Calculations of half-widths, their temperature dependence, and line shifts for the carbon dioxide-water vapor collision system

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Half-widths, γ, line shifts, δ, and the temperature dependence of the half-width, *n*, were calculated for the CO_2 transitions in the 00011 ← 00001 band with H_2O as the perturbing gas. The calculations employed the complex Robert-Bonamy formalism with trajectories determined by solving Hamilton's equations, real and imaginary components of the intermolecular potential, explicit solution of the velocity integral, and an atom-atom potential expanded to 20^{th} *order* and *rank* 4. Using the γ and *n* measurements of Sung *et al.* [1] the intermolecular potential for the CO_2-H_2O system was adjusted. Since a 20 4 4 potential run takes ~ 30 days computer time on a 12 processor 3.02 GHz Mac Pro, the potential was first adjusted at 8^{th} *order rank* 2. After 68 iterations, calculations using the 20 4 4 potential were then made. Six additional iterations were needed to give the final potential. The comparison with Sung *et al.* gives an average percent difference of -0.02 and a standard deviation of 0.94 percent.

Using this potential, calculations were made for 24 vibrational bands to study the vibrational dependence of the line shape parameters. These data will be used in the line shape prediction routine [2] for CO_2-H_2O.

[1] K. Sung, L. R. Brown, R. A. Toth, T. J. Crawford, Can. J. Phys. 87: 469, 2009.
[2] R. R. Gamache, J. Lamouroux, J. Quant. Spectrosc. Radiat. Transfer, in Press, 2013.