Spectroscopy

SFIT Retrieval Workshop

J Hannigan

NCAR, Boulder, CO
November 2019

Outline

- HITRAN
- ATM
- Structure of SFIT4 line listings
- Pseudolines
- hbin
- Retrieving isotopes in SFIT4
- TIPS

HITRAN 1/3

- *"The database is a long-running project started by the Air Force Cambridge Research Laboratories (AFCRL) in the late 1960s in response to the need for detailed knowledge of the infrared properties of the atmosphere."*
- See http://www.hitran.org
- HITRAN if a funded, curated spectral line parameter list in wide global use, it is not the only one, but may be the most widely used, and is often considered a standard list. (Hence the reluctance in the IRWG to move away from it.)
- It is supported and contributed to by a long standing global molecular spectroscopy community. Who continually check and revise and republish the list.
- And it continues to exhibit issues.
- When changing lists there is no substitute for extensive testing.

HITRAN 2/3

- SFIT uses a subset of parameters for Voigt & extra parameters for the few species these are available for other line shapes including Galatry or line mixing

```
For the Voigt line function:
INTEGER  :: MO              ! MOL ID
INTEGER  :: IS              ! ISOTOPE ID #
REAL(8)  :: NU              ! WAVENUMBER
REAL(8)  :: SL              ! INTENSITY [CM-1/(MOLEC/CM-2)]
REAL(4)  :: EA              ! EINSTEIN A COEFF
REAL(4)  :: AH              ! AIR BROADENED HALFWIDTH [CM-1/ATM]
REAL(4)  :: SH              ! SELF BROADENED HALFWIDTH [CM-1/ATM]
REAL(8)  :: EL              ! LOWER STATE ENERGY [CM-1]
REAL(4)  :: TX              ! TEMPERATURE EXPONENT
REAL(4)  :: PS              ! PRESSURE SHIFT [CM-1]
```

- Line files are copied verbatim to the SFIT linelist folders except
  - After molecule id 21 numbering is different
  - Note some numbering has changed with version 1.0pr from previous SFIT4 versions (but gases that are new of little used)
  - See file LineLists_Map.xlsx

HITRAN 3/3

Documentation for HITRAN:

- *The HITRAN2016 Molecular Spectroscopic Database*. Gordon, I., et al., (2017). Journal of Quantitative Spectroscopy and Radiative Transfer.
- sfit-core-code/docs/linelist/HITRAN_Units-definitions.pdf
- sfit-core-code/docs/linelist/HITRAN16_isotopePage.pdf
- sfit-core-code/docs/linelist/LineLists_Map.xlsx
- sfit-core-code/docs/linelist/Molecules.txt
- sfit-core-code/docs/linelist/molparam.txt
- sfit-core-code/docs/linelist/Uncertainty Indices.pdf

ATM 1/1

- The ATM list is managed by G Toon, JPL. Began as his best list for his MKIV solar spectra analysis. Was then adopted (in the near IR) for TCCON. Geoff is very active in the HITRAN activities.
- Geoff periodically updates the ATM list.
- The current list ATM20190910 has been updated with Geoff's best estimate of water lines.
- This list is reformatted with updated numbering and is currently on the SFIT wiki merged into linelist-core-20191030.zip
- The base of the list is HITRAN 16 so should be compatible with SFIT4 v1.0pr

Pseudolines 1/2

What do you do when you do not have HITRAN type line parameters for a gas you are interested in?

1. Use cross-section data in a forward model, or
2. Use cross-section data and value-add a line model (like Voigt) to create pseudo lines.

- We opt for the second choice in SFIT.
- Typically (or historically) pseudolines are made for complex molecules that are hard to calculate or measure directly. But broad cross-sections are measurable.
- Pseudolines are made from a set of cross-sections measures at varying temperatures and pressures that (hopefully) span those in the atmosphere.
- They are often done on an monotonic grid for simplicity sake so long as the cross-section spectra can be completely resolved. Except in the case of some for instance recent C2H6 (Harrison et al., 2010).

Pseudolines 2/2

- Pseudolines released in **linelist-core-20191030.zip** are G Toon. More info on this can be had from his website https://mark4sun.jpl.nasa.gov/pseudo.html
  - You are advised to visit if you use pseudolines. A subset of information is included in the SFIT4 linelist folders.

Structure of SFIT4 line listings 1/3

- Previous to SFIT4, the linelist files contained all species for a particular wavenumber region e.g. cfgl2020 contained parameters for all gases from wn 2020 to 2040
  - This required more deliberate management. A particular set of cgfl files were made for a specific version of SFIT.
  - In particular, other molecular parameters embedded in the SFIT code was often unique to a particular cfgl set of line parameters.

- SFIT4 is much more flexible wrt ingesting a variety of line parameter lists but:

Its incumbent on the user to know if components are not compatible and make it so if needed. There is not really any algorithmic check.

Structure of SFIT4 line listings 2/3

	SFIT Molecule #	SFIT NAME	HITRAN LINES	HITRAN Molecule #	HITRAN NAME	HITRAN LINES	NO_LINES EXIST	PSEUDO LINES	ATM LINES
	DATA	&		/					
	1	H2O	X	1	H2O	X			X
	2	CO2	X	2	CO2	X			X
	3	O3	X	3	O3	X			X
	4	N2O	X	4	N2O	X			X
	5	CO	X	5	CO	X			X
	6	CH4	X	6	CH4	X			X
	7	O2	X	7	O2	X			X
	8	NO	X	8	NO	X			X
	9	SO2	X	9	SO2	X			X
	10	NO2	X	10	NO2	X			X
	11	NH3	X	11	NH3	X			X
	12	HNO3	X	12	HNO3	X			X
	13	OH	X	13	OH	X			X
	14	HF	X	14	HF	X			X
	15	HCL	X	15	HCL	X			X
	16	HBR	X	16	HBR	X			X
	17	HI	X	17	HI	X			X
	18	CLO	X	18	CLO	X			X
	19	OCS	X	19	OCS	X			X
	20	H2CO	X	20	H2CO	X			X
Same above	21	HOCL	X	21	HOCL	X			X

	SFIT Molecule #	SFIT NAME	HITRAN LINES	HITRAN Molecule #	HITRAN NAME	HITRAN LINES	NO_LINES EXIST	PSEUDO LINES	ATM LINES
	DATA	&		/					
	22	HO2	X	33	HO2	X		X	X
	23	H2O2	X	25	H2O2	X			X
	24	HONO					X		
	25	HO2NO2					X		
	26	N2O5						X	
	27	CLONO2		35	CLONO2			X	
	28	HCN	X	23	HCN	X			X
	29	CH3F							
	30	CH3CL	X	24	CH3CL	X			X
	31	CF4		42	CF4			X	
	32	CCL2F2						X	
	33	CCL3F						X	
	34	CH3CCL3							
	35	CCL4						X	
	36	COF2	X	29	COF2	X	X		X
	37	COCLF						X	
	38	C2H6	X	27	C2H6	X			X
	39	C2H4	X	38	C2H4	X			X
	40	C2H2	X	26	C2H2	X			X
	41	N2	X	22	N2	X			X
	42	CHF2CL						X	
	43	COCL2	X	49	COCL2	X		X	
	44	CH3BR	X	40	CH3Br	X			
	45	CH3I					X		
	46	HCOOH	X	32	HCOOH	X		X	X
	47	H2S	X	31	H2S	X			X
	48	CHCL2F						X	
	49	O2CIA							X
	50	SF6		30	SF6			X	
	51	NF3						X	
	52	N2CIA							X
	53	OTHER							
	54	OTHER							
	55	OTHER							
	56	OTHER							
	57	OTHER							
	58	OCLO					X		
	59	F134A					X		
	60	C3H8						X	
	61	F142B						X	
	62	CFC113						X	
	63	F141B					X		
	64	CH3OH	X		CH3OH	X			
	65	CH3CNPL						X	
	66	C2H6PL						X	
	67	PAN						X	
	68	CH3CHO						X	
	69	CH3CN	X		CH3CN	X			
	70	OTHER							
	71	CH3COOH						X	
	72	C5H8						X	
	73	MVK						X	
	74	MACR						X	
	75	C3H6						X	
	76	C4H8						X	

Structure of SFIT4 line listings 3/3

- The only real check is the isotope numbers.
- Line parameter storage is a folder by gas. Allowing multiple lists and auxiliary parameter files to be conveniently stored.
- Files names are not so important, but the number and name of the folder is! (see hbin section)

hbin 1/1

- hbin.f90 –Consolidates the necessary portion of line parameters into a **fast** reading binary data file for a specific retrieval setup.
- It specifically depends on:
  - Wavenumber range for each bandpass
  - Specific line parameter files
  - Any isotope separation
  - Specific lineshape model

✓ SFIT tests each line before calculating the absorption. If it is weak it is ignored to save calculation time. If you know the VMR * line intensity is low you can speed up the retrieval by excluding these lines from the hbin output before SFIT.

✓ hbin.f90 also reads non-Voigt parameters from auxiliary files and stores them with inclusion flags to the appropriate line – a functional and speed improvement.

Retrieving isotopes in SFIT4 1/4

- The line parameter files contain all HITRAN isotopes for that gas. (We used to separate HDO and CH3D)
- Isotope separation is now generalized and can be performed for any isotope in HITRAN using the same mechanism.
- An isotope renamed to a new species need not be retrieved.
- You need to supply a new molecule ID (molid) – Choose one that is currently labeled OTHER.
- Documents:
  - sfit_isotope_descrip.docx
  - molparam.txt – gives isotope info all gases in HITRAN (or see the isotope page on the HITRAN web site).
  - Of particular importance for SFIT is the iso id, mass and abundance

Retrieving isotopes in SFIT4 2/4

```
6    42             ! number of isotope seperation species (blocks), # of VMR values
CO2                 ! old name
2 2 0               ! ld molec id, isotope id, f_isovmr (0 read vmr below, 1 read below but use vmr in reference.prf, 2 use vmr in reference.prf)
O13CO               ! new name
53 1 45.0 3 1. 1.   ! new molec id, isotope id, mass, mode, tdep, intensity scale
1334,1,  649,2, 2283,1
   7.411e-05,   1.290e-04,   2.101e-04,   2.593e-04,   2.931e-04,
   3.283e-04,   3.493e-04,   3.593e-04,   3.631e-04,   3.651e-04,
   3.666e-04,   3.675e-04,   3.672e-04,   3.672e-04,   3.671e-04,
   3.671e-04,   3.671e-04,   3.671e-04,   3.671e-04,   3.670e-04,
   3.670e-04,   3.669e-04,   3.668e-04,   3.667e-04,   3.667e-04,
   3.668e-04,   3.673e-04,   3.687e-04,   3.706e-04,   3.717e-04,
   3.719e-04,   3.724e-04,   3.732e-04,   3.734e-04,   3.736e-04,
   3.736e-04,   3.735e-04,   3.732e-04,   3.728e-04,   3.726e-04,
   3.724e-04,   3.724e-04,
CO2                 ! old name
2 3 0               ! old molec id and isotope id
CO18O               ! new name
54 1 46.0 3 1. 1.   ! new molec id, isotope id, mass, mode, tdep, intensity scale
1333,1,  667,2, 2349,1
   7.411e-05,   1.290e-04,   2.101e-04,   2.593e-04,   2.931e-04,
   3.283e-04,   3.493e-04,   3.593e-04,   3.631e-04,   3.651e-04,
   3.666e-04,   3.675e-04,   3.672e-04,   3.672e-04,   3.671e-04,
   3.671e-04,   3.671e-04,   3.671e-04,   3.671e-04,   3.670e-04,
   3.670e-04,   3.669e-04,   3.668e-04,   3.667e-04,   3.667e-04,
   3.668e-04,   3.673e-04,   3.687e-04,   3.706e-04,   3.717e-04,
   3.719e-04,   3.724e-04,   3.732e-04,   3.734e-04,   3.736e-04,
   3.736e-04,   3.735e-04,   3.732e-04,   3.728e-04,   3.726e-04,
   3.724e-04,   3.724e-04,
```

Intensity scale accounts for **abundance** that HITRAN already accounts for.

HITRAN isotope line intensities are scaled by the 'natural' abundance fractionation.

Here you can reset the intensity to its appropriate value using the abundance value from the tables in the molparam.txt file.

Retrieving isotopes in SFIT4 3/4

```
H2O                 ! old name
1 4 0               ! old molec id and isotope id
HDO                 ! new name
55 1 19.0 3 1.5 1.  ! new molec id, isotope id, mass, mode, tdep, intensity scale
2724,1, 1403,1, 3707,1
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.5000E-06,  5.0000E-06,
  9.2373E-06,  2.9235E-05,  1.3056E-04,  2.9550E-04,  6.7797E-04,
  1.5391E-03,  3.3744E-03,  6.9752E-03,  1.3268E-02,  2.2671E-02,
  3.5250E-02,  4.1415E-02,
H2O                 ! old name - Add as second HDO isotope
1 5 2               ! old molec id and isotope id
HDO                 ! new name
55 2 21.0 0 1.5 1.  ! new molec id, isotope id, mass, mode, tdep, intensity scale
H2O                 ! old name - Add as third HDO isotope
1 6 2               ! old molec id and isotope id
HDO                 ! new name
55 3 20.0 0 1.5 1.  ! new molec id, isotope id, mass, mode, tdep, intensity scale
H2O                 ! old name
1 2 0               ! old molec id and isotope id
H218O               ! new name
56 1 20.0 3 1.5 1.  ! new molec id, isotope id, mass, mode, tdep, intensity scale
3650,1, 1588,1, 3742,1
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.0000E-06,
  4.0000E-06,  4.0000E-06,  4.0000E-06,  4.5000E-06,  5.0000E-06,
  9.2373E-06,  2.9235E-05,  1.3056E-04,  2.9550E-04,  6.7797E-04,
  1.5391E-03,  3.3744E-03,  6.9752E-03,  1.3268E-02,  2.2671E-02,
  3.5250E-02,  4.1415E-02,
```

✓ If mode is 0 then no modes are read

Retrieving isotopes in SFIT4 4/4

- Once the isotope.input file is read in:
  - A new species exists and assigned a new:
    - Molecule name
    - Molecule ID, isotope id and mass
  - It may inherit or be assigned a:
    - Modes and degeneracies
    - Temperature dependence value
    - Intensity scaling
    - VMR

TIPS 1/1

- TIPS – Total Internal Partition Function
  - *"Total internal partition sums for 166 isotopologues of 51 molecules important in planetary atmospheres: Application to HITRAN2016 and beyond."* Gamache, R. R. et al., (2017). Journal of Quantitative Spectroscopy and Radiative Transfer, 203:70 – 87. HITRAN2016 Special Issue.
- Definitive and compatible partitioning calculation for HITRAN 2016. It is publicly available from Bob Gamache as FORTRAN codes and data files.
- We reformat for SFIT4.
  - It is slow.
- SFIT originally used a function based on FASCOD1C that works for all species with modes and degeneracies defined
- ✓ Tips for TIPS – Turn off TIPS when testing, turn on for final retrievals –
  - ✓ See switch fw.tips

end

Notes