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Ab-Initio Based Computation of Rate Constants of Spin Forbidden Transitions in (Bio)inorganic Complexes and Metalloproteins[1] ABDULLAH OZKANLAR, JORGE H. RODRIGUEZ — Some (bio)chemical reactions are non-adiabatic processes whereby the total spin angular momentum, before and after the reaction, is not conserved. These are named spin- forbidden reactions. The application of spin density functional theory (SDFT) to the prediction of rate constants is a challenging task of fundamental and practical importance. We apply non-adiabatic transition state theory in conjunction with SDFT to predict the rate constant of the spin- forbidden dihydrogen binding to iron tetracarbonyl. To model the surface hopping probability between singlet and triplet states, the Landau-Zener formalism is used. The lowest energy point for singlet-triplet crossing, known as minimum energy crossing point (MECP), was located and used to compute, in a semi-quantum approach, reaction rate constants at 300 K. The predicted rates are in good agreement with experiment. In addition, we present results which are relevant to the ligand binding reactions of metalloproteins. This work is supported in part by NSF via CAREER award CHE-0349189 (JHR).

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