Effects of solvents, ligand aromaticity, and coordination sphere on the g tensor of anionic *o*-semiquinone radicals complexed by Mg^{2+} ions : DFT studies.

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Streszczenie

Density functional theory (DFT) was employed to study the impact of Mg^{2+} ions on the *o*-semiquinone radical anions of different aromaticity in protic and aprotic solvents. After the geometry optimization of ligands and complexes, their **g** tensors were computed at the UBP86/TZVP and UB3LYP/TZVP theory levels. The suitability of various model systems, assuming continuum dielectric approaches, different Mg^{2+} coordination spheres (completed by solvent molecules), and inclusion of additional solvent molecules H-bonded to the ligands, was tested in terms of correlation between the experimental and calculated *g*-shifts. The effects of complexation, ligands aromaticity, and solvents on the electron spin density for *o*-semiquinones are discussed. To recognize clearly the changes in the nature of the **g** tensor components, the contributions from particular excited states were analyzed. A structural characterization of the tested complexes is expected to be helpful in investigations on the complicated biosystems in which the similar paramagnetic units are present.

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https://www.acs.org/content/acs/en.html