ENTRANCE CHANNEL COMPLEXES X-HX (X=Cl and Br) IN SOLID PARAHYDROGEN

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We report high-resolution vibrational spectra of the entrance channel complexes X-HX (X=Cl and Br) isolated in solid parahydrogen. The related X-HF complexes have been successfully synthesized in liquid helium droplets and rotationally resolved spectra reported at an earlier meeting.[a] These free radical complexes are formed by co-depositing X_2 and HX into solid parahydrogen followed by 355 nm in situ photodissociation of the X_2. The crystal is then thermally annealed to allow the X-HX complexes to form. Initial studies focused on the Br-HCl complex because it is non-reactive at the 4 K temperatures studied. These spectroscopic studies revealed both HCl donor and HCl acceptor absorption peaks that could be assigned to the isolated dimer via isotopic shifts due to ^{35}Cl and ^{37}Cl present in natural abundance. These studies suggest that both conformers of the Br-HCl complex, HCl donor and HCl acceptor, have nearly equal populations within the parahydrogen matrix. These results are interesting since intermolecular potentials that include relativistic effects disagree on the relative stabilities of these two conformers. Present studies focus on forming the homodimers (Br-HBr and Cl-HCl) where H-atom tunneling may be observed spectroscopically. The latest results and analysis will be presented at the meeting.

[a] J. M. Merritt, J. Kupper, and R. E. Miller, talk WH01, 58^{th} International Symposium on Molecular Spectroscopy, 18 June, 2003.