

IS HO₂⁺ A DETECTABLE INTERSTELLAR MOLECULE?

SUSANNA L. WIDICUS WEAVER^a, *Departments of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801*; DAVID E. WOON, *Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801*; BRANKO RUSCIC, *Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439*; BENJAMIN J. McCALL, *Departments of Chemistry and Astronomy, University of Illinois at Urbana-Champaign, Urbana, IL 61801*.

Although molecular oxygen, O₂, has long been thought to be present in interstellar environments, it has only been tentatively detected toward one molecular cloud. The fractional abundance of O₂ determined from these observations is well below that predicted by astrochemical models. Given the difficulty of O₂ observations from ground-based telescopes, identification of a molecule that could be used as a tracer of O₂ in interstellar environments would be quite useful.

To this end, we have begun a collaborative examination of HO₂⁺ in an attempt to evaluate the feasibility of its detection in interstellar clouds. The formation reaction for HO₂⁺ is nearly thermoneutral, and so a full thermochemical evaluation of its formation mechanism is required. In addition to this uncertainty, no laboratory spectroscopic information is available for HO₂⁺, and previous *ab initio* calculations are not sufficiently accurate to guide observational searches. Here, we will present highly accurate spectral predictions based upon the new high-level *ab initio* calculations presented in the preceding talk. We will also report the HO₂⁺ formation reaction enthalpy and equilibrium constant, which were obtained from an Active Thermochemical Tables (ATcT) analysis and are the most accurate values available to date. Additionally, we will discuss the potential formation and destruction pathways for HO₂⁺ in interstellar environments. Based on this information, we will estimate the HO₂⁺ column density in molecular clouds and discuss the feasibility of its detection. Progress on obtaining the high-resolution infrared laboratory spectroscopy on the ν_1 band of HO₂⁺ will also be reported.

^aCurrent address: Department of Chemistry, Emory University, Atlanta, GA 30322