Magnetic field sensitivity in plants: A case study of *Arabidopsis* CRY-1 protein

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Abstract

Experimentally, it has been shown that magnetic field sensitivity in living organisms is connected to the presence of blue-light photoreceptors cryptochromes. Cryptochromes transduce a light signal through a chain of chemical reactions involving the formation of intermediate biradicals. It was proposed that an external magnetic field affects the interconversion between singlet and triplet states of biradicals and thus interferes with the signal transduction chain. Theoretical modeling of this process requires an accurate evaluation of all interactions important for singlet-triplet interconversion: electron-electron, spin-orbit, spin-spin, hyperfine, and Zeeman. In the current study we investigate these interactions at the CIS level of theory applied to representative fragments of the CRY-1 protein in the plant *Arabidopsis thaliana*. We find, in contrast to previous simplified modeling [O. Efimova and P. J. Hore, Biophys. J. **94**, 1565 (2008)], that the spin-spin interaction is significantly larger than the "exchange" interaction. Thus it is not cancelled by the latter but rather dies off with the inter-radical separation. Also, it has been found that the spin-orbit interaction can play a significant role in singlet-triplet interconversion for short inter-radical distances, and the hyperfine interaction becomes the only coupling interaction for long inter-radical distances.