THE Cl+H₂ \rightarrow HCl+H REACTION INDUCED BY IR + UV IRRADIATION OF Cl₂ IN SOLID PARAHYDROGEN

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Matrix isolation spectroscopy is a technique which enables highly reactive species to be trapped in a host environment and studied spectroscopically. Solid parahydrogen (pH_2) has been employed as a matrix host because of its interesting quantum mechanical properties and also because of its general inertness towards trapped dopants. However, in some cases pH_2 can react with impurities yielding new product molecules and providing insight into non-classical reaction pathways. In this talk I will present the results from a series of experiments where molecular chlorine (Cl₂) doped pH_2 crystals were exposed to two different irradiation schemes (namely UV only or IR + UV conditions) that gave rise to very different products. Cl₂ doped pH_2 crystals irradiated with 355 nm UV light produced almost exclusively (99%) isolated Cl-atom photofragments, indicating the reaction Cl+H₂($\nu = 0, J = 0$) \rightarrow HCl+H is not readily occurring. Cl₂ doped pH_2 exposed simultaneously to 355 nm UV irradiation and broadband cwIR light yielded HCl photoproducts indicating that the following reaction is playing a significant (15%) role in the *in situ* photochemistry: Cl+H₂($\nu = 1, J = 0$) \rightarrow HCl+H. The kinetic analysis of these experiments with two very different reaction pathways for UV only or IR + UV conditions will be presented. Further, the results of current investigations involving spin-orbit excited Cl-atoms generated using 416 nm UV photons will be discussed in order to explore the intriguing possibility of non-Born Oppenheimer reaction dynamics in the simple Cl+H₂ reaction.