

Mulliken population analysis (MPA)

A partitioning scheme based on the use of density and overlap matrixes of allocating the electrons of a molecular entity in some fractional manner among its various parts (atoms, bonds, orbitals). As with other schemes of partitioning the electron density in molecules, MPA is arbitrary and strongly dependent on the particular basis set employed. However, comparison of population analyses for a series of molecules is useful for a quantitative description of intra-molecular interactions, chemical reactivity and structural regularities.

Source:

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1953