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Title:	A Comprehensive study of theoretical and computational aspects of concepts of aromaticity and anti-aromaticity.
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Abstract:	This thesis is devoted to a discussion of various aspects arising from the concept of aromaticity. Beginning with a short historical exploration of this concept, the thesis traces its development and understanding over a period of time. After a discussion on Hückel Molecular Orbital (HMO) method, we have used it to present a detailed mathematical derivation of the energy levels of a general monocyclic conjugated polyenes exhibiting both Huckel and Möbius topologies. This derivation augments the brief derivations of ten found in the literature, particularly for Möbius topology. Following this, the thesis then presents a survey of various indicators used to quantify aromaticity. Finally, the thesis explores the concept of multidimensional nature of aromaticity, highlighting its implications for comprehending aromaticity..
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