Summary of the tool for the CO_2 line-mixing package

The package contains the FORTRAN code (calculation of the absorption coefficients for CO_2-air taking (or not) into account the line-mixing effects). This package is based on the HITRAN 2016 database and format (Gordon et al., JQSRT (2017) doi:10.1016/j.jqsrt.2017.06.038). Note that the calculation is being done only for the first 10 isotopologues of CO_2 at the moment.

References: Lamouroux et al., JQSRT 111 (2010), 2321-2331; Lamouroux et al., JQSRT 151(2015), 88–96; and references therein. *Please cite these references along with HITRAN2016 paper if you are using the present tools.*

The structure of the package is the following:
|>Data_new (output): *contains the spectroscopic files, "bandinfo.dat", and the elements of the relaxation matrix files.*

|>The main code used for the calculation of CO_2-air absorption coefficient : *LM_calc_CO2_2017.for* and the file "parameters.inc" that contains some parameters used in the main code.

|>>> Input parameters:

- sgmin, sgmax, dsg [cm^{-1}] : Min and Max wavenumbers and step of the calculation
- sTotMax [cm^{-1}/(molecule.cm^{-2}) at 296K]: Total band intensity cut-off
- xCO_2 [no unit] : CO_2 molefraction
- xH_2O [no unit] : H_2O molefraction
- Temp [K] : Temperature of the calculation
- Ptot [atm] : Total pressure
- MixFull = Switch to full diagonalization line-mixing
- MixSDV = Switch to a Speed-dependent Voigt profile
  !!Note that at the moment the full diagonalization line-mixing is not possible when a Speed-dependent Voigt profile is used.!!

|>>> Output results:

- AbsV : Absorption Coefficient neglecting LineMixing (assuming Voigt Line-Shapes) (cm^{-1})
- AbsY : Absorption Coefficient predicted using the First (Order Line-Mixing Approximation) (cm^{-1})
- AbsW : Absorption Coefficient predicted using Full (diagonalization Line-Mixing) (cm^{-1})

From all these files, the absorption coefficient can be calculated using the main code "LM_calc_CO2_2017.for" and the file "parameters.inc" that must be included into the directory. In output of this main code are the frequency, the absorption coefficient using a Voigt (or Speed-dependent Voigt) profile (no line-mixing), the absorption coefficient using a Voigt (or Speed-dependent Voigt) profile using the first order approximation (Y coefficients) for line-mixing, and the absorption coefficient using a Voigt profile and the full relaxation matrix. **Note that at the moment no Speed-dependent Voigt profile can be used when the full relaxation matrix is used for the line-mixing calculation.**