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Ab-Initio Based Computation of Rate Constants for Spin Forbidden Metalloprotein-Substrate Reactions[1] ABDULLAH OZKANLAR, JORGE H. RODRIGUEZ, Department of Physics, Purdue University, West Lafayette, IN 47907-2036, RODRIGUEZ RESEARCH TEAM — Some chemical and biochemical 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 ab-initio methods, such as 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 (NA-TST) in conjuntion with SDFT to predict the rate constant of the spin-forbidden recombination of carbon monoxide with 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 very good agreement with experiment. In addition, we present results for the spin- forbidden ligand binding reactions of iron-containing heme proteins such as myoglobin.

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