

**Elucidation of the Chemo- and Regioselectivity of Polar Diels-Alder
Reactions involving Thiophene-1, 1-Dioxides Using DFT-Based
Reactivity Indexes**

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Abstract :

The analysis of the global electrophilicity indexes of some substituted thiophene-1,1-dioxides shows that these species act as potential electrophiles in polar Diels – Alder reactions with diene systems. The chemo- and regioselectivity of these cycloadditions are rationalized using local electrophilicity and local nucleophilicity indexes recently proposed by Domingo's group [Domingo, L. R.; Aurell, M. J.; Perez, P.; Contreras, R. Quantitative Characterization of the Local Electrophilicity of Organic Molecules. Understanding the Regioselectivity on Diels Alder Reactions. *J. Phys. Chem. A.*, 2002, 106(29), 6871-6875; Perez, P.; Domingo, L. R.; Duque-Norena, M.; Chamorro, E. A Condensed-to-Atom Nucleophilicity Index. An Application to the Director Effects on the Electrophilic Aromatic Substitutions. *J. Mol. Struct. THEOCHEM*, 2009, 895, 86-91]. The cyclization modes, predicted using these static DFT-based reactivity indexes, are in good agreement with experimental outcomes.

Keywords : Diels-Alder reactions, thiophene-1,1-dioxides, Chemoselectivity, Regioselectivity, DFT-based reactivity indexes, stereoselectivity, the transition state, frontier molecular orbital (FMO) theory.

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