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A vibronic approach to the hyperfine interaction observed in biomagnetosensors

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The interactions of biological processes with magnetic fields can have significant impacts, with a strong example of this being magnetosensitivity in avian proteins allowing for migration[1]. The two main biological systems for optically-driven magnetosensing are cryptochrome (CRY) and light-oxygen-voltage (LOV) proteins[2,3], where each can be broadly summarised by 4 steps: photoactivation, radical pair generation, hyperfine hopping, and recombination/recycling. Understanding each through experimental observations and theoretical modelling is key to understanding and controlling the biomagnetoptical mechanism. The third step, whereby an induced coupling between the electronic and nuclear magnetic moments results in rapid spin-inversion, is incredibly sensitive to magnetic fields. Existing theoretical models typically consider the nuclei as frozen, however this neglects temperature-based effects, such as those due to vibronic oscillations (Herzberg-Teller contributions). In this work, I show that omission of these second-order contributions will result in a grossly underestimated kinetic model. Rate constants will be shown to increase by several orders of magnitude when incorporating vibronic effects, and will shift state lifetimes from microseconds to nanoseconds. This work addresses the hyperfine interaction taking into account these Herzberg-Teller terms to the correlated electronic-spin state matrix element. The second-order perturbative term is derived and applied to the magnetosensitive active site of a LOV protein. This approach more readily incorporates realistic temperature-based phenomena as vibronic contributions to the hyperfine interaction are explored, and acts as a solid first step towards a complete kinetic model within a complete protein system, which will ultimately require both temperature-dependant conformational sampling and anisotropic contributions to the second-order corrected isotropic matrix coupling element.

1. Ritz, Wiltschko, Hore, Rodgers, et al.; Biophysical Journal, 2009; 96, 8, 3451-3457.
2. Solov'yov; Quantum Effects in Biology; C10; Cambridge University Press, 2014; 218-236.
3. Abrahams, Spreng, Štuhec, Kempf, et al.; bioRxiv, 2024.

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