

From Distance to Distance Distribution Measurements by Pulsed Double Electron-Electron Double Resonance (PELDOR).

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PELDOR spectroscopy theory used for the analysis of the experiments will be described. It is shown that by analyzing the kinetics of PELDOR signal decay it is possible to find the distance between paramagnetic centers in a pair in the range 15-65 Å, to identify the radical assembling in groups and to estimate the number of the radicals in the groups. The distances determination by PELDOR in different systems will be exemplify.

By distance measurements the conformations of the double labeled peptides (trichogines and its dimmers) were determined for the polar glassy frozen solutions. In apolar solutions the self-assembling of peptides was found. The structures of aggregates based on the geometrical parameters obtained by PELDOR are proposed.

For the analysis of PELDOR signal decay due to dipole-dipole interaction between spins we used the approach based on the numerical solution of inverse problem which supplies us not only the distance but the distance distribution function between spins. The distance distribution functions between spin labels in the peptide molecules and their aggregates in solution were investigated as a function of the solvent composition. Peptide molecules (double labeled trichogine dimmers) in the aggregates in solutions with low methanol content display two types of structures, *i.e.* the α -helix with the 2.8 nm distance between labels and the 3_{10} -helix with the 3.2 nm distance between labels. As the methanol content of the solvent increases, a structure arises with the distance of 3.2 nm between labels, which corresponds to the 3_{10} -helical peptide molecule. An increase of the methanol content leads to the disruption of the aggregates and a change to the peptide conformation as well. The peptides fail to form aggregates in the pure methanol and a wide distribution of distances between labels were observed.

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