Description of isotope.input file contents for Sfit4 c0.9
Update : 1 August 2012- JWH

This document describes the contents of a "isotope.input" file used with SFIT4 b3.999.

Lines beginning with a *number* and are **bold** are from a sample "isotope.input" file for a generic SFIT4 run. Note the name 'isotope.input' is a variable and provided to Sfit4 from the sfit4.ctl file. The first number on these lines is a line number and not part of the contents of the file. This example is for file option description only! See test cases included in SFIT4 release for more examples (e.g. x.co2.isotope). Following each input line is the variable name where each parameter is stored and a description. The next line is the parameter type and size and how each is read.

The *isotope.input* file is required by both hbin & sfit4.

In this example we saparate H2O into 4 species. (see the HITRAN doc ByMolecule-Readme.pdf). H2O has 6 isotopermers:

Old gas name	HITRAN Iso Designation	Isotope ID	New Gas Name	New Gas ID	New Iso ID
H2O	161	1	H2O	1	1
H2O	171	2	H217O	65	1
H2O	181	3	H218O	66	1
H2O	162	4	HDO	53	1
H2O	172	5	HDO	53	2
H2O	182	6	HDO	53	3

> ***1 4   41***

NISOSEP – the number of isotopes that will be separated out to new species. This then is also the number of repeated data blocks in this file
NISOVMR - number of VMR values. These vmr profiles are pre-raytrace so they are on the same reference grid as in the reference.prf file. This value must match number of layers in reference.prf file.

> (2) INTEGER, list-directed i/o

> ***2 H2O***

OLDNAME(I) – name of gas from which an isotope will be separated. Must match a gas name in reference.prf.

> CHAR*7, format(a7)

> ***3 1   2***

OLDID(I) – Sfit2 gas id of gas from which an isotope will be separated (OLDNAME(I))
OLDISO(I) – isotope id of gas from which an isotope will be separated (OLDNAME(I))

> (2) INTEGER, list-directed i/o

> ***4 H218O***

NEWNAME(I) – name of 'new' gas, does not have to be retrieved.

CHAR*7, format(a7)

```
    5  65 1 20.0 3 1.5
```
NEWID(I)   – gas id for 'new' gas, check reference.prf for an empty vmr block designated by gas name 'OTHER' & vmr of zero's.
NEWISO(I)   – isotope id for 'new' gas, id of 'OTHER' block above.
NEWMASS(I) – mass of 'new' gas.
NEWMODE(I) – number of rotational modes for 'new' gas, *to start** copy from main isotope see vibfcn.f90
NEWTDEP(I)   – temperature dependence, *to start** copy from main isotope see molcparam.f90
ISOSCALE(I) – line intensity scale factor, *to start*** use 1.0D0*

(2) INTEGER, (1) REAL, (1) INTEGER, (2) REAL, list-directed i/o

```
    6  3657,1, 1595,1, 3756,1
```
IIVIB(2,:,I) – rotational band centers and degeneracy pairs, provide for NEWMODE(I) pairs, *to start** copy from main isotope see vibfcn.f90

(NEWMODE(I)) REAL, list-directed i/o

```
    7  5.3669E-06 5.4567E-06 5.7056E-06 6.1999E-06 5.1364E-06 5.3619E-06
    8  5.3226E-06 5.4317E-06 5.6051E-06 5.6490E-06 5.7683E-06 5.7257E-06
    9  5.7200E-06 5.7331E-06 5.7177E-06 5.7168E-06 5.6837E-06 5.6365E-06
   10 5.6016E-06 5.5089E-06 5.4460E-06 5.3348E-06 5.2177E-06 5.1049E-06
   11 4.9422E-06 4.8004E-06 4.5971E-06 4.4103E-06 4.2114E-06 4.0010E-06
   12 3.8008E-06 3.6896E-06 3.9076E-06 5.1472E-06 8.4035E-06 1.5453E-05
   13 2.9829E-05 5.6825E-05 1.0753E-04 1.8584E-04 2.7377E-04
```

NEWVMR(:KMAX,I) – NLEV (IRTYPE) mixing ratio values same as those in (reference.prf). Generally copy/paste from the reference.prf file the profile of the main isotopomer to the separated specie here.

(NISOVMR) REAL, list-directed i/o

Next is the complete block for separating H2O 1/3 to H218O 66/1

```
   14  1 3                    ! old molec id and isotope id
   15  H217O                  ! new name
   16  66 1 19.0 3 1.5    ! new molec id, isotope id, mass, mode, tdep
   17  3657,1, 1595,1, 3756,1, 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
   18  5.3669E-06 5.4567E-06 5.7056E-06 6.1999E-06 5.1364E-06 5.3619E-06
   19  5.3226E-06 5.4317E-06 5.6051E-06 5.6490E-06 5.7683E-06 5.7257E-06
   20  5.7200E-06 5.7331E-06 5.7177E-06 5.7168E-06 5.6837E-06 5.6365E-06
   21  5.6016E-06 5.5089E-06 5.4460E-06 5.3348E-06 5.2177E-06 5.1049E-06
   22  4.9422E-06 4.8004E-06 4.5971E-06 4.4103E-06 4.2114E-06 4.0010E-06
   23  3.8008E-06 3.6896E-06 3.9076E-06 5.1472E-06 8.4035E-06 1.5453E-05
   24  2.9829E-05 5.6825E-05 1.0753E-04 1.8584E-04 2.7377E-04
```

This block separate H2O 1/4 to HDO 53/1

```
   25 H2O                     ! old name
   26 1 4                     ! old molec id and isotope id
   27 HDO                     ! new name
```

```
28 53 1 19.0 3 1.5 1. ! new molid, isoid, mass, mode, tdep, inten scale
29 2724,1, 1403,1, 3707,1
30 4.0222E-06 4.0091E-06 4.0001E-06 4.0008E-06 4.0025E-06 4.0022E-06
31 4.0020E-06 4.0009E-06 4.0002E-06 4.0000E-06 4.0000E-06 4.0001E-06
32 4.0001E-06 4.0001E-06 4.0001E-06 4.0001E-06 4.0001E-06 4.0001E-06
33 4.0001E-06 4.0001E-06 4.0001E-06 4.0001E-06 4.0002E-06 4.0217E-06
34 4.2680E-06 4.5724E-06 4.8661E-06 6.0691E-06 8.5766E-06 1.4688E-05
35 2.6803E-05 5.4395E-05 1.1161E-04 2.3303E-04 4.8531E-04 9.8322E-04
36 1.9118E-03 3.5303E-03 6.1168E-03 9.8928E-03 1.5014E-02 2.1326E-02
37 2.8491E-02 3.6855E-02
```

This block separates to a second HDO isotope

```
38 H2O                     ! old name - Add as second HDO isotope
39 1 5                     ! old molec id and isotope id
40 HDO                     ! new name
41 53 2 21.0 0 0. 0. 0     ! new molec id, isotope id, mass, mode
```

    (2) INTEGER, (1) REAL, (1) INTEGER, (2) REAL, list-directed i/o

A second isotopomer of water is added to the HDO isotopomer ie. H2O 1/5 -> 53/2. When the nmode variable s set to 0 no vibrational data or VMR data are read in. Values for tdep and intensity scale factor variables needed for the read: set them to zero.

The VMR and vibrational data must be given for the first isotope of this new species.

When changing more than one isotope to a new species put isotopes in order starting at 1 both as the isotope ID and also in this input file.

This block separates to a third HDO isotope

```
38 H2O                     ! old name - Add as second HDO isotope
39 1 6                     ! old molec id and isotope id
40 HDO                     ! new name
41 53 3 20.0 0 0. 0. 0     ! new molec id, isotope id, mass, mode
```

*some molecular parameters (eg band centers) are not strictly the same for all isotopes, better values may be found via your literature search.

**in HITRAN line strengths are scaled by the terrestial isotopic fraction so that a single vmr will retreive the same amount from all isotopic lines of a particular – unless fractionation at the time of the measurement is different. When this is set to unity copy the main isotope vmr to this file for the separated specie and all is well.