Relationships between structure, EPR, and NMR parameters for inorganic and biological molecules

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Abstract. Parameters of electron paramagnetic resonance (EPR) and nuclear magnetic resonance (NMR) spectroscopies are of increasing importance for the determination of molecular structure and dynamics at various fields of chemistry. While several structure-NMR and structure-EPR relationships have been established in the past, their parameterization is in general dependent on the type of system in question; hence the combination of an experiment with a quantum chemical calculation is of interest. First, the relationship between a molecular structure and electronic energy will be discussed on the example of an unusual structure of the AuI_3 molecule stabilized in the interlayer space of the $Bi_2Sr_2CaCu_2O_8$ superconductor. Second, we will concentrate on the relationship between the molecular structure, the EPR hyperfine splitting tensor and the EPR g-tensor of VO^{2+} complexes and of amavadin. Third, we will focus on Karplus relationships between three-bond NMR spin-spin coupling constants and the related torsion angle in nucleosides. Fourth, relationships between the phosphorus chemical shift in a nucleic acids backbone and the two closest torsion angles will be considered. Finally, the quantum chemical view of NMR parameters will be connected to that of EPR parameters via focusing on a spin-orbit contribution to the chemical shift which in transition metal complexes follows similar structural trends as the g-tensor of EPR spectroscopy.