

STEERING H-ATOM DIFFUSION THROUGH IMPURITY-DOPED SOLID PARAHYDROGEN: THE ROLE OF DIFFERENTIAL SOLVATION ENERGIES

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Ultraviolet irradiation of solid parahydrogen (pH₂) matrices doped with suitable H-atom precursor molecules generates H atoms *in situ* through a series of photoinitiated chemical reactions; these H atoms move through the pH₂ matrix through a quantum diffusion process that involves the tunneling-mediated process $\text{H} + \text{H}_2 \rightarrow \text{H}_2 + \text{H}$. The mobile H atoms may react chemically with other species that are also embedded in the pH₂ matrix; an investigation of the kinetics of these H-atom chemical reactions provides us with information about reaction dynamics in the pH₂ matrix environment. A recent study of the $\text{H} + \text{N}_2\text{O} \rightarrow \text{HNNO}$ reaction in solid pH₂ [Mutunga, Follett, and Anderson, *J. Chem. Phys.* **139**, 151104 (2013)] demonstrates that this reaction exhibits strongly non-Arrhenius behavior, proceeding at measurable rates only when the temperature of the system drops below $T \approx 2.4$ K. A molecular-level understanding of these findings requires information about how the solid pH₂ matrix environment affects the long-range entrance channel of the $\text{H} + \text{N}_2\text{O}$ reaction. Here, we carry out quantum Monte Carlo simulations of a simple model system (Ar-doped solid pH₂) to investigate matrix-induced changes to long-range interactions between H atoms and other impurities embedded in solid pH₂ matrices. Our results suggest that the pH₂ matrix creates an effective long-range repulsion between the H atom and the Ar impurity, which we explain in terms of differential solvation energies of Ar and H atoms in solid pH₂.