Field dependence of ^{1}H optical nuclear polarization in organic molecular crystal powder: experiments and modeling

Zhukov Ivan V.,[1*] Kiryutin Alexey S.,[1] Vieth Hans-Martin,[1,2]
Matysik Jörg,[3] Yurkovskaya Alexandra V.[1]

[1] *International Tomography Center SB RAS, Institutskaya 3a, 630090, Novosibirsk, Russia*

[2] *Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany*

[3] *Institut für Analytische Chemie, University of Leipzig, Linnéstraße 3, 04103 Leipzig, Germany*

** E-mail: i.zhukov@tomo.nsc.ru*

Optical nuclear polarization (ONP) is the effect of nuclear spin hyperpolarization build up as a result of optical cycle “excitation-relaxation” of a dye molecule incorporated in a host molecular crystal structure. To show ONP, the optical cycle of a dye molecule must proceed through an optically excited triplet state $|T_1\rangle$ characterized by the strong non-equilibrium populations of the electron spin sublevels $|T_{1X}\rangle$, $|T_{1Y}\rangle$, $|T_{1Z}\rangle$, i.e. optical electron polarization (OEP), defined with respect to the molecular-fixed frame [1]. The electron spin sublevels of the excited triplet state are coupled to local nuclear spins through hyperfine interaction (HFI), which transfers part of this strong non-equilibrium electron spin order to the local nuclear spins. The transfer might be either coherent (which is especially pronounced in a level avoided crossing (LAC) region) [1], i.e., mediated by the static HFI of a local magnetic nucleus with the excited tripled state of a trapped dye molecule, or incoherent [2], i.e., mediated by time-dependent HFI of a local magnetic nucleus with mobile triplet excitons. Recently, a complete theoretical approach has been developed, which is focused on description of static ONP field dependence in terms of level crossing and level avoided crossings [3].

Previously, ONP studies were preferably done using single crystals, allowing to investigate in detail the LAC-ONP field and orientation effects. These investigations impose quite strict requirements on the experimental setup and on the quality of crystals used, and are challenging to implement. On the other hand, ONP studies on powder samples are relatively simple to implement, both in static and MAS conditions. However, to extract quantitative data on the properties of the system under study, a challenging numerical modeling should be exploited. Results of experiments and numerical modeling of on ^{1}H ONP field dependence studies will be presented.

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