OTTOSSON'S CUBE

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Many of the quintessential aromatic compounds present high symmetry. Symmetry is one of the usual features of aromatic compounds. Although not all aromatic species are symmetric, the most archetypal aromatic compounds are highly symmetric and possess degenerate highest-occupied molecular orbitals. These orbitals can be fully occupied resulting in a closed-shell structure or can be same-spin half-filled. This closed-shell or same-spin half-filled electronic structure, which provides an extra stabilization, is the origin of several rules of aromaticity such as the Hückel 4n+2 rule,[1-4] the lowest-lying triplet excited state Baird's rule,[5,6] the Soncini and Fowler extension of the Baird rule,[7] or the 4n rule followed by monocyclic conjugated hydrocarbons in a Möbius-type conformation.[8,9] All these rules of (anti)aromaticity are nicely summarized in the so-called Ottosson's cube.[10] Some examples of the applications of these rules performed in our group will be reviewed in the seminar. The validity of some of these rules will be assessed. We will conclude by showing a somewhat extended version of the Ottoson cube.

References

(1) Hückel, E. *Z. Physik* **1931**, *70*, 104.
(2) Hückel, E. *Z. Physik* **1931**, *72*, 310.
(3) Hückel, E. *Z. Physik* **1932**, *76*, 628.
(4) Hückel, E. *Z. Elektrochemie* **1937**, *43*, 752.
(5) Baird, N. C. *J. Am. Chem. Soc.* **1972**, *94*, 4941.
(6) Ottosson, H. *Nat Chem* **2012**, *4*, 969.
(7) Soncini, A.; Fowler, P. W. *Chem. Phys. Lett.* **2008**, *450*, 431.
(8) Heilbronner, E. *Tetrahedron Lett.* **1964**, 1923.
(9) Ajami, D.; Oeckler, O.; Simon, A.; Herges, R. *Nature* **2003**, *426*, 819.
(10) Rosenberg, M.; Dahlstrand, C.; Kilsa, K.; Ottosson, H. *Chem. Rev.* **2014**, *114*, 5379.