SEMIEMPIRICAL H_2O HALF WIDTHS CALCULATIONS

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Impact theory has been modified on the wider use of empiric data by introducing of the additional parameters taking into account the trajectory bending, effects of vibrational excitation, corrections to the scattering matrix obtained from the perturbation theory, etc. Model parameters were determined by fitting the broadening coefficients to experimental data. This allows sufficiently accurate prediction of the parameters of line profiles, which were not measured.

The Anderson theory [1] employs the simplest (straight path) representation of the relative motion and the intermolecular potential is taken as the long range expansion. For the case of weak interactions ($r_c > b_0$) this method does not provide a good description, and therefore several authors proposed various versions of cut-off-free method taking into account increasingly subtle effects (atom-atom potential, trajectory curvature, accounting for the imaginary part of the interruption function for broadening calculation [2-4]). Some versions of the cut-off-free method describe the processes rather well, but due to the complexity of the calculations, do not allow visualizing and analyzing processes occurring in colliding molecules, in particular, the effect of compensation for contributions of different scattering channels in the pressure-induced shift. Therefore, we have corrected the Anderson method trying to eliminate its main disadvantages, but to held its advantages. So, we are able to analyze different dependencies of line contour parameters such as vibrational-rotational, thermal ones as well as dependence on perturbing particle.

Using semiempiric method the coefficients of H_2O broadening by nitrogen pressure, as well as the coefficients of thermal dependence of line profiles were calculated. J-dependence of line shifting and broadening coefficients for water ν_2 band (R-branch) lines induced by N_2 pressure in a wide range of J quantum numbers up to 18 was analysed. The H_2O shifts of the same lines induced by pressure of different buffer gases were compared, and the roles of different terms of the intermolecular potential in the formation of line shifts were studied.

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[1]. C.J. Tsao, B. Curnutte, J.Quant.Spectrosc.Radiat.Transfer, 2, 41-91 (1961).
[2]. D Robert and J. Bonamy, J. de Physique, 40, 923–943 (1979).
[3]. R. Lynch, R. Gamache, S. P. Neshyba, J. Chem. Phys., 105, N 14, 5711–5721 (1996).
[4]. A.D. Bykov, N.N. Lavrent'eva, and L.N. Sinitsa, Atmos. Oceanic Opt. 5, No. 9, 587–594 (1992).