

MODELING THE INFLUENCE OF NUCLEAR SPIN IN THE REACTION OF H_3^+ WITH H_2

KYLE N. CRABTREE, BRIAN A. TOM,^a BENJAMIN J. McCALL, *Department of Chemistry, University of Illinois, Urbana, IL 61801, USA.*

The reaction $\text{H}_3^+ + \text{H}_2 \rightarrow \text{H}_2 + \text{H}_3^+$ is among the simplest of bimolecular chemical reactions, and may play an important role in determining the *ortho:para* ratios of H_3^+ and H_2 in interstellar environments. Despite its apparent simplicity, the kinetics of this reaction is not well understood, particularly the branching fractions of the proton hop and hydrogen exchange reaction pathways. In this contribution, we present a series of steady state chemical models that show how this reaction can be studied in the laboratory with spectroscopy. Our first model is based entirely on nuclear spin statistics, appropriate for high temperature, low pressure plasmas. This model is then extended to account for the possibility of a small number of three-body collisions which could influence the interpretation of spectroscopic measurements of the $\text{H}_3^+ + \text{H}_2$ binary reaction. Our final model employs rate coefficients calculated using a microcanonical statistical approach which takes into account energetic restrictions on certain reaction pathways, which may become important at lower temperatures. These models are directly aimed at extracting kinetic information about the $\text{H}_3^+ + \text{H}_2$ reaction from laboratory spectra of hydrogenic plasmas.

^aPresent Address: Department of Chemistry, United States Air Force Academy, Air Force Academy, CO 80840, USA