity" it still remains an intriguing topic with immense potential as it is aptly said by Schleyer that, "aromaticity has been a time-dependent phenomenon."