# Influence of Pb(II) on the radical properties of humic substances and model compounds.

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The influence of Pb(II) ions on the properties of the free radicals formed in humic acids and fulvic acids was investigated by electron paramagnetic resonance spectroscopy. It is shown that, in both humic acid and fulvic acid, Pb(II) ions shift the radical formation equilibrium by increasing the concentration of stable radicals. Moreover, in both humic acid and fulvic acid, Pb(II) ions cause a characteristic lowering of the stable radicals' *g*-values to *g* = 2.0010, which is below the free electron *g*-value. This effect is unique for Pb ions and is not observed with other dications. Gallic acid (3,4,5-trihydroxybenzoic acid) and tannic acid are shown to be appropriate models for the free radical properties, i.e., *g*-values, Pb effect, pH dependence, of humic and fulvic acid, respectively. On the basis of density functional theory calculations for the model system (gallic acid−Pb), the observed characteristic *g*-value reduction upon Pb binding is attributed to the delocalization of the unpaired spin density onto the Pb atom. The present data reveal a novel environmental role of Pb(II) ions on the formation and stabilization of free radicals in natural organic matter.

Słowa kluczowe

Ions, Gallic acid, Electron paramagnetic resonance spectroscopy, pH, Quantum mechanics

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