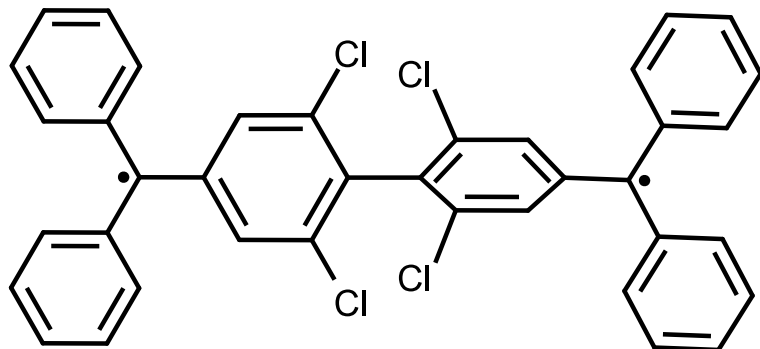


## biradical

An even-electron molecular entity with two (possibly delocalized) radical centres which act nearly independently of each other, e.g.



Species in which the two radical centres interact significantly are often referred to as 'biradicaloids'. If the two radical centres are located on the same atom, the species are more properly referred to by their generic names: carbenes, nitrenes, etc. The lowest-energy triplet state of a biradical lies below or at most only a little above its lowest singlet state (usually judged relative to  $k_B T$ , the product of the Boltzmann constant  $k_B$  and the absolute temperature  $T$ ). The states of those biradicals whose radical centres interact particularly weakly are most easily understood in terms of a pair of local doublets. Theoretical descriptions of low-energy states of biradicals display the presence of two unsaturated valences (biradicals contain one fewer bond than permitted by the rules of valence): the dominant valence bond structures have two dots, the low energy molecular orbital configurations have only two electrons in two approximately nonbonding molecular orbitals, two of the natural orbitals have occupancies close to one, etc. Although this term has been recommended in the past for diradicals, specialists working in the field prefer the latter term.

**See also:** carbenes, nitrenes

### Source:

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1089

PAC, 1995, 67, 1307 (*Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995)*) on page 1322