DATE: Day 17 Month 04 Year 2023

SUMMARY of
2022 RESEARCH RESULTS REPORT
For International Collaborative Research with IPR, Osaka University

Research Title		Temperature Dependence of Methyl-Driven Overhauser DNP
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	Affiliation	**Ames National Laboratory**
	Present Title	**Scientist III**
Research Collaborator (Host PI)		**Yoh Matsuki (Associated Professor)**

Summary

The Overhauser effect in the dynamic nuclear polarization (DNP) of non-conducting solids has drawn much attention due to the potential for efficient high-field DNP as well as a general interest in the underlying principles that enable the Overhauser effect in small molecules. We recently reported the observation of ^{1}H and ^{2}H Overhauser effects in H_3C- or D_3C-functionalized Blatter radical analogs, which we presumed to be caused by methyl rotation. With this collaborative project, we looked at the mechanism behind methyl-driven Overhauser DNP using ultralow temperature MAS-DNP. We hypothesized that three possible dynamic modes could contribute to the effect, namely, methyl librations and tunneling in addition to classical rotation and used DFT and spin dynamics simulations to predict their temperature dependences. Comparisons between the DNP results and the simulations revealed that cross-relaxation at temperatures above 60 K originates from both libration and rotation, while librations dominate at lower temperatures. Due to the zero-point vibrational nature of these motions, they are not quenched by very low temperatures, and methyl-driven Overhauser DNP is expected to increase in efficiency down to 0 K, predominantly due to increases in nuclear relaxation times. These results suggest that a broader class of radicals than initially though may be able to perform methyl-driven Overhauser DNP, which could have important implications for high field DNP.

***Deadline: May 12, 2023**
***Please submit it to E-mail: tanpakuken-kyoten@office.osaka-u.ac.jp.**
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