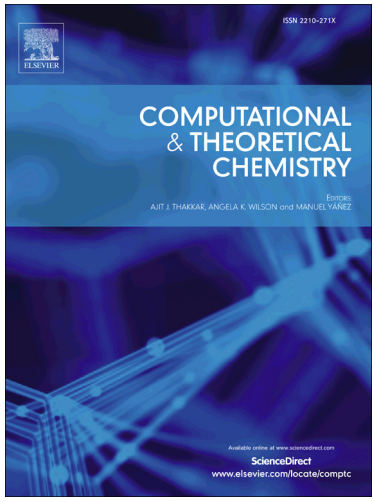

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PII: S2210-271X(16)30210-9
DOI: http://dx.doi.org/10.1016/j.comptc.2016.06.004
Reference: COMPTC 2155

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

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

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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

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