Local electrophilicity

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© 2018, Springer-Verlag GmbH Germany, part of Springer Nature. In this work some possibilities for deriving a local electrophilicity are studied. First, we consider the original definition proposed by Chattaraj, Maiti, and Sarkar (J Phys Chem A 107:4973, 2003), in which the local electrophilicity is given by the product of the global electrophilicity, and the Fukui function for charge acceptance is derived by two different approaches, making use of the chain rule for functional derivatives. We also modify the proposals based on the electron density so as to have a definition with the same units of the original definition, which also introduces a dependence in the Fukui function for charge donation. Additionally, we also explore other possibilities using the tools of information theory and the temperature dependent reactivity indices of the density functional theory of chemical reactivity. The poor results obtained from the last two approaches lead us to conjecture that this is due to t