

LINE SHAPE CALCULATIONS FOR THE H₂O-O₂ COLLISION SYSTEM

R. GAMACHE **N. ORPHANOS**, *University of Massachusetts Lowell, 265 Riverside Street, 01854, Lowell, MA, USA*; **B. VISPOEL**, *Research unit Lasers and Spectroscopies (LLS), Institute of Life, Earth and Environment (ILEE), University of Namur, 61 Rue de Bruxelles, Namur, Belgium*; **K. SUNG**, **G. TOON**, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109-8099, USA*

Modified Complex Robert-Bonamy (MCRB) calculations were made for the H₂O-O₂ collision system using an intermolecular potential comprised of dipole-quadrupole, quadrupole-quadrupole, atom-atom component expanded to 20th order and rank 4, induction and London dispersion terms. The intermolecular potential was refined using the high-precision measurements of half-widths and line shifts made in this work. The final potential gives results that compare very well with the measurements; average percent difference of 0.052 and a standard deviation of 5.108 percent. With previous data sets the agreement was never better than ~15 percent standard deviation. Calculations employing this intermolecular potential were then made for some fourteen thousand water vapor transition in the 5680-9090 cm⁻¹ range and for the temperature range 200-3000 K for the H₂O-O₂ collision systems. These data were combined with H₂O-N₂ data to produce line shape data for H₂O-air. The temperature dependence of the half-widths and line shifts were determined with the Double Power Law model of Gamache and Vispoel¹. The final line shape data were added to a HITRAN-like line list for use in modeling telluric features toward extreme precision radial velocity measurements made by the Palomar Radial Velocity Instrument (PARVI), which is a near infrared fiber-fed diffraction limited high resolution spectrograph built for Doppler measurements of the host stars of extrasolar planets.

¹[doi:10.1016/j.jqsrt.2018.05.019](https://doi.org/10.1016/j.jqsrt.2018.05.019), R.R. Gamache and B. Vispoel, *J. Quant. Spectrosc. Radiat. Transfer* **217**, 440-452, (2018).