

Protonated o-semiquinone radical as a mimetic of the humic acids *native* radicals: a DFT approach to the molecular structure and EPR properties.

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Streszczenie

Organic radicals are known to be an indispensable component of the humic acids (HA) structure. In HA two forms of radicals, stable (*native*) and short-lived (*transient*), are identified. Importantly, these radical forms can be easily differentiated by electron paramagnetic resonance (EPR) spectroscopy. This article provides a DFT-based insight into the electronic and molecular structure of the *native* radicals. The molecular models including an increase of the radical aromaticity and the hydrogen bonding between the radical and other functional groups of HA are taken under investigation. In consequence the interesting pieces of information on the structure of the *native* radical centers in HA are revealed and discussed, especially in terms of differences between the electronic structure of the *native* and *transient* forms.

Adres publiczny

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