

The pH-induced shift in the g -tensor components of semiquinone-type radicals in humic acids-DFT and EPR studies.

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DFT method has been applied to calculate pK_a and g -tensors values of semiquinone radicals mimicking the radicals present in humic acids. The results obtained support the hypothesis that naturally occurring stable semiquinone radicals (*native* form) are trapped in the humic acid macromolecule matrices which unables their direct involvement in the acid-base equilibrium with short-lived radicals (*transient* form). The differences between calculated g parameters for protonated and deprotonated model radicals are similar to those observed for humic acids allowing to attribute the stable radicals to protonated semiquinones and the short-lived radicals to deprotonated forms.

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