

Hückel ($4n + 2$) rule

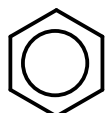
Monocyclic planar (or almost planar) systems of trigonally (or sometimes digonally) hybridized atoms that contain $(4n + 2)$ π -electrons (where n is a non-negative integer) will exhibit aromatic character. The rule is generally limited to $n = 0$ –5. This rule is derived from the Hückel MO calculation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



cyclopropenyl cation
($= 3, = 0$) mn



cyclopentadienyl anion
($= 5, = 1$) mn



benzene
($= 6, = 1$) mn

Systems containing $4n$ π -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