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EPR and DFT studies on heterometallic polynuclear compounds and Pb(II) complexes with semiquinone radicals

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Applications of High-Field and High-Frequency EPR (HF EPR) to study the nature of anisotropic exchange interactions between the paramagnetic centers present in different heterometallic systems, in correlation with their isotropic exchange interactions of different character and crystal and molecular structure, are reviewed. The report presents also the results of the DFT calculations of geometry, g parameters and distribution of unpaired electron density performed to explain the significant effects of Pb(II) ions on natural and model semiquinone radicals, which are pronounced in the changes of EPR spectral properties.