LINE SHAPE PARAMETERS FOR CO_2 TRANSITIONS: ACCURATE PREDICTIONS FROM COMPLEX ROBERT-BONAMY CALCULATIONS

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A model for the prediction of the vibrational dependence of CO_2 half-widths and line shifts for several broadeners, based on a modification of the model proposed by Gamache and Hartmann[a], is presented. This model allows the half-widths and line shifts for a ro-vibrational transition to be expressed in terms of the number of vibrational quanta exchanged in the transition raised to a power p and a reference ro-vibrational transition. Complex Robert-Bonamy calculations[b] were made for 24 bands for lower rotational quantum numbers J'' from 0 to 160 for N_2-, O_2-, air-, and self-collisions with CO_2. In the model a Quantum Coordinate is defined by $(c_1\Delta\nu_1 + c_2\Delta\nu_2 + c_3\Delta\nu_3)^p$ where a linear least-squares fit to the data by the model expression is made. The model allows the determination of the slope and intercept as a function of rotational transition, broadening gas, and temperature. From these fit data, the half-width, line shift, and the temperature dependence of the half-width can be estimated for any ro-vibrational transition, allowing spectroscopic CO_2 databases to have complete information for the line shape parameters.

[a] R. R. Gamache, J.-M. Hartmann, *J. Quant. Spectrosc. Radiat. Transfer.* **83** (2004), 119.
[b] R. R. Gamache, J. Lamouroux, *J. Quant. Spectrosc. Radiat. Transfer.* **117** (2013), 93.