THEORETICAL CALCULATION OF THE N_2 BROADENED HALF-WIDTHS OF H_2O

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The water molecule is the most important Greenhouse gas and thus plays a pivotal role in atmospheric spectra. In addition to accurate intensities and frequencies, one also needs accurate self and foreign half-widths and shifts, and their temperature dependence. Over the years, a large number of theoretical calculations have been carried out by Gamache and his collaborators[a]. They used the complex Robert-Bonamy theory with a sophisticated interaction potential. The drawback of this method is that one has to carry out the calculations to a high-order perturbation in order to obtain converged results. However, by using the coordinate representation one is able to obviate the perturbation expansion and obtain results corresponding to a high cut-off order[b]. We present comparisons for the H_2O-N_2 system for a few lines using the same interaction potential for a comparison between the methods. We conclude that for lines having a large half-width, the convergence is rapid but, on the other hand, for lines with relatively small half-widths the convergence is very slow.

[a]I. E. Gordon et al., J.Q.S.R.T. **108**, 389 (2007) and references therein.
[b]Q. Ma, R. H. Tipping, and C. Boulet, J. Chem. Phys. **124**, 014109 (2006).