Interstitial hydrogen in vanadium dioxide\footnote{Supported by NSF grant DMR-1160756.} W. B. FOWLER, M. STAVOLA, WEIKAI YIN, YING QIN, Lehigh University, L. A. BOATNER, Oak Ridge National Laboratory — It has long been recognized that VO$_2$ has a monoclinic-to-rutile phase transition as the temperature increases through 340K, accompanied by a remarkable increase in conductivity from insulator to metal\cite{1,2}. Recently it has been found that interstitial hydrogen can modify both the structural and the electronic phase transition\cite{3}. The way hydrogen does this has only recently begun to be studied\cite{4}. We are using infrared spectroscopy to study the properties of H$_i$, and are also using the CRYSTAL06 code\cite{5} with hybridized DFT Hamiltonian to determine equilibrium positions and vibrational frequencies. IR spectroscopy finds several OH vibrational lines in hydrogenated VO$_2$ samples. Within the monoclinic structure of VO$_2$ there are four inequivalent sites for H$_i$ which may lead to distinct spectroscopic signatures. \cite{1} F. J. Morin, Phys. Rev. Lett. \textbf{3}, 34 (1959). \cite{2} A. Zylbersztejn and N. F. Mott, Phys. Rev. B \textbf{11}, 4383 (1975). \cite{3} J. Wei \textit{et al.}, Nature Nanotechnology \textbf{7}, 357 (2012). \cite{4} K. H. Warnick \textit{et al.}, Appl. Phys. Lett. \textbf{104}, 101913 (2014). \cite{5} R. Dovesi \textit{et al.}, \textit{Crystal06 User’s Manual} (University of Torino, Torino, 2006).