Predicting kinetics of spin-dependent reactions in an external magnetic field with nonadiabatic statistical theory

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The application of an external magnetic field to chemical reactions holds significance as it provides a novel element for controlling the reaction rate, potentially leading to the development of more efficient reactions that rely on magnetic properties of molecules. In this study, we explore a theoretical framework aimed at modeling spin-orbit coupling mediated transitions between electronic states with different spin multiplicities in the presence of an external magnetic field. Our approach incorporates the Zeeman interaction (interaction of electron spin with an external magnetic field) into the spin-dependent kinetics equations, alongside the spin-orbit interaction. The foundational equations of this investigation are derived within the framework of nonadiabatic statistical theory (NAST). We have integrated the external magnetic field effect into our NAST software package. The approach relies on electronic structure calculations to compute the Landau-Zener transition probabilities and the associated rate constants for spin-dependent processes. Our primary focus centers on the application of an external magnetic field to singlet-triplet transitions. We systematically examine the influence of the magnetic field on the spin adiabatic states for various field strengths, covering examples that span different spin-orbit coupling regimes. This comprehensive analysis allows us to gain a deeper understanding of the intricate interplay between the spin-orbit coupling and magnetic field effects in spin-dependent chemical reactions. As an example, we calculate the rate constants for singlet-triplet transitions in $Ni(dpp)Cl_2$ (dpp=1,3-bis(diphenylphosphino)propane) in the presence of an external magnetic field.