**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:
   1. 0 -> 10
   2. A -> 11
   3. 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 engages 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. LLLLL.llllll-HHHHH.hhhhhh.hbin – this is a binary file with all HITRAN data, line-mixing data, Galatry data and separated isotopes for this run of sfit. LLLLL.llllll is the lowest wavenumber from all bandpasses and HHHHH.hhhhhh is the highest.
2. LLLLL.llllll-HHHHH.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 then 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 windws. 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/band.x.opd\_max + 4.0 [1/cm]

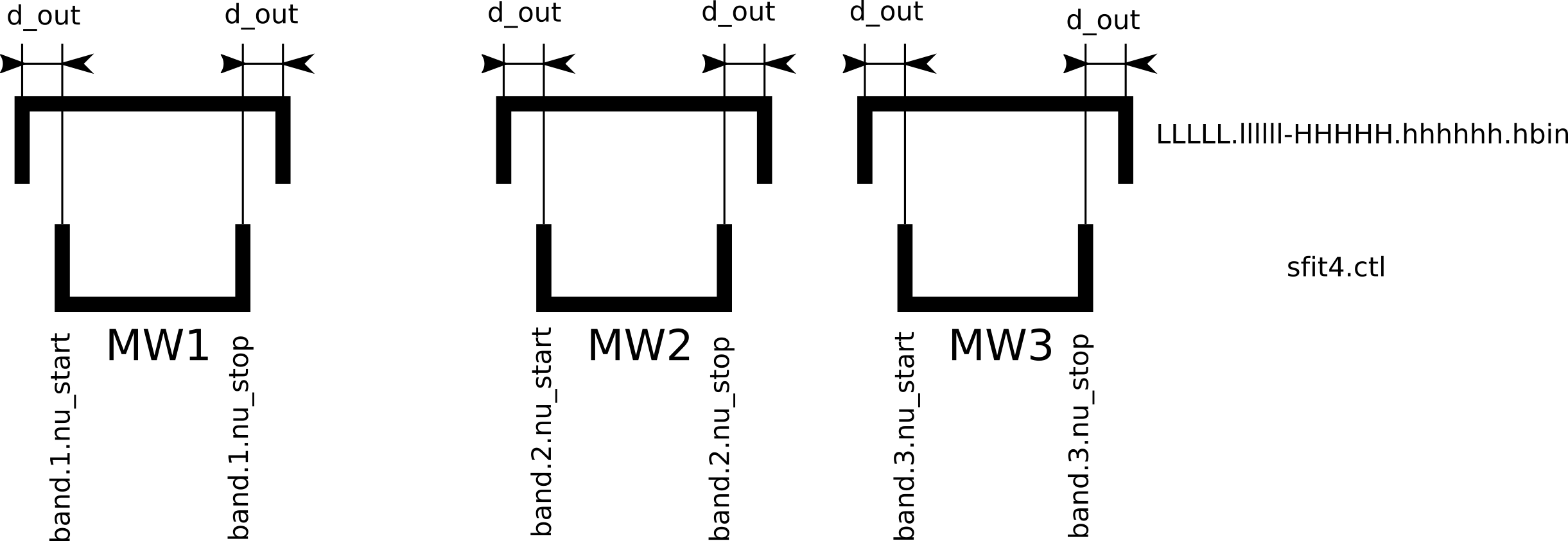


Figure 1: Structure of LLLLL.llllll-HHHHH.hhhhhh.hbin. For the definition of d\_out see text.

A

new xxx-xxx.hbin needs to be calculated if the microwindows in sfit4.ctl get beigger 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.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.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.prf file

# eg a files containing hitran lines is read from one subdir in linelist then the molid will be changed

# to the 2digit integer 0N of the subdir name and assumed to be for gas 'abcdef' from subdir to be for gas 'abcdef' from subdir 0NN\_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 wavenember 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

#

#