

Comparison among four different ways to condense the Fukui function

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Four different ways to condense the Fukui function are compared. Three of them perform a numerical integration over different basins to define the condensed Fukui function, and the other one is the most traditional Fukui function using Mulliken population analysis. The basins are chosen to be the basins of the electron density (AIM), the basins of the electron localization function (ELF), and the basins of the Fukui function itself. The use of the last two basins is new and presented for the first time here. It is found that the last three methods yield results which are stable against a change in the basis set. The condensed Fukui function using the basins of the ELF is not able to give information on the reactivity of an acceptor molecule. In general, the condensed Fukui function using the basins of the density or the basins of the Fukui function describe the reactivity trends well. The latter is preferred, because it only contains information about the Fukui function itself and it g