pH-dependent formation of Hg(II)-semiquinone complexes from natural phenols.

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The ability of various natural phenols to form Hg(II)-semiquinone complexes was tested in the pH range of 2.8–12. EPR experiments performed at 9.6 and 34 GHz (the X- and Q-band, respectively) revealed that the complexes formed at low and high pH values exhibit a significant dissimilarity between their *g*-matrices (*g*-tensors), strongly suggesting that the complexes differ structurally. Our previous investigation on the low pH complex (Chemosphere 2015, 119, 479–484) had shown the Hg(II) ion to be tetracoordinated by two ligands, one of the ligands being monoprotonated with the unpaired electron mainly located on it. In order to reveal the molecular structure of the high pH form a DFT-based theoretical analysis was carried out in this work. For all the optimized model structures the *g*-matrices were computed and compared with their experimental counterparts. Good agreement was observed only if the geometry of the model Hg(II) complex was planar and the coordination sphere was composed of one fully deprotonated radical ligand and hydroxyl anions.

Słowa kluczowe

semiquinone radicals, EPR spectroscopy, density functional calculations, hgII

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