

RECENT STUDIES ON ASPECTS RELATED TO AROMATICITY

M. Solà¹, F. Feixas¹, E. Matito², J. Poater¹

¹Institut de Química Computacional and Departament de Química, Universitat de Girona, Campus de Montilivi, Girona, 17071

² Kimika Fakultatea, Euskal Herriko Unibertsitatea and Donostia International Physics Center (DIPC), P.K. 1072, 20018 Donostia

In this seminar, we will discuss some recent studies we have performed on different topics related to aromaticity. First, we will show that more stable isomers are not always those that display higher aromaticity. Second, we will discuss the aromaticity of a Cu(II) complex used in therapeutic treatment of Alzheimer's disease. Molecular orbitals and aromaticity descriptors confirm that this complex exhibits interesting Möbius metalloaromaticity. Finally, we will analyze the possible extension of $4N$ Baird's rule of aromaticity in annulenes to spherical compounds having a same-spin half-filled last energy level. This situation is reached in spherical systems for a number of electrons equal to $2N^2+2N+1$. We prove this rule by showing that open-shell icosahedral fullerenes following the $2N^2+2N+1$ rule are aromatic. This $2N^2+2N+1$ rule for spherical systems is linked to $4N$ Baird's rule for annulenes in the same way $2(N+1)^2$ Hirsch's rule for spherical compounds is the analog of $4N+2$ Hückel's rule.