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Optimization of ¹³C dynamic nuclear polarization: isotopic labeling of free radicals¹ PETER NIEDBALSKI, CHRISTOPHER PARISH, AND-HIKA KISWANDI, LLOYD LUMATA, University of Texas at Dallas — Dynamic nuclear polarization (DNP) is a physics technique that amplifies the nuclear magnetic resonance (NMR) signals by transferring the high polarization of the electrons to the nuclear spins. Thus, the choice of free radical is crucial in DNP as it can directly affect the NMR signal enhancement levels, typically on the order of several thousand-fold in the liquid-state. In this study, we have investigated the efficiency of four variants of the well-known 4-oxo-TEMPO radical (normal 4-oxo-TEMPO plus its ¹⁵N-enriched and/or perdeuterated variants) for use in DNP of an important metabolic tracer [1-13C] acetate. Though the variants have significant differences in electron paramagnetic resonance (EPR) spectra, we have found that changing the composition of the TEMPO radical through deuteration or ¹⁵N doping yields no significant difference in ¹³C DNP efficiency at 3.35 T and 1.2 K. On the other hand, deuteration of the solvent causes a significant increase of ¹³C polarization that is consistent over all the 4-oxo-TEMPO variants. These findings are consistent with the thermal mixing model of DNP.

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