Quantum Diffusion of Impurities in Solid Parahydrogen

Anderson, D.T.[1]* Muddasser, I.[2] Nguyen, A.[2]

*presenter
[1] danderso@uwyo.edu, Department of Chemistry, University of Wyoming, USA.
[2] Department of Chemistry, University of Wyoming, USA.

Over the last twenty years solid parahydrogen (pH_2) has emerged as an alternative host for matrix isolation studies in comparison to the more traditional noble gas solids. The physical and chemical properties of solid pH_2 distinguish it from noble gas solids in three important ways as a host for matrix isolation: (1) the weak cage effect of solid pH_2 allows *in situ* photolysis to be used as an effective means to produce isolated photoproducts, (2) several dopants species can readily diffuse in solid pH_2 permitting bimolecular solid-state reaction studies, and (3) the individual pH_2 host molecules can participate in chemical reactions while noble gas atoms are essentially chemically inert. This second distinction for a pH_2 host crystal has been leveraged by our research group[1] and others[2,3] to study hydrogen atom (H atom) reactions with various chemical species in solid pH_2 where the H atom is mobile via a quantum diffusion process. Recently, we have observed the $O(^3P) + O_2(X\ ^3\Sigma_g^-) \rightarrow O_3(X\ ^1A_1)$ reaction following the 193 nm *in situ* photolysis of O_2. This suggest that $O(^3P)$ atoms are mobile in solid pH_2 opening new opportunities to study O atom reactions. In fact, even stable molecules such as HF[4] and H_2O[5] have been reported to quantum diffuse in solid pH_2. We therefore have become interested in investigating which dopant species can diffuse, and which species are immobilized within solid pH_2. In this study we will focus on the diffusion properties of $O(^3P)$ and $Cl(^2P_{1/2})$ atoms in solid pH_2.

1. Mutunga, F.M.; Olenyik, K.M.; Strom, A.I.; Anderson, D.T. Hydrogen atom quantum diffusion in solid parahydrogen: The $H+N_2O \rightarrow$ *cis*-HNNO $\rightarrow$ *trans*-HNNO reaction. *J. Chem. Phys.* **2021**, *154*, 014302.
2. Tsuge, M.; Tseng, C.-Y.; Lee, Y.-P. Spectroscopy of prospective interstellar ions and radicals isolated in solid *para*-hydrogen matrices. *Phys. Chem. Chem. Phys.* **2018**, *20*, 5344.
3. Schneiker, A.; et al. Non-energetic, low-temperature formation of C_α-glycyl radical, a potential interstellar precursor of natural amino acids. *J. Phys. Chem. Lett.* **2021**, *12*, 6744.
4. Ooe, H.; et al. Diffusion of hydrogen fluoride in solid parahydrogen. *J. Chem. Phys.* **2013**, *138*, 2104309.
5. Moore, B.; Djuricanin, P.; Momose, T. Diffusion of water molecules in quantum crystals. *J. Phys. Chem. Lett.* **2018**, *9*, 6475.