

atomic charge

The charge attributed to an atom A within a molecule defined as $\zeta = Z_A - q_A$, where Z_A is the atomic number of A and q_A is the electron density assigned to A . The method of calculation of q_A depends on the choice of the scheme of partitioning electron density. In the framework of the Mulliken population analysis q_A is associated with the so-called gross atomic population: $q_A = \sum q_\mu$, where q_μ is a gross population for an orbital μ in the basis set employed defined according to

$$q_\mu = P_{\mu\mu} + \sum_{\nu \neq \mu} P_{\mu\nu} S_{\mu\nu}$$

where $P_{\mu\nu}$ and $S_{\mu\nu}$ are the elements of density matrix and overlap matrix, respectively (see overlap integral). In the Hückel molecular orbital theory (where $S_{\mu\nu} = \delta_{\mu\nu}$), $q_\mu = n_\mu P_{\mu\mu}$, where n_μ is the number of electrons in the MO μ .

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1924