

antiaromaticity (antithetical to aromaticity)

Those cyclic molecules for which cyclic electron delocalization provides for the reduction (in some cases, loss) of thermodynamic stability compared to acyclic structural analogues are classified as antiaromatic species. In contrast to aromatic compounds, antiaromatic ones are prone to reactions causing changes in their structural type, and display tendency to alternation of bond lengths and fluxional behavior (see fluxional molecules) both in solution and in the solid. Antiaromatic molecules possess negative (or very low positive) values of resonance energy and a small energy gap between their highest occupied and lowest unoccupied molecular orbitals. In antiaromatic molecules, an external magnetic field induces a paramagnetic electron current. Whereas benzene represents the prototypical aromatic compound, cyclobuta-1,3-diene exemplifies the compound with most clearly defined antiaromatic properties.

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1923