Hückel \((4n + 2)\) rule

Monocyclic planar (or almost planar) systems of trigonally (or sometimes digonally) hybridized atoms that contain \((4n + 2)\) \(\pi\)-electrons (where \(n\) is a non-negative integer) will exhibit aromatic character. The rule is generally limited to \(n = 0\)–5. This rule is derived from the Hückel MO calculation on planar monocyclic conjugated hydrocarbons \((\text{CH})_m\) where \(m\) is an integer equal to or greater than 3 according to which \((4n + 2)\) \(\pi\)-electrons are contained in a closed-shell system. Examples of systems that obey the Hückel rule include:

- \(\text{cyclopropenyl cation} = (3, 0)mn\)
- \(\text{cyclopentadienyl anion} = (5, 1)mn\)
- \(\text{benzene} = (6, 1)mn\)

Systems containing \(4n\) \(\pi\)-electrons (such as cyclobutadiene and the cyclopentadienyl cation) are 'antiaromatic'.

See also: conjugation, Möbius aromaticity

Source:
PAC, 1994, 66, 1077 (Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)) on page 1122