

Saturation factor of nitroxide radicals in liquid DNP by pulsed ELDOR experiments at 0.34 T and 3.4 T

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Dynamic nuclear polarization (DNP) in aqueous solution is a major topic of current efforts to enhance the sensitivity of high resolution NMR and magnetic resonance imaging.¹

In recent studies, nitroxide radicals have been favoured as polarizing agents for DNP since they are soluble in water, non-toxic and have been found to account for large DNP enhancements up to 9 T. However, the determination of the saturation factor for this class of polarizers has emerged as one of the major difficulties in rationalizing the observed enhancements in terms of the Overhauser equation since the NMR signal enhancement depends on the saturation level of all EPR lines of the polarizer.

Therefore, the theory for saturation transfer between the hyperfine states of nitroxides has been re-examined.² We exemplarily show at 0.34 T and 3.4 T that the effective saturation factor in Overhauser DNP can be directly determined in a pulsed electron-double-resonance (ELDOR) experiment, which measures the intensity of a hyperfine line when pumping a coupled line.³ The obtained values for ¹⁵N-²H-TEMPONE and ¹⁵N-Fremy's Salt at different concentrations are rationalized in terms of spin relaxation and are shown to fulfil the Overhauser theory.

A comparison of the two widely used radicals at 0.3 T yields similar maximum DNP enhancements but clearly different power dependence of their saturation behaviour.

1. Special Issue in *Phys. Chem. Chem. Phys.*, 2010, **12**, 5725-5928
2. S. Hyde, J. C. W. Chen and J. H. Freed, *J. Chem. Phys.*, 1968, **48**, 4211-4226.
3. M.-T. Türke, M. Bennati, *Phys. Chem. Chem. Phys.*, 2011, **13**, 3630-3633