

Accepted Manuscript

Local reactivity through fukui function on endohedral mono-metallofullerenes

J.G. Rodríguez-Zavala

PII: S1386-9477(18)30300-X

DOI: [10.1016/j.physe.2018.08.027](https://doi.org/10.1016/j.physe.2018.08.027)

Reference: PHYSE 13272

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

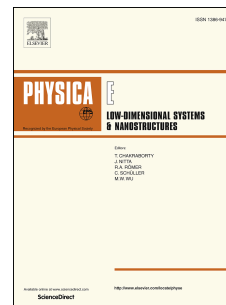
Received Date: 28 February 2018

Revised Date: 11 July 2018

Accepted Date: 22 August 2018

Please cite this article as: J.G. Rodríguez-Zavala, Local reactivity through fukui function on endohedral mono-metallofullerenes, *Physica E: Low-dimensional Systems and Nanostructures* (2018), doi: <https://doi.org/10.1016/j.physe.2018.08.027>.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Local Reactivity Through Fukui Function on Endohedral Mono-metallofullerenes

J. G. Rodríguez-Zavala^{a,*}

^a*Departamento de Ciencias Exactas y Tecnología, Centro Universitario de los Lagos, Universidad de Guadalajara, Enrique Díaz de León, 1144, Lagos de Moreno, Jalisco, México*

Abstract

Analysis of local reactivity through f^- , f^0 and f^+ Fukui functions was performed for (La, Ce, Y, Sc, Gd, Nd, Eu, Tm and Yb)@C₈₂-C_{2v}(9) mono-endohedral fullerenes. A clear difference was observed for trivalent and divalent compounds. For trivalent systems an amphoteric behavior was observed, which confirms the similarity found in previous studies about chemical reactivity in (La, Ce, Y, Sc, Gd)@C₈₂-C_{2v}(9) compounds. However, in spite of Nd@C₈₂-C_{2v}(9) is a trivalent compound, this system does not present an amphoteric behavior. In addition, divalent systems have not an amphoteric behavior either. Interestingly, in scientific literature there are several studies on functionalization of (La, Ce, Y, Sc, Gd)@C₈₂-C_{2v}(9) endohedral fullerenes, which are trivalent systems and are the ones who present the amphoteric behavior, however, there is nothing of literature about functionalization of divalent systems, one of the reasons could be that divalent systems have a low yield in comparison with trivalent systems, however, Nd@C₈₂-C_{2v}(9) is a trivalent system and has a high yield, nonetheless, this system has not been functionalized either and one of the answers could be in the amphoteric or non amphoteric behavior of the compounds. Additionally, it is worth to mention that this study is the first local reactivity analysis through Fukui functions on these compounds.

Keywords: Mono-endohedral fullerene; DFT calculations; Fukui function.

*Corresponding author

Email address: jgrz@culagos.udg.mx (J. G. Rodríguez-Zavala)

Download English Version:

<https://daneshyari.com/en/article/11026674>

Download Persian Version:

<https://daneshyari.com/article/11026674>

[Daneshyari.com](https://daneshyari.com)