CALCULATION OF LINESHAPE PARAMETERS FOR SELF-BROADENING OF WATER VAPOR TRANSITIONS VIA COMPLEX ROBERT-BONAMY THEORY

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Water vapor in the Earth's atmosphere is being studied in the 3.2–17.76μm spectral region by the atmospheric infrared sounder (AIRS) on Aqua, the troposphere emission spectrometer (TES) and the high-resolution dynamics limb sounder (HIRDLS) on Aura both part of the NASA EOS mission[a]. However, the lack of sufficient data on spectral parameters will hamper the prospect of accurate retrievals of temperature and concentration profiles. The spectral parameters for thousands of water vapor transitions are required, which are hard to determine by measurements alone. As reported previously,[b] of the 10 602 measurements of H_2O self-broadening half-widths only 440 intercomparisons with more than 3 data points have estimated uncertainty less than 10%. In this work, we have employed the mean relative thermal velocity approximation of the complex implementation of Robert–Bonamy formalism[c] to obtain the self-broadened half-widths and self induced line shifts for 5442 water vapor transitions in the 3.2–17.76μm region. From these calculations a number of hidden aspects of broadening and shifting mechanisms can be understood. Here we consider the dependence of the line shape parameters on rotational state, vibrational state, temperature, intermolecular potential, collision dynamics, and method of calculation.

[a] http://eospso.gsfc.nasa.gov/eos_homepage/mission_profiles/index.php
[b] R. R. Gamache and J.-M. Hartmann, *Can. J. Chem.* **82**, 1013-1027 2004.
[c] R. R. Gamache *J. Mol. Spectrosc.* **229**, 9-18, 2005.