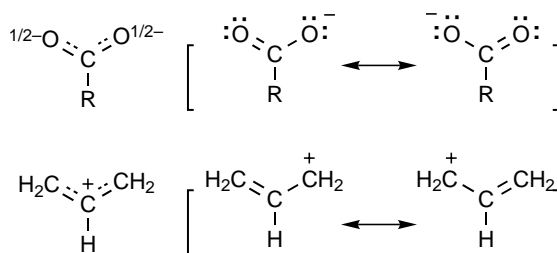


delocalization

A quantum mechanical concept most usually applied in organic chemistry to describe the π -bonding in a *conjugated system*. This bonding is not localized between two atoms: instead, each link has a ‘fractional double bond character’ or *bond order*. There is a corresponding ‘delocalization energy’, identifiable with the stabilization of the system compared with a hypothetical alternative in which formal (localized) single and double bonds are present. Some degree of delocalization is always present and can be estimated by quantum mechanical calculations. The effects are particularly evident in *aromatic* systems and in symmetrical *molecular entities* in which a lone pair of electrons or a vacant p-orbital is conjugated with a double bond (e.g. carboxylate ions, nitro compounds, enamines, the allyl cation). Delocalization in such species may be represented by partial bonds or as resonance (here symbolized by a two-headed arrow) between *contributing structures*.



These examples also illustrate the concomitant delocalization of charge in ionic conjugated systems. Analogously, delocalization of the spin of an unpaired electron occurs in conjugated *radicals*.

See also *mesomerism*.

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N.B. This is superseded by a *later definition*.