Ústav systémové biologie a ekologie
AKADEMIE VĚD ČESKÉ REPUBLIKY

Filip Zimandl: Conformational Study of a Flexibility of the Fluorescence Dye QSY 21

Review of the bachelor thesis

The bachelor thesis of Filip Zimandl can be separated in five chapters. In introduction part author introduced the aim of the work which is application of computational methods to study conformational changes and finding the most stable conformers of of the isolated QSY 21 probe and estimate the barrier height of the rotation of most flexible parts of the molecule.

In second part which is devoted to theoretical background and quantum mechanical methods the author introduced the approximations have been used in the methods such as Born-Oppenheimer approximation, central field approximation. Also molecular orbital theory and Ab-initio calculations such as Hartree-Fock method, Møller-Plesset perturbation theory and quenching molecular dynamics have been introduced.

In third part which is methods part molecular dynamics/quenching (MD/Q) calculations and correlated Ab-initio quantum calculations of isolated dye in order to estimate the rotational barrier height of the DIHI rings are developed. The author quite intensively described the methodology of the work and in results and discussion part discussed the conformational flexibility of the QSY 21 dye and the rotation barriers of the aromatic side ring of the above mentioned dye. The emphasis of this work which also demonstrates the application of the quantum mechanical methods has been presented in this thesis submitted as a scientific paper in the Journal of Phys. Chem. Chem. Phys. which is in press.

Thesis is well organized and the language of the thesis is quite good, clear and understandable.

At the end I must state that Filip Zimandl with this work and publishing one paper in high impact factor journal as Phys. Chem. Chem. Phys., in his bachelor study without any doubts fullfills all criteria for being awarded a bachelor degree. Therefore with pleasure I recommend Filip Zimandl for being awarded the bachelor degree.

Question: Author in the table 2 summarized the energy profile of the rotation of the DIHI ring employing various method and basis set in vacuum an in the implicit water. Did author try to see the effect of explicit water in the calculations?

Nove Hrady, May 31st 2010

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