PRECISION MEASUREMENTS and MODELING OF H2O SPECTROSCOPY BROADENED BY O_2 and N_2

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Previously we produced precision measurements of H_2O transitions broadened by O_2, which has improved intermolecular potential of the collisional pair, H_2O-O_2, to a sub-percent level [See Gamache et al. [a]]. Now it has turned out that the modeling precision of Air-broadened spectroscopy of H_2O is limited by the accuracy of the intermolecular potential of the H_2O-N_2, which can be semi-empirically determined from the measurements of line shape parameters. Thus we have extended our laboratory measurements to H_2O transitions broadened by N_2. For this, we have obtained three N_2-mixture spectra in the ν_2 band at room temperature using the same high-resolution Fourier transform spectrometer (Bruker IFS-125HR) at the Jet Propulsion Laboratory, as previously used for the O_2-broadened H_2O study. For the sake of the best consistency, we have also used the same high-precision spectrum fitting package, Labfit, which adopts non-linear least squares curve fitting algorithm based on a Voigt line shape profile. We have retrieved their line widths and pressure-shifts by fitting all the three N_2-broadened H_2O spectra simultaneously, but while holding their line intensities to the HITRAN values. Results from this work have been combined to derive Air-broadened widths and pressure-shifts, which are compared to be lower than the HITRAN values by about 2 - 5%, depending transitions. Using these new measurements, the H_2O-N_2 intermolecular potential for the Complex Robert-Bonamy-Ma calculations is being developed, which leads to precision modeling of Air-broadened line shape parameters for the H_2O transitions in the entire infrared region. In this talk, we present and discuss the retrieval methodology and the improvement on the modeling of the line shape parameters expected for the rovibrational transitions of H_2O in the infrared.[b]

[a] Gamache et al. 2023 https://doi.org/10.1080/00268976.2023.2281592

[b] Government support acknowledged.