Proposal of a simple and effective local reactivity descriptor through a topological analysis of an orbital-weighted fukui function

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The prediction of reactivity is one of the long-standing objectives of chemistry, contributing to enforce the link between theory and experiment. In particular, the regioselectivity of aromatic molecules has motivated the proposal of different reactivity descriptors based on foundational theories, like Frontier Molecular Orbital (FMO) theory and density functional theory, to predict and rationalize such regioselectivity. This article examines cases where reactivity descriptors, based on FMO theories, are known to have failed, specifically on electrophilic aromatic substitution reactions, through a simple but effective new reactivity model: the Orbital-weighted Fukui function ((Formula presented.)) and its topological analysis. Interestingly, this descriptor proves to be effective in adequately predicting regioselectivities where other approximations failed. © 2017 Wiley Periodicals, Inc.

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