

Solvent effect on EPR, molecular and electronic properties of semiquinone radical derived from 3,4-dihydroxybenzoic acid as model for humic acid transient radicals: high-field EPR and DFT studies.

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Rok wydania

2009

Czasopismo

Chemical Physics Letters

Numer woluminu

473

Strony

160-166

DOI

10.1016/j.cplett.2009.03.035

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The *g*-tensor components and isotropic hyperfine constants of solvent-affected radical anion from 3,4-dihydroxybenzoic acid were computed at UBP86/EPR-II level and correlated with the molecular and electronic structures. The role of solvent was considered in two ways: by using a conductor-like screening model (COSMO) and by adding water molecules, hydrogen bonded to the radical. To reach the best efficiency of the calculations, the theoretical EPR parameters were compared with experimental derived from high-field (406.4 GHz) and X-band spectra. Inclusion of water molecules in the first hydration sphere of the radical appears to be mandatory for correct prediction of its properties.

Adres publiczny<https://doi.org/10.1016/j.cplett.2009.03.035>Strona internetowa wydawcy<http://www.elsevier.com>