Spin dynamics simulation package for fixed-geometry charge-separated systems

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Charge-separated radical intermediates of photoinduced chemical reactions with rather rigid molecular geometry and strong coupling between unpaired electrons participate in various important processes, for example, in photosynthesis of plants [1]. It is tempting to construct an artificial organic photosynthetic system which is mimicking the processes in the natural one to tackle the world's growing energy consumption challenge in a "green" way. This requires deep understanding of photochemical processes taking place both in natural and artificial systems. Both coherent and incoherent spin selective processes strongly affect the chemical properties of such charge-separated states, thus modulating the efficiency of the overall processes [2], but sometimes it is difficult to separate the influence of different processes involved. Experimental methods developed in spin chemistry: magnetic field affected reaction yield (MARY), chemically induced electron and nuclear polarization (CIDEP and CIDNP, correspondingly) can be applied to disentangle contributions from different channels, but they are effective only in combination with thorough analytical and numerical calculations.
In this contribution, the newly written Matlab based script package will be introduced, which allows to calculate the magnetic field effect of any observable, including CIDNP [3], CIDEP, MARY [4], and is freely available on request. It has been successfully applied for simulating proton and carbon-13 solution-CIDNP field dependences of a series of donor-linker-acceptor systems with at least 23 magnetic nuclei with non-zero hyperfine coupling in charge-separated state [3]. It's architecture and approximations made will be described, and the influence of model parameter's variations will be shown.

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References

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