Accepted Manuscript

Conformational and electronic properties of hydroquinone adsorption on C60 fullerenes: Doping atom, solvent and basis set effects

Orkun Ergürhan, Cemal Parlak, Özgür Alver, Mustafa Şenyel

PII: S0022-2860(18)30542-8

DOI: 10.1016/j.molstruc.2018.04.092

Reference: MOLSTR 25165

To appear in: Journal of Molecular Structure

Received Date: 24 January 2018

Revised Date: 10 April 2018

Accepted Date: 27 April 2018

Please cite this article as: O. Ergürhan, C. Parlak, Öü. Alver, M. Şenyel, Conformational and electronic properties of hydroquinone adsorption on C60 fullerenes: Doping atom, solvent and basis set effects, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.04.092.

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.



Conformational and electronic properties of hydroquinone adsorption on

C60 fullerenes: Doping atom, solvent and basis set effects

Orkun Ergürhan¹, Cemal Parlak¹, Özgür Alver^{2*} and Mustafa Şenyel²

¹Department of Physics, Science Faculty, Ege University, Izmir, 35100, Turkey

²Department of Physics, Science Faculty, Anadolu University, Eskişehir, 26470, Turkey

* Corresponding author:

E-mail: cemal.parlak@ege.edu.tr

Tel: +90 232 311 23 83

Download English Version:

https://daneshyari.com/en/article/7807082

Download Persian Version:

https://daneshyari.com/article/7807082

Daneshyari.com