

ANALYSIS OF THE CHEMICAL BONDING AND AROMATICITY BASED ON THE STUDY OF ELECTRON DELOCALIZATION

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The purpose of this lecture is to discuss some recent advances in the analysis of aromaticity and chemical bonding using electron delocalization measures in the framework of the Atoms-in-Molecules (AIM) theory of Bader and coworkers.^[1-4] We will show how through the N-order electron density, the AIM theory allows to define localization (LI), delocalization indices (DI), and multicenter indices that give relevant information on the localization and delocalization of the electronic charge.^[5-8] From these indices, one can analyse the chemical bond and define new indicators of local aromaticity,^[7,8] which are founded on the fact that aromaticity is related to the cyclic delocalized distribution of π electrons. The results obtained with these new indexes in comparison with previous measures of aromaticity for a series of aromatic systems are presented.

References

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