

bond order

The electron population in the region between atoms A and B of a molecular entity at the expense of electron density in the immediate vicinity of the individual atomic centers. Different schemes of partitioning electron density give rise to different definitions of bond orders. In the framework of the Mulliken population analysis, bond order is associated with the total overlap population

$$q_{AB} = 2 \sum_{\mu}^A \sum_{\nu}^B P_{\mu\nu} S_{\mu\nu}$$

where $P_{\mu\nu}$ and $S_{\mu\nu}$ are respectively the elements of the density matrix and overlap matrix (see overlap integral). A large positive value of bond order signifies strong bonding between the atoms of the molecular entity, whereas negative values of q_{AB} imply that electrons are displaced away from the inter-atomic region and point to an anti-bonding interaction. In valence bond theory, bond order is given by a weighted average of the formal bond orders (i.e. by the number of electron pairs in a given Lewis structure) between the atoms in the resonance structures (see resonance hybrid).

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1927