THEORETICAL AND EXPERIMENTAL WATER COLLISIONS WITH NORMAL AND PARAHYDROGEN

BRIAN J. DROUIN, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109-8099*; LAURENT WIESENFELD, *UJF-Grenoble 1/CNRS, Institut de Planétologie et d'Astrophysique de Grenoble (IPAG) UMR 5274, Grenoble, F-38041, France*.

The experimental data set of water-hydrogen collisions has been expanded and added to previously reported data[1]. In all, three rotational transitions of water; $1_{11} \leftarrow 0_{00}$, $2_{02} \leftarrow 1_{11}$ and $1_{10} \leftarrow 1_{01}$, have been studied in the 20-250 K range via lineshape measurements in a collisional cooling system with buffer gas of both normal and parahydrogen. Unlike previous studies with the same apparatus, these measurements have a verified, stable, ortho-parahydrogen ratio and qualitatively follow trends previously predicted from collision theory. However, the agreement with theory was not uniform, and measurements of pressure-shifts were not following the predicted trends. Since these measurements provide a valuable probe of the $H_2O$-$H_2$ potential energy surface (PES), we decided to repeat the theoretical calculations with the most current PES. To improve precision of the collisional energy calculations, several more time consuming steps were applied (1) Tighter convergence of inelastic scattering was forced through a summation in partial waves up to $J$ = 10; (2) Even tighter convergence of elastic scattering was forced through a summation up to $J^{Total}$ = 55 (3) the parahydrogen basis sets always included the $j$ = 2 level of $H_2$. Finally, the detailed resonances observed (especially in parahydrogen) required a fine energy grid for conversion of the collisional energy cross sections into temperature dependent cross-sections. The resulting data-sets are compared for each rotational transition and found to be in tight agreement ($<$ 30%) for two of the three transitions. Comparisons of the other transition, the fundamental transition of water ($1_{11} \leftarrow 0_{00}$), disagree up to 80%. We will discuss these results and their pertinence to models of cold interstellar material.

[1] B.J. Drouin, J.C. Pearson, L. Wiesenfeld and A. Faure - TF13, International Symposium on Molecular Spectroscopy, Ohio State University, 2011.