A prediction algorithm for CO_2 line-shape parameters for spectroscopic databases

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An algorithm to predict the half-width, its temperature dependence, and the line shift for CO_2 in collision with air and CO_2 was developed based on the work of Gamache and Lamouroux [1]. In the method the half-widths and line shifts for a ro-vibrational transition are expressed in terms of a reference rotational half-width/line shift and a coefficient times a *Quantum Coordinate* defined by $(c_1|\Delta\nu_1| + c_2|\Delta\nu_2| + c_3|\Delta\nu_3|)^p$. Data are available to predict half-widths and line shifts for J" up to 200 at eleven temperatures; 125, 150, 200, 250, 296, 350, 500, 700, 1000, 1500, and 2000 K. The predicted semi-empirical data show excellent agreement with the calculated and measured half-widths and line shifts. Studies indicate that the power law model does not work well over large temperature ranges [2] and that temperature exponents vary with the temperature range of the fit [3]. As such, temperature exponents should be determined for the particular application in mind. A new approach was developed for the Ames databases. These data have been added to the 471,847 CO_2 transitions on the HITRAN database, to the AMES 296 K database (~24 million transitions) and the Ames 1000 K database (~543 million transitions) [5]. The new structure for the Ames databases is presented.

[1] R. R. Gamache and J. Lamouroux, J. Quant. Spectrosc. Radiat. Transfer 2013, In Press.
[2] G. Wagner et al., J. Quant. Spectrosc. Radiat. Transfer 2005, 92, 211-30.
[3] J. Lamouroux et al., J. Quant. Spectrosc. Radiat. Transfer 2012, 113, 1536-46.
[4] L.S. Rothman et al., J. Quant. Spectrosc. Radiat. Transfer 2013, submitted.