

The Electron Paramagnetic Resonance technique for the study of the structural and dynamical properties of biomacromolecules

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Electron Paramagnetic Resonance (EPR) is a spectroscopic method for determining the structure and dynamics and the spatial distribution of paramagnetic species. Such species with at least one unpaired electron are often chemically reactive. Compounds with transition metal ions feature prominently as catalysts in different branches of chemistry, and free radical intermediates are observed in many organic reactions and in one-electron transfer processes. In nature, transition metal catalysis is realized by a number of metalloproteins and free radical intermediates play a central role in photosynthesis. Paramagnetic defects and impurities in crystal and glasses can influence the electrical and optical properties of a material even at low concentrations. They can also be used as spin probes, for example, to obtain insight into solid-state dynamics and phase transitions. Finally, stable free radicals such as nitroxides can be deliberately introduced as spin probes and spin labels into complex biological and synthetic materials.

In all these systems, continuous wave (CW) EPR and pulse related techniques (ENDOR, DEER/PELDOR) can provide unique information on the electronic structure since the magnetic parameters are related on the electronic wavefunction and the configuration of the surrounding nuclei with non-zero spins. With a frequency range up to several hundred gigahertz, EPR spectroscopy can also access molecular and chemical dynamics down to the nanosecond timescale.

In the lesson, after a brief introduction on the general and theoretical aspects of CW- and pulse EPR, examples covering the different aspects of EPR applications will be presented.