FCIA and SCIA PSEUDO-LINELISTS FOR COLLISION-INDUCED ABSORPTION

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INTRODUCTION

This file gives an introduction to the latest version (April 20, 2006) of the pseudo-linelists for collision induced absorption. Separate pseudo-linelists are given for foreign-collision induced absorption (FCIA) and self-collision induced absorption (SCIA). They contain pseudolines for O2 and N2. In the mid-infrared they cover the fundamental O2 band around 1550 cm-1, the fundamental N2 band around 2330 cm-1, and the first overtone band of N2 around 4630 cm-1. In near-infrared pseudo-lines are given for the O2 bands around 7900, 9400 cm-1, and 13250 cm-1. Each linelist consists of 5909 pseudolines with a spacing of 1 cm-1.

ABSORPTION CALCULATIONS

The pseudo-linelists are in the HITRAN format. However, as they describe collision induced absorption, the line strength is given in the unit cm-1/molec2/cm-5. To calculate the correct absorption, the SCIA absorption coefficients derived from the pseudolines must be multiplied by the number density times the volume mixing ratio of the considered gas, and the FCIA absorption coefficients must be multiplied by the number density times (1 - volume mixing ratio).

   Absorption = S_scia * d^2 * v^2 +   S_fcia * d^2 * v*(1-v)

The sum of both contributions can then be used to calculate optical thicknesses or transmittances. Note that the units of the line strengths and hence the calculation of the absorption is different from previous versions of the CIA linelists, in which units were given in cm-1/molec/cm-2/atm and absorption was calculated by multiplicating the coefficients with the pressure.

DERIVATION OF THE LINELISTS

For the O2 and N2 fundamental bands tabulated values from empirical models were converted to HITRAN units (line strength and ground state energy). For the N2 overtone band absorptions were read from a figure and converted to HITRAN units. In all three cases it was necessary to fit an exponential function to the linear temperature dependence of (T/T_hitran), which originates from the rotational partition function. This fit has an accuracy of 2% in a temperature range between 190-295 K.

The O2 fundamental band is based on the measurements and the empirical model given in Tab. 1 by Thibault et al. (1997), which gives parameters for O2-air collision induced absorption. Separation in FCIA and SCIA was done by assuming a temperature independent effectiveness of
O2-O2 collisions = 0.94 * effectiveness of O2-N2 collisions
estimated from data in Tab. 1 of Orlando et al. (1991). The linelist has been extrapolated to zero line strengths at 2*FWHM from the maximum absorption towards lower wavenumbers and 2.5*FWHM towards higher wavenumbers. This covers the range from 1275-1905 cm-1, giving a total of 631 pseudo-lines.

The N2 fundamental band is based on the measruements and the empirical model given in Tab. 1 by Lafferty et al. (1996). They give their empirical model for

N2-N2 collisions, which could be directly converted to HITRAN units for SCIA. N2-O2 collisions were calculated from the N2-N2 collisions using their temperature dependent conversion factor, which parameterizes a linear temperature dependence based on Menoux et al. (1993). For this, an exponential function has been fitted to the product of (T/T_hitran) and the N2-O2 conversion factor, the accuracy of which is 0.3% between 190-295 K. The new linelist has been extrapolated to zero line strengths at 2*FWHM from the maximum absorption towards lower wavenumbers and 2.5*FWHM towards higher wavenumbers. This covers the range from 2030-2705 cm-1, giving a total of 676 pseudo-lines.

The N2 first overtone band is based on absorption data given by Shapiro and Gush (1966). The absorption was digitized from Fig. 8 of the paper, and converted to pseudoline strengths assuming similar ground state energies as for the fundamental band. Shapiro and Gush (1966) give the absorption for N2-N2 collisions. Separation to SCIA and FCIA was done assuming an effectiveness of N2-O2 collisions = 0.92 * effectiveness of N2-N2 collisions as suggested by Menoux et al. (1993) for the fundamental N2 band (Tab. 4), however, no possible temperature dependence has been taken into account. The new linelist covers a range of 4330-4930 cm-1 with 601 pseudo-lines.

For the O2 CIA in the 7900 and 9400 cm-1 bands pseudolines were derived by fitting laboratory spectra from Smith and Newnham (2000). These lab spectra covered 198 to 295K and O2 vmrs from 21% to 75%. The pseudo-lines are able to reproduce the O2 slant column amounts in the lab spectra to within 1% rms (2.4% max).

The O2 A-band CIA pseudo-linelist was derived by fitting the absorptions given in Fig. 7 of the paper "Line-Mixing and collision-induced absorption by O2 in the A-band" by H.Tran, C. Boulet, and J.-M.Hartmann. Since no lab spectra were available, we simply fitted the two curves in the paper.

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