

Accepted Manuscript

DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs

Mahmoud Mirzaei, Oğuz Gülseren, Nasser Hadipour

PII: S2210-271X(16)30210-9
DOI: <http://dx.doi.org/10.1016/j.comptc.2016.06.004>
Reference: COMPTC 2155

To appear in: *Computational & Theoretical Chemistry*

Received Date: 2 March 2016
Revised Date: 6 June 2016
Accepted Date: 6 June 2016



Please cite this article as: M. Mirzaei, O. Gülseren, N. Hadipour, DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs, *Computational & Theoretical Chemistry* (2016), doi: <http://dx.doi.org/10.1016/j.comptc.2016.06.004>

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.

DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs

Mahmoud Mirzaei^{a,*}, OğuzGülseren^b, Nasser Hadipour^c

^a*Bioinformatics Research Center, School of Pharmacy and Pharmaceutical Sciences,
Isfahan University of Medical Sciences, Isfahan, Iran*

^b*Department of Physics, Faculty of Science, Bilkent University, Ankara, Turkey*

^c*Department of Chemistry, Faculty of Science, Tarbiat Modares University, Tehran, Iran*

ABSTRACT

Atomic scale properties of quadrupole coupling constants (C_Q) have been evaluated for singular and paired 5-fluorouracil (FU) models. Structural possibilities and properties for various types of hydrogen bonded (HB) homo pairs of FU have been investigated based on density functional theory (DFT) calculations. The models have been optimized to obtain the minimum energy level structures and only the planar molecular pairs have been considered. Various types of HB interactions have also managed the molecular shapes for the FU pairs. Different types of energies and also electron transferring properties have been investigated by the evaluated optimized properties. The atomic scale results indicated different strengths of HB interactions for FU pairs according to the changes of C_Q properties for atoms in the singular and paired systems depending on the strength of interactions.

Keywords: Fluorouracil; Hydrogen bond; Density functional theory; Quadrupole coupling constant

* Corresponding author. Fax: +98-31-36680011; E-mail: mdmirzaei@pharm.mui.ac.ir

Download English Version:

<https://daneshyari.com/en/article/5392754>

Download Persian Version:

<https://daneshyari.com/article/5392754>

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