An Improved Version of the CO_2 Line-mixing Database and Software: Update and Extension

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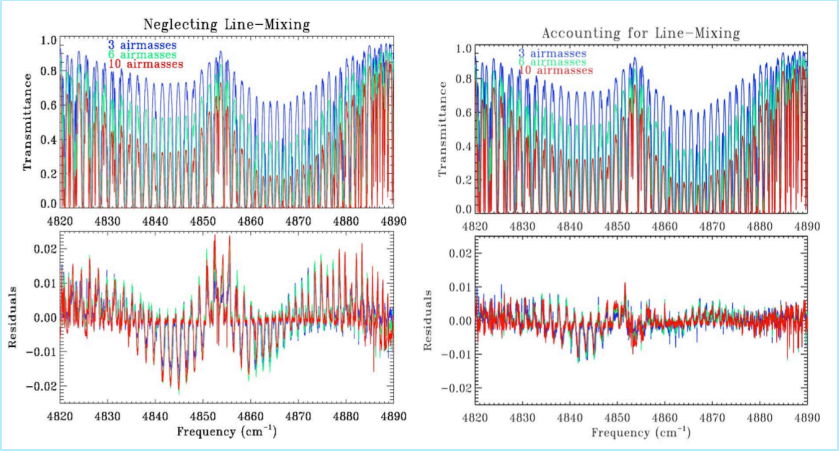
The importance line-mixing for CO_2



From Hartmann *et al.* (2009). Residuals obtained from fits of ground-based atmospheric solar-absorption spectra in the region from 4765 to 4915 cm^{-1} for various airmasses.

Previous work

- In a previous study, Niro *et al.* (2005) presented a database and software package which provided for the calculation of the absorption coefficients of CO_2 that included the effects of line-mixing.

- J.-M. Hartmann *et al.* (2009) concluded that the CO_2 database and software of Niro *et al.* needed to be updated and improved. The present work provides this update.

The present work was driven by the need for a line-mixing database consistent with the CO_2 database on HITRAN. The new database being presented goes hand-in-hand with HITRAN2008.

Line-mixing

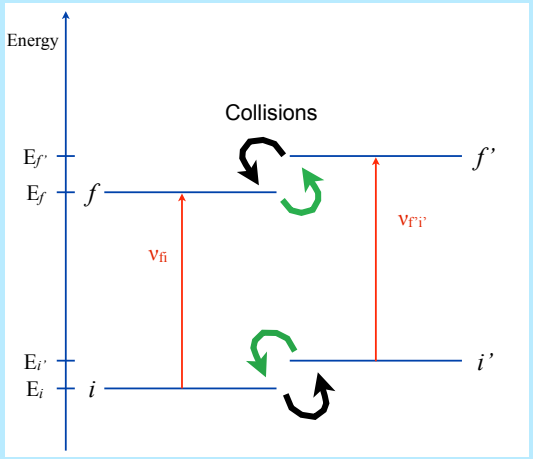


Illustration of line-mixing between two optical transitions, f ← i and f' ← i' (Hartmann *et al.* 2008).

The previous database

Spectroscopic files – data files for each band
Bandinfo – statistical information for each band
Software – computes the absorption coefficients

The off-diagonal elements of the relaxation matrices, *W(T)*, are computed, and from the *W's* the line-mixing coefficients, Y_k, are calculated. The *Y's* are then used to calculate absorption coefficients.

Procedure for the construction of the new database

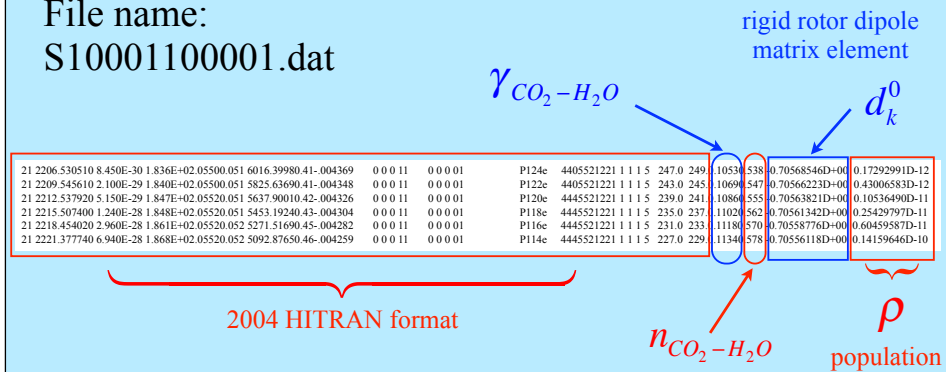
- Took HITRAN2008, CDSD-296 and CDSD-1000 and separated into files by isotopologue and by vibrational band.
- Checked for $J_{max} \geq 70$ in HITRAN, if not then checked for the missing transitions in CDSD-296, and in CDSD-1000 (if not in CDSD-296).
- For bands where the $J_{max} \geq 70$ condition could not be met with the inclusion of the 3 databases, line-mixing effects were not included in the calculation of absorption coefficients. Note that these bands are weak bands and are for minor isotopologues.
- For each band with $J_{max} \geq 70$, the same procedure from the previous model is used to calculate absorption coefficients.

The new line-mixing database

Previous version (Niro *et al.*, 2005)	**Updated version (Lamouroux *et al.*, 2010)**
HITRAN 2000 (Rothman *et al.*, 2003)	HITRAN 2008 (Rothman *et al.*, 2009) CDSD-296 (Tashkun *et al.*, 2003) CDSD-1000 (Tashkun *et al.*, 2008)
~ 600 vibrational bands	~ 3600 vibrational bands
~ 78,000 lines	~ 450,000 lines
Half-widths	
CO_2–CO_2 CO_2–air	CO_2–CO_2 (Rothman *et al.*, 1992) CO_2–air (Rothman *et al.*, 1992) CO_2–H_2O (Sung *et al.*, 2009) mass dependence (Lamouroux *et al.*, 2010)
Temperature Dependence	
CO_2–air	CO_2–air (Rothman *et al.*, 1992) CO_2–H_2O (Sung *et al.*, 2009)
Line Shifts	
Some CO_2–air	CO_2–air (J.-M. Hartmann, 2009)

Example of the new database - Spectroscopic files

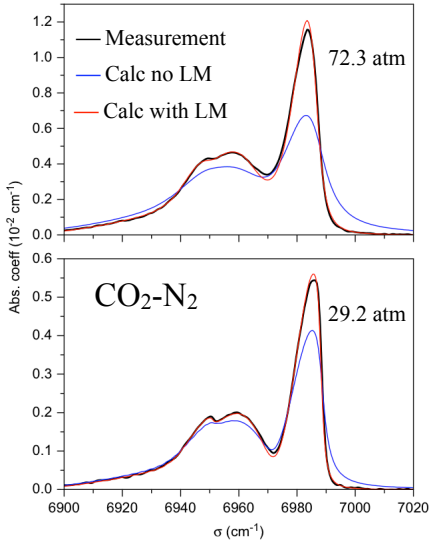
File name:
S10001100001.dat



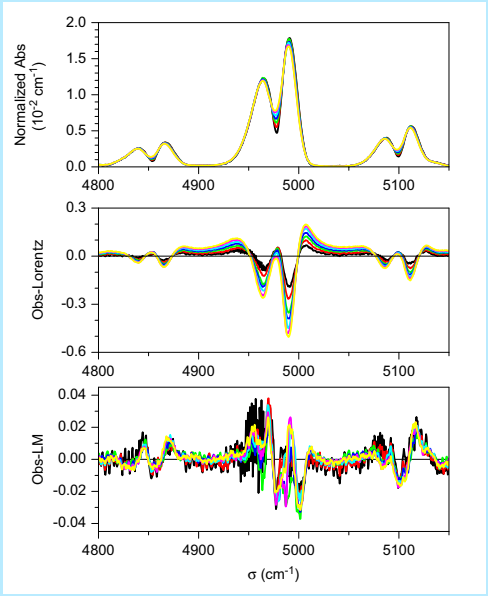
The user will receive:

- Database files (like above) and a file with information on each band
- Software to process these files (i.e. calculate absorption coefficients via W and Y_k)

Comparison with measured laboratory spectra



Comparison between measured and calculated CO_2 absorption coefficients in the $3\nu_3$ band. The black line is measured values, red and blue are calculated values from the new version of the database and software taking line mixing into account and neglecting line-mixing, respectively. (Lamouroux *et al.*, 2010)



Absorption coefficients and measured-calculated residuals for 1% CO_2 in seven pressures (from 19 to 76.0 atm) of N_2 at 295.15 K in the region of the ($2\nu_1 + \nu_3$) triad. The top panel displays the measured absorptions normalized to unity area through integration over σ. The middle and lower panels display the residuals (meas-calc) obtained from calculations with our new database, respectively, neglecting line-mixing and taking this process into account (Lamouroux *et al.*, 2010).

Conclusions

- The new line-mixing database includes the best available data for CO_2 line-mixing calculations.
- It includes many more lines than the previous Niro *et al.* 2005 database.
- More parameters are included such H_2O-broadening parameters of CO_2.
- The new database is consistent with HITRAN2008.
- The calculated absorption coefficients agree very well with measurement.
- Important for GOSAT, OCO-2, ACE-FTS, and any other high-precision remote sensing measurements.

Future research

- Software is being tested on atmospheric spectra simulations.
- Procedure for creating future CO_2 line-mixing database has been somewhat automated so that updates corresponding to future HITRAN editions can be easily done.
- Go from the empirically determined values of half-width and line shift used in this work to experimental/calculated values.

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