

Accepted Manuscript

Electrostatic properties of fullerenes under an external electric field: First-principles calculations of energetics for all IPR isomers from C_{60} to C_{78}

Jun-ya Sorimachi, Susumu Okada

PII: S0009-2614(16)30417-1

DOI: <http://dx.doi.org/10.1016/j.cplett.2016.06.022>

Reference: CPLETT 33931

To appear in: *Chemical Physics Letters*

Received Date: 19 February 2016

Accepted Date: 7 June 2016

Please cite this article as: J-y. Sorimachi, S. Okada, Electrostatic properties of fullerenes under an external electric field: First-principles calculations of energetics for all IPR isomers from C_{60} to C_{78} , *Chemical Physics Letters* (2016), doi: <http://dx.doi.org/10.1016/j.cplett.2016.06.022>

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.



Electrostatic properties of fullerenes under an external electric field: First-principles calculations of energetics for all IPR isomers from C₆₀ to C₇₈

Jun-ya Sorimachi*, Susumu Okada

Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8571, Japan

Abstract

Based on first-principles total energy calculations, we analyze the energetics of the fullerene isomers from C₆₀ to C₇₈, all of which satisfy the isolated pentagon rule, under a parallel electric field. Our calculations show that the total energy of the fullerene is proportional to the square of the external electric field. On the other hand, the coefficient of the quadratic energy profile is sensitive to the fullerene species and their orientation. Furthermore, fullerenes possessing lower symmetry exhibit asymmetric quadratic energy profiles with respect to the field, indicating that they possess intrinsic polarization along particular molecular orientations.

Keywords: Fullerene, Electric field, Spherical dielectric, Intrinsic polarization

1. Introduction

For the past three decades, fullerenes have maintained a premier position in the fields of nanoscience and nanotechnology as representatives of nanometer-scale materials exhibiting unusual chemical and physical properties not seen in conventional carbon allotropes [1]. Because of the huge number of possible arrangements of 12 pentagonal rings and the appropriate

*TEL/FAX: +81-298535600 (ext. 8233)/+81-298535924

Email addresses: jsorimachi@comas.frsc.tsukuba.ac.jp (Jun-ya Sorimachi), sokada@comas.frsc.tsukuba.ac.jp (Susumu Okada)

Download English Version:

<https://daneshyari.com/en/article/5378765>

Download Persian Version:

<https://daneshyari.com/article/5378765>

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