Protic and aprotic solvent effect on molecular properties and g-tensors of *o*-semiquinones with various aromacity and heteroatoms: A DFT study.

Autorzy

Maciej Witwicki

Julia Jezierska

Rok wydania

2010

Czasopismo

Chemical Physics Letters

Numer woluminu

493

Strony

364-370

DOI

10.1016/j.cplett.2010.05.063

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The UB3LYP/EPR-II, UPBE0/EPR-II and UBP86/EPR-II DFT methods have been applied to study the protic and aprotic solvent effect on the ***g***-tensor and molecular properties of*o*-semiquinone radicals. The solvent effect has been taken into account in two ways: by employing continuum dielectric approach and by explicit solvent molecules inclusion. Choice of the investigated systems has allowed to determinate the influence of increased aromaticity and the presence of heteroatoms on the radical properties. To reach the best efficiency of the theoretical studies the calculated Δg_{iso} values have been compared with these experimentally observed.

Adres publiczny

https://doi.org/10.1016/j.cplett.2010.05.063

Strona internetowa wydawcy

http://www.elsevier.com