INFRARED SPECTROSCOPIC STUDIES OF ORTHO-PARA CONVERSION IN SOLID HYDROGEN CATALYZED BY HYDROGEN ATOMS

DAVID T. ANDERSON, MORGAN E. BALABANOFF, AARON I. STROM, *Department of Chemistry, University of Wyoming, Laramie, WY, USA*.

Our group has been studying the reactions of hydrogen atoms (H atoms) with various molecules (NO, N_2O, CH_3OH) in solid hydrogen for the last several years.[abc] One interesting puzzle that we have been unable to solve is how to detect the concentration of H atoms using FTIR spectroscopy. One possibility to estimate the H atom concentration is to measure the conversion of ortho-H_2 to para-H_2 within the solid that is catalyzed by the presence of H atoms. The H atom is a good ortho-para catalyst because it is paramagnetic and mobile within the solid even at extremely low temperatures. We have recently conducted a number of studies where we purposely synthesize solid para-H_2 samples with approximately 3% ortho-H_2 concentrations (slightly elevated). In the absence of H atoms, the ortho-H_2 concentration in the solid is stable on the order of days due to slow self-conversion. We can quantitatively detect the ortho-H_2 fraction using the overlapping $Q_1(0)$+$S_0(1)$ and $Q_1(1)$+$S_0(1)$ double transitions of solid molecular hydrogen. By rapidly generating H atoms via in situ photolysis of various H atom precursor molecules (NO and N_2O), we can initiate ortho-para conversion and follow the ortho-H_2 fraction in real time. This H atom catalyzed ortho-para conversion data therefore has the time dependent H atom concentration encoded in the signal; the challenge is to extract it. We observe qualitative differences in the shape of the ortho-H_2 fraction decay curve depending on the specific precursor used, the specific photolysis conditions, and the temperature of the sample. We will present the latest results and analysis at the meeting.

[a] F.M. Mutunga, S.E. Follett, D.T. Anderson, *J. Chem. Phys.* **139**, 151104 (2013).

[b] M. Ruzi, D.T. Anderson, *J. Phys. Chem. A* **119**, 12270 (2015).

[c] M.E. Balabanoff, M. Ruzi, D.T. Anderson, *Phys. Chem. Chem. Phys.* **20**, 422 (2018).