

Description of hbin.ctl for SFIT4 v1.0

Update : June 2020 - MP

Included linemixing files for CO2 created from Lamouroux software (comes with HITRAN), compare docs/linelist/Get_ExtraParameters.txt

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

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.ctl – a list of the HITRAN and Galatry input files
2. sfit4.ctl - defines the bandpasses
3. isotope.input – if this is engaged via logical switch in sfit4.ctl 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 – its creation is switched on by setting file.out.ascii = T in hbin.ctl.

hbin builds a linelist file from HITRAN by-molecule files, pseudo line list files, line-mixing data files and Galatry beta files. It reads faster than previous ascii files. It will contain only lines required for the bandpasses in a given fit. It does not require rerunning for each sfit run, if the microwindows are not changed. Please compare figure 1 for how the xxx-xxx.hbin file is structured.

In order to accommodate for wavenumber shift the lines have to be calculated outside the actual windows. Extra space will be needed when the following options in sfit4.ctl are switched on:

rt.wshift = T – retrieves a wavenumber shift

or

band.x.wave_factor <> 1.0 this option multiplies the wavenumbers given in spectrum. Changes by 1e-6 can already cause the wavenumber range in the spectrum to be outside hbin.

The extra space is calculated by:

$$d_out = 10.5/\text{band.x.opd_max} + 4.0 \text{ [1/cm]}$$

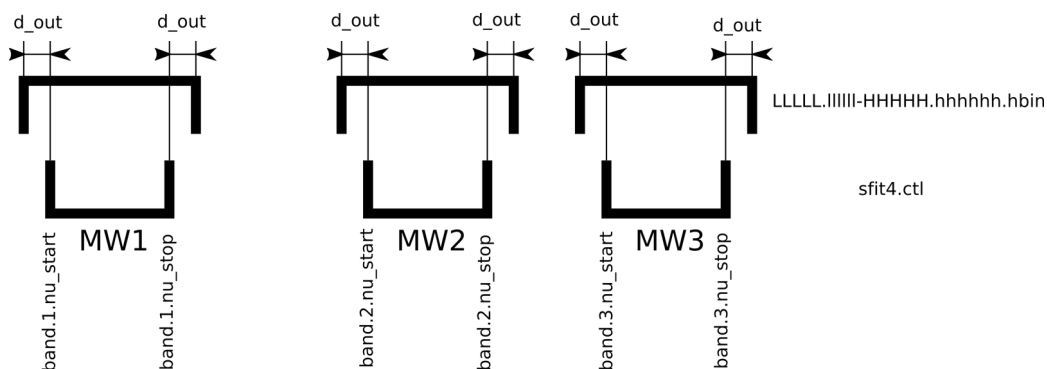


Figure 1: Structure of LLLLL.Llllll-HHHHH.hhhhhh.hbin. For the definition of d_out see text.

A

new xxx-xxx.hbin needs to be calculated if the microwindows in sfit4.ctf get bigger than the ones in the xxx-xxx.hbin file.

Directory structure

Dirs look like this:

001_H2O/001_H2O.hit16.20181107

002_CO2/002_CO2.hit16.20181107

.
.
.

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.ctf 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.ctl.

hbin.ctl:

```
# hbin.input for Testing HITRAN 2016
#
# implemented in version v1.0:
# the linelist directory structure is the key to the gas names and the molecule id numbers
# those id's and names must be the same in the reference.prp file
# eg a files containing hitran lines is read from one subdir in linelist then the molid will be
changed
# to the 2digit integer ON of the subdir name and assumed to be for gas 'abcdef' from subdir to
be for gas 'abcdef' from subdir ONN_abcdef
#
# Save an ascii (HITRAN format) list file (True / False)
file.out.ascii = T
#
# Path to the directory tree where the gas subdirectories are
file.in.linelist = /Users/jamesw/FDP/sfit/400/linelist-core/
#
# ids are dealt with differently
#
# Number of path/files to look for
hitran.nr = 99
#
# Then the next lines are paths to each gas file that will be searched for lines in the
# desired wavenumber region. The id numbers are in sfit order - not HITRAN, BUT KEEP
# these directory names the files are in HITRAN format. File names can be anything.
#
# Tip: put a blank after the '/' to skip that gas or just remove it (and decrease hitran.nr)
#
# 049_O2CIA/o2cia_20060420.101 - this file is a special case, molid & isotope
#
hitran.files =
001_H2O/001_H2O.hit16.20181107
002_CO2/002_CO2.hit16.20181107
003_O3/003_O3.hit16.20181107
004_N2O/004_N2O.hit16.20181107
005_CO/005_CO.hit16.20181107
```

006_CH4/006_CH4.hit16.20181107
007_O2/007_O2.hit16.20181107
008_NO/008_NO.hit16.20181107
009_SO2/009_SO2.hit16.20181107
010_NO2/010_NO2.hit16.20181107
011_NH3/011_NH3.hit16.20181107
012_HNO3/012_HNO3.hit16.20181107
013_OH/013_OH.hit16.20181107
014_HF/014_HF.hit16.20181107
015_HCL/015_HCL.hit16.20181107
016_HBR/016_HBR.hit16.20181107
017_HI/017_HI.hit16.20181107
018_CLO/018_CLO.hit16.20181107
019_OCS/019_OCS.hit16.20181107
020_H2CO/020_H2CO.hit16.20181107
021_HOCL/021_HOCL.hit16.20181107
022_HO2/033_HO2.hit16.20181107
023_H2O2/025_H2O2.hit16.20181107
024_HONO/
025_HO2NO2/
026_N2O5/2007.sudo.n2o5
027_CLONO2/2007.sudo.clono2
028_HCN/023_HCN.hit16.20181107
029_CH3F/
030_CH3CL/024_CH3CL.hit16.20181107
031_CF4/2007.sudo.cf4
032_CCL2F2/2007.sudo.ccl2f2
033_CCL3F/2007.sudo.ccl3f
034_CH3CCL3/
035_CCL4/2007.sudo.ccl4
036_COF2/029_COF2.hit16.20181107
037_COCLF/2007.sudo.coclf
038_C2H6/027_C2H6.hit16.20181107
039_C2H4/038_C2H4.hit16.20181107
040_C2H2/026_C2H2.hit16.20181107
041_N2/022_N2.hit16.20181107
042_CHF2CL/2007.sudo.chf2cl
043_COCL2/049_COCL2.hit16.20181107
044_CH3BR/040_CH3Br.hit16.20181107
045_CH3I/
046_HCOOH/032_HCOOH.hit16.20181107
047_H2S/031_H2S.hit16.20181107
048_CHCL2F/
049_O2CIA/o2cia_20060420.101
050_SF6/2007.sudo.sf6
051_NF3/nf3.101.511.txt
052_N2CIA/
053_OTHER/

054_OTHER/
055_OTHER/
056_OTHER/
057_OTHER/
058_OCLO/
059_F134A/
060_C3H8/2005ppn.sudo.c3h8
061_F142B/2007.sudo.f142b
062_CFC113/2007.sudo.f113
063_F141B/
064_CH3OH/039_CH3OH.hit16.20181107
065_OTHER/
066_OTHER/
067_PAN/2007.sudo.pan
068_CH3CHO/2007.sudo.ch3cho
069_CH3CN/041_CH3CN.hit16.20181107
070_OTHER/
071_CH3COOH/ch3cooh_1100_pll.txt
072_C5H8/c5h8_885_pll.txt
073_MVK/mvk_910_pll.txt
074_MACR/macr_890_pll.txt
075_C3H6/c3h6_850_pll.txt
076_C4H8/c4h8_750_pll.txt
077_OTHER/
078_OTHER/
079_OTHER/
080_OTHER/
081_OTHER/
082_OTHER/
083_OTHER/
084_OTHER/
085_OTHER/
086_OTHER/
087_OTHER/
088_OTHER/
089_OTHER/
090_OTHER/
091_OTHER/
092_OTHER/
093_OTHER/
094_OTHER/
095_OTHER/
096_OTHER/
097_OTHER/
098_OTHER/
099_OTHER/

#

```
# Galatry parameters
# molecule id numbers in these files have to match the sfit molecule id
aux = gal sdv lm
aux.gal.nr = 2
aux.gal.files =
014_HF/14_hit16_Galatry.txt
015_HCL/15_hit16_Galatry.txt
#
# Speed Dependent Voigt parameter files
aux.sdv.nr = 1
aux.sdv.files =
005_CO/05_hit16_SDV.txt
#
#
# Line mixing parameters
aux.lm.nr = 1
aux.lm.files =
002_CO2/002_CO2.hit16_LM1ST.par
#
#
```