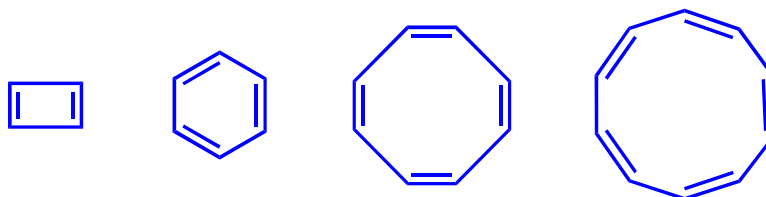


## Aromaticity. Molecular Orbital Picture of an Intuitive Concept.

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Recently, we have shown that the propensity of the  $\pi$  electrons in 1,3-cyclobutadiene (or [4]annulene) as well as in benzene (or [6]annulene) is always to localize the double bonds, against the delocalizing force of the  $\sigma$  electrons. More importantly, we have also shown that the  $\pi$  electrons nevertheless decide about the localization or delocalization of the double bonds. Here, based on accurate Kohn-Sham DFT computations, we explain the mechanism behind this behavior and we show that larger [n]annulenes are subject to the same electronic mechanisms (see illustration). The geometry and nature of (anti)aromatic rings is compared to that of the corresponding saturated ones. We also address the issue that aromatic character fades out if one goes to larger annulenes, such as, [10]annulenes.



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