HALFWIDTHS AND LINE SHIFTS OF H_2O TRANSITIONS BROADENED BY CO_2

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The complex semiclassical formalism of Robert and Bonamy [a,b] is used to calculate both halfwidths and line shifts for water vapor in a bath of carbon dioxide gas. The assumed intermolecular potential is a combination of electrostatic, Lennard-Jones 6-12 atom-atom (expanded to 8th order), induction, and dispersion terms. Calculations are made for transitions in the ν_1, $2\nu_2$, and ν_3 vibrational band and are compared with the measurements of Gamache et al. [c] Good agreement with the experimental results is observed for both the halfwidth and line shifts. It is shown that the imaginary parts are important for both the line shift and halfwidth calculations.

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[a] D. Robert and J. Bonamy, "Short range force effects in semiclassical molecular line broadening calculations", *J. Phys.* (Paris) **40**, 923 (1979).

[b] R. Lynch, R. R. Gamache, and S. P. Neshyba, "Fully Complex Implementation of the Robert- Bonamy Formalism: Halfwidths and Line Shifts of H_2O Broadened by N_2," submitted to *J. Chem. Phys.* November, 1995.

[c] R. R. Gamache, S. P Neshyba, J. J. Plateaux, A. Barbe, L Rgalia, and J. B. Pollack, *J. Mol. Spectrosc.* **170**, 131 (1995).