

Accepted Manuscript

The effect of substituents on energy splitting in organic radicals : Quantitative cognizance from *ab initio* studies

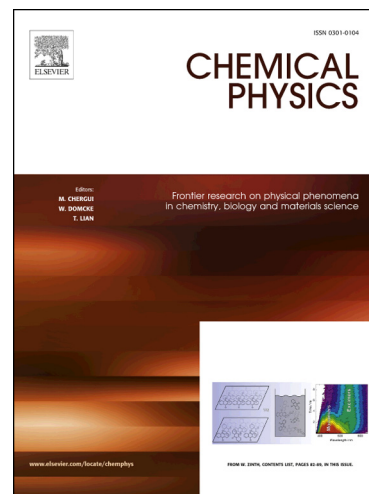
Sudip Chattopadhyay

PII: S0301-0104(18)30556-1

DOI: <https://doi.org/10.1016/j.chemphys.2018.08.008>

Reference: CHEMPH 10124

To appear in: *Chemical Physics*



Please cite this article as: S. Chattopadhyay, The effect of substituents on energy splitting in organic radicals : Quantitative cognizance from *ab initio* studies, *Chemical Physics* (2018), doi: <https://doi.org/10.1016/j.chemphys.2018.08.008>

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.

Manuscript ID: CHEMPHYS-2018-464

The effect of substituents on energy splitting in organic radicals : Quantitative cognizance from *ab initio* studies

Sudip Chattopadhyay*

*Department of Chemistry, Indian Institute of Engineering
Science and Technology, Shibpur, Howrah 711103, India*

(Dated: July 30, 2018)

The effect of substituents on the electronic states ordering in trimethylenemethane and *m*-xylylene diradicals, has been studied at the quantitative level through the estimations of separate individual state energies and the gap between them using our computationally economical perturbative *ab initio* method directed at describing one specific state, in contrast to multistate treatments. To provide reliable and chemically accurate estimates for energy differences between multiple states of different nature appropriate computational protocol is needed which is built on a democratic and consistent description of target electronic states of different spin-multiplicity. As the energy gap between electronic states of the radicals treated here is relatively small, order of the states can be tuned by using suitable substituents. Our present estimates are well supported by the experimental findings. Present work may serve as a guide for the study of similarly large radicaloid systems for which the use of wavefunction methods becomes challenging.

I. INTRODUCTION

There are many reasons to be surprised of in the study of radicals, although traditional radical chemistry is regarded by some chemists as a mature domain of science. A plethora of chemical processes involve radicals (a class of reactive molecules in which N unpaired electrons occupy N quasidegenerate orbitals) which exhibit high reactivity and also show

*Electronic address: sudip_chattopadhyay@rediffmail.com

Download English Version:

<https://daneshyari.com/en/article/7837097>

Download Persian Version:

<https://daneshyari.com/article/7837097>

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