



Molecular Structure, HOMO-LUMO, MEP and Fukui Function Analysis of Some TTF-donor Substituted Molecules Using DFT (B3LYP) Calculations

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Authors' contributions

This work was carried out in collaboration between all authors. The synthesis part of this work was carried out under the direction of author AKG; the computational study was carried out under the direction of authors DV, TA and AB realized and wrote the work. All authors read and approved the final manuscript.

Article Information

DOI: 10.9734/IRJPAC/2016/27066

Editor(s):

(1) Wolfgang Linert, Institute of Applied Synthetic Chemistry Vienna University of Technology Getreidemarkt, Austria.

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Complete Peer review History: <http://sciencedomain.org/review-history/15084>

Original Research Article

Received 17th May 2016
Accepted 14th June 2016
Published 20th June 2016

ABSTRACT

In this letter, through computational study based on density functional theory (DFT/B3LYP) using basis set 6-31G (d,p) a number of global and local reactivity descriptors were computed to predict the reactivity and the reactive sites on the molecules. The molecular geometry and the electronic properties such as frontier molecular orbital (HOMO and LUMO), ionization potential (I) and electron affinity (A) were investigated to get a better insight of the molecular properties. Molecular electrostatic potential (MEP) for all compounds were determined to check their electrophilic or nucleophilic reactivity. The chemometric methods PCA and HCA were employed to find the subset of variables that could correctly classify the compounds according to their reactivity.

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