aromatic

- 1. In the traditional sense, 'having a chemistry typified by benzene'.
- 2. A cyclically conjugated molecular entity with a stability (due to delocalization) significantly greater than that of a hypothetical localized structure (e.g. Kekulé structure) is said to possess aromatic character. If the structure is of higher energy (less stable) than such a hypothetical classical structure, the molecular entity is 'antiaromatic'. The most widely used method for determining aromaticity is the observation of diatropicity in the ¹H NMR spectrum.

See also: Hückel (4n + 2) rule, Möbius aromaticity

3. The terms aromatic and antiaromatic have been extended to describe the stabilization or destabilization of transition states of pericyclic reactions. The hypothetical reference structure is here less clearly defined, and use of the term is based on application of the Hückel (4n + 2) rule and on consideration of the topology of orbital overlap in the transition state. Reactions of molecules in the ground state involving antiaromatic transition states proceed, if at all, much less easily than those involving aromatic transition states.

Source:

PAC, 1994, 66, 1077 (Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)) on page 1086

See also:

PAC, 1995, 67, 1307 (Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995)) on page 1319