CO LINESHAPES: A COMPARISON BETWEEN AB INITIO CALCULATIONS AND HIGH-RESOLUTION MEASUREMENTS

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The role of inelastic collisions in the formation of infrared spectral line shapes is explored through a comparison of spectroscopic measurements and ab initio calculations. The shapes of a set of CO-Ar spectral lines in the fundamental band were recorded between -50°C and $+25^\circ$C, and between 0.05 atm and 1 atm, by a difference-frequency laser spectrometer with a resolution of less than 2 MHz and a signal-to-noise ratio greater than 4000:1. The ab initio line shape calculations used broadening coefficients obtained from fully quantal close-coupled calculations, which were in turn based on an assumed molecular potential energy surface. It is found that a failure to distinguish elastic and inelastic collisions in the CO-Ar system leads to incorrect line shape calculations at low pressures.