ATOMIC BROADENING OF WATER VAPOR TRANSITIONS

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Pressure-broadened halfwidths and pressure-induced line shifts are determined for water vapor transitions with atomic collision partners. Calculations based on the Complex Robert-Bonamy (CRB) formalism are made for a number of vibrational bands, for which there are experimental data to compare with. The intermolecular potential is taken as a sum of Lennard-Jones (6-12) atom-atom, isotropic induction, and dispersion components. The dynamics of the collision process are correct to second order in time. A new feature in the CRB approach is that the real and imaginary components of the Liouville S matrix affect both the halfwidth and the line shift. The calculations investigate the order of the expansion of the atom-atom potential and the role of the imaginary parts of the S matrix on the calculated halfwidths. The calculated values are compared with those obtained in a number of experimental studies. In general, good agreement is observed between the CRB calculations and the measured values for both halfwidths and line shifts. It is also clear that some parameters describing the intermolecular potential need to be better determined.