

bond order, p_{rs}

Theoretical index of the degree of bonding between two atoms relative to that of a single bond, i.e. the bond provided by one localized electron pair. In molecular orbital theory it is the sum of the products of the corresponding atomic orbital coefficients (weights) over all the occupied molecular spin-orbitals.

G.B. 17; see also 1994, 66, 1090

N.B. This is superseded by a *later definition*.