HOW CHLORINE ATOM REACTS WITH H_2 IN IR-IRRADIATED SOLID PARA-HYDROGEN

JEN-YU WU, MOHAMMED BAHOU, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan*; AND YUAN-PERN LEE, *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan and Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 10617, Taiwan*.

The use of solid para-hydrogen (p-H_2) as a matrix host has generated considerable interest in recent years. Solid p-H_2 is considered as a quantum solid; hence it is softer than noble gas matrices and has several unique properties such as narrow bandwidths, feasibility of molecular and internal rotation, and a diminished cage effect, which is particularly relevant to the formation of atoms and radicals in a matrix using photolysis $insitu$. Raston and Anderson employed laser emission at 355 nm to photodissociate Cl_2 trapped in solid p-H_2 at 2 K and produced isolated Cl atoms.[a] Excitation of the solid p-H_2 with IR light in the range 4000-5000 cm^{-1} from a globar source induces reactions of Cl atoms with p-H_2 to form HCl.[b] We investigated the reaction of Cl with solid p-H_2 with a tunable IR laser and a FTIR spectrometer. The Cl atoms were produced on irradiation of a Cl_2/p-H_2 (1/1000-1/4000) matrix with light at 365 nm from a light-emitting diode. By monitoring continuously the formation of HCl while tuning the wavelength of the IR laser, we obtained the relative yield of HCl as a function of excitation wavelength. We found that absorption of the Cl-H_2 complex and solid H_2, but not the Cl_2-H_2 complex, induced the reaction Cl + H_2. In separate experiments we irradiated a selective area of the matrix with UV light and compared the yields of HCl in this area when we irradiated IR light at various locations. When the IR laser light irradiated outside the UV-irradiated area, excitation of p-H_2 near 4229 cm^{-1}, but not the Cl-H_2 complex at 4148.5 cm^{-1}, still produced HCl. In contrast, when the IR light irradiated inside the UV-irradiated region, more HCl was produced at 4148.5 cm^{-1}. This indicates that the excited H_2 can move around and react with Cl located far away from the originally excited area, whereas the IR excited Cl-H_2 complex reacts directly to form HCl. We also found that irradiation of H_2 produced some dimers of HCl, whereas irradiation at the Cl-H_2 complex produced only HCl monomer.

[a] P. L. Raston and D. T. Anderson, *J. Chem. Phys.* **126**, 021106 (2007).
[b] P. L. Raston and D. T. Anderson, *Phys. Chem. Chem. Phys.* **8**, 3124 (2006).