Quantitative characterization of the local electrophilicity of organic molecules. Understanding the regioselectivity on Diels-Alder reactions

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Regional electrophilicity at the active sites of the reagents involved in polar Diels-Alder processes may be described on a quantitative basis using an extension of the global electrophilicity index recently introduced by Parr et al. (J. Am. Chem. Soc. 1999, 121, 1922). The local or regional electrophilicity provides useful clues about the expected regioselectivity of the products on Diels-Alder reactions showing significant polar character. The local (regional) electrophilicity index shows significant advantages over other unnormalized definitions of relative electrophilicity proposed in the literature in the sense that it clearly identifies the relevant electrophilic sites in a molecule without restricting the search to those sites having comparable values of regional electrophilic/nucleophilic softness.