

Description of isotope.input file contents for Sfit4 v0.9

Update : November 2018 -JWH

Now accommodates HITRAN 16

1. CO₂ has 12 isotopes , we map these:
 - a. 0 -> 10
 - b. A -> 11
 - c. B -> 12

Update : 4 December 2012- JWH

For beta version b003.991 beta and higher.

Note don't mix input files and the HITRAN directory tree of different versions. Use only b3.991 or later!

This document describes the files and directories required to create the binary hitran data input file for sfit4.

Components:

Hbin.f90 – FORTRAN code that creates a binary hitran linelist file for a specific sfit4 run. It is compiled along with sfit4. It uses many of the same modules. It compiles to hbin.

Input:

1. hbin.input – a list of the HITRAN and Galatry input files
2. sfit4.ctf - defines the bandpasses
3. isotope.input – if this is engaged via logical switch in sfit4.ctf then it is read too. Isotopes are separated at this level so sfit4 does not perform this task.
4. Linelist/ - is a fixed directory structure providing for 99 gases (don't mix versions)

Output:

1. LLLLLL.llllll-HHHHHH.hhhhhh.hbin – this is a binary file with all HITRAN data, line-mixing data, Galatry data and separated isotopes for this run of sfit. LLLLLL.llllll is the lowest wavenumber from all bandpasses and HHHHHH.hhhhhh is the highest.
2. LLLLLL.llllll-HHHHHH.hhhhhh.hasc – this is for a sanity check to see what lines are in the .hbin file – someday we'll make its creation an option.

Hbin builds a linelist file from HITRAN by-molecule files, pseudo line list files, line-mixing data files and Galatry beta files. It will contain only lines required for the bandpasses in a given fit. It does not require rerunning for each sfit run. It reads faster than previous ascii files.

Directory structure:

Dirs look like this:

001_H2O/01_hit09.par
002_CO2/02_hit08_f53.par

.
.
.

The first 3 digits of the molecule sub-directory in the linelist directory structure is the key to the gas names and the molecule id numbers and need to match the HITRAN gas file in that directory and the gas ID in the reference.prf file and in molcparam.f90 and vibfcn.f90. For some gases the 'HITRAN' ID in the by-molecule file is not the same as the SFIT ID. Hbin will change it to these 3 digits from the directory name. All this is correct if you keep versions together and don't change anything.

Data files for O2 CIA, CO2 line-mixing and HCl & HF Galatry parameters are included. See switches in sfit4.ctl to engage these parameters.

Tips:

See the hbin.input file for more details. hbin.input should be in the local directory where hbin is run. Its name is fixed and read only by hbin.f90.

To include/exclude certain gases from a fit include/exclude those pathnames from the hbin.input file. Change the number of gases at the top to reflect the new number of by-molecule files to search through.

Or to exclude looking at a file put a blank after the '/' at the end of the sub-directory name in hbin.input.

Hbin.input:

A line starting with a # is a comment

first non-comment line is a path to the directory tree where the gas subdirectories are
#

/Users/jamesw/FDP/sfit/400/linelist/

#

next non-comment entry is the number of path/files to look for

99

#

Then the next lines are paths to each gas file that will be searched for lines in the

desired wavenumber region

#

001_H2O/01_hit09.par

002_CO2/02_hit08_f53.par

.
.
.

099_OTHER/

#

```
#
# Galatry parameters
# molecule id numbers in these files have to match the sfit molecule id
2
014_HF/hf_galatry.txt
015_HCL/hcl_galatry.txt
#
#
# CO2 Line mixing parameters for Boone implementation
1
002_CO2/co2_lm.dat
#
```