

Tentative Outline Special Issue for LETTERS IN ORGANIC CHEMISTRY

Guest Editor: Luis R. Domingo

Application of the density functional based reactivity indices to the study of the organic reactions. The case of the diels-alder reaction.

Aims & Scope:

This special issue is aimed to providing a recent update on the application of the based reactivity indices to the study of the Diels-Alder reactions, and thus to evince that concepts defined within the FMO theory as pericyclic reaction, normal and inverse electron demand, and HOMO and LUMO interactions should not be used in the recent DFT analysis. Due to the relevance that is developing the conceptual DFT within the modern bibliography, this issue will be of grant interest for the organic chemist community.

Key words: Polar Diels-Alder reactions, Reactivity, Regioselectivity, Quimioselectivity, Electrophilicity, Nucleophilicity, Local electrophilicity, Local nucleophilicity, Charge transfer processes.

Subtopics:

Cycloaddition reactions.

Polar mechanisms.

Density functional reactivity indices.

Submission Deadline for Authors: September 2010.