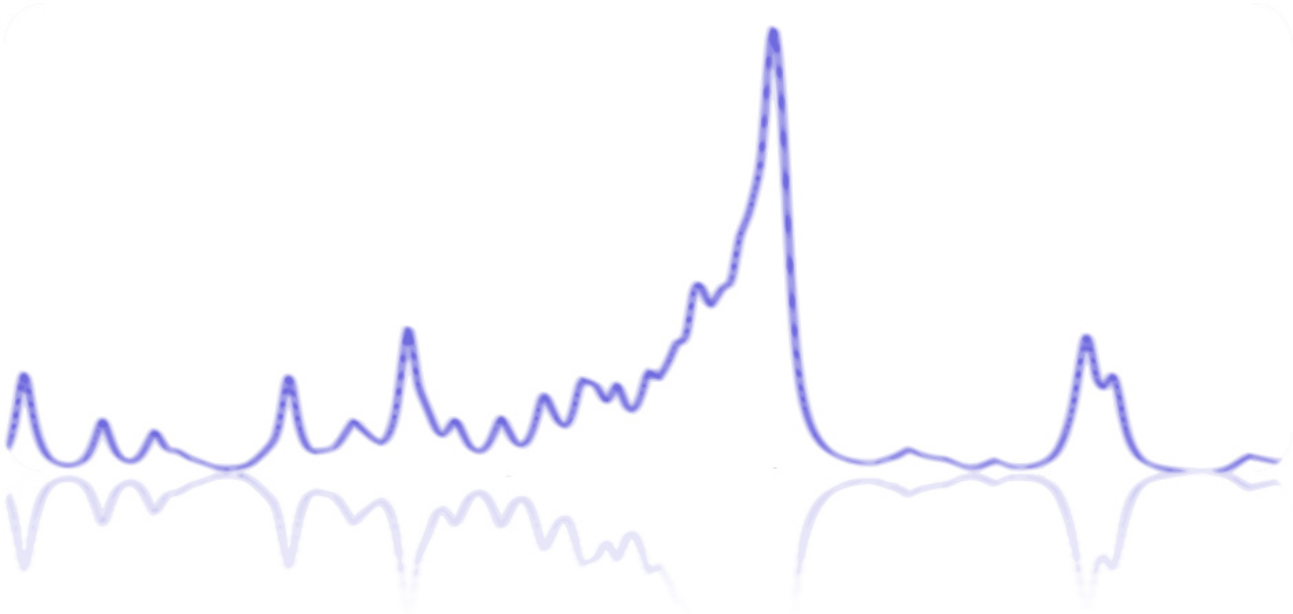
HITRAN **A**pplication **P**rogramming **I**nterface (HAPI)

User Guide



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I. INTRODUCTION

1.1. PREFACE

HITRAN **A**pplication **P**rogramming **I**nterface (HAPI) is a set of routines in Python which is aimed to provide a remote access to functionality and data given by the new project HITRANonline (http://hitranazure.cloudapp.net)[1].

At the present time, the API can download, filter and process data on molecular and atomic line-by-line spectra which is provided by the HITRANonline portal.

One of the major purposes of introducing this API is to extend the functionality of the main site, particularly providing a possibility to calculate several types of spectral functions based on the flexible HT (Hartmann-Tran) profile [1] and optionally accounting for instrumental functions.

Each feature of the API is represented by a Python function with a set of parameters providing a flexible approach to the task.

The current version is at the beta stage. All comments and suggestions are welcome!
The HAPI library doesn't require installation by itself. The user just needs to install prerequisites (see Section II).

HAPI is a completely free product and uses only open-source libraries. The user is free to modify and use it with no licensing fees or limitations.

1.2. FEATURES SUMMARY

Some of the prominent current features of HAPI are:
1) Downloading line-by-line data from the HITRANonline site to a local machine.
2) Filtering and processing the data in SQL-like fashion.
3) Conventional Python structures (lists, tuples, and dictionaries) for representing spectroscopic data.
4) Possibility to use a large set of third-party Python libraries to work with the data.
5) Python implementation of the HT profile [1-3] which can be used in spectra simulations. This line shape can also be reduced to a number of conventional line profiles such as Gaussian (Doppler), Lorentzian, Voigt, Rautian, Speed-dependent Voigt and speed-dependent Rautian.
6) Python implementation of total internal partition sums (TIPS-2011 [4]) which is used in spectra simulations as well as scaling some HITRAN [5] parameters.
7) High-resolution spectra simulation accounting for pressure, temperature and optical path length. The following spectral functions can be calculated:
   a) absorption coefficient
   b) absorption spectrum
   c) transmittance spectrum
   d) radiance spectrum
8) Spectral calculation using a number of instrumental functions to simulate experimental spectra.
9) Possibility to extend the user's functionality by adding custom line shapes, partition sums and apparatus functions.

[1] The link to the site will be different when HITRANonline is officially released.

II. PREREQUISITES

HITRAN API has the following two prerequisites:

1) Python 2.6+:
   https://www.python.org/
2) Numpy:
   http://www.numpy.org/

These two entities can be installed either separately (see the links given) or in one shot using a scientific Python distribution:

http://continuum.io/downloads ("Anaconda")
https://www.enthought.com/products/canopy ("Canopy")
http://www.sagemath.org ("Sage")

… or any other similar package.

To be able to go through tutorials the user would need to have the Matplotlib installed:
http://matplotlib.org/

To have a nice Mathematica-style interface for Python the user can install IPython notebook:
http://ipython.org/

Note that all listed prerequisites are open source and free to use.

III. WORKING WITH DATA

Welcome to the manual on retrieving and processing the data from HITRANonline.
This manual will give you an insight of how to use HAPI's capabilities for working with data.

3.1. LOCAL DATABASE STRUCTURE

The local data is downloaded from the HITRANonline portal (http://hitranazure.cloudapp.net) using API functions (fetch and fetch_by_ids). Downloaded data is stored in the folder which was specified in a call to db_begin().

The structure of a local data folder is as follows (assuming that you have already downloaded several tables from HITRANonline):

Folder name
|
|----- *table1.data*
| *table1.header*
|
|----- *table2.data*
| *table2.header*
…
|----- *tableN.data*
tableN.header

The typical format is as follows: **<table_name>.data** for line-by-line data, and **<table_name>.header** for table description (field names and positions, format, number of lines etc...). The default file format is 160-character HITRAN format (see Ref [5] and links within).

Besides working with downloaded HITRANonline data, HAPI can also deal with custom data files. It is sufficient to copy HITRAN-formatted files with an extension ".par" into the database directory, and HAPI will detect them automatically after the db_begin() call.

3.2. DOWNLOADING AND DESCRIBING DATA

To start working with HAPI, the user should import all functions from the module "hapi.py":

```
from hapi import *
```

First, let's choose a folder for our local database. Every time you start your Python project, you have to specify explicitly the name of the database folder.

```
db_begin('data')
```

N.B. It's important to note that commands in Python are case sensitive!

So, let's download some data from the server and do some processing on it. Suppose that we want to get line-by-line data on the main isotopologue of H_2O.

For retrieving the data to the local database, the user has to specify the following parameters:
1) Name of the local table which will store the downloaded data.
2) Either a pair of molecule and isotopologue HITRAN numbers (M and I), or a "global" isotopologue ID (iso_id).
3) Wavenumber range (nu_min and nu_max)

N.B. If you specify a name which already exists in your local folder, the existing table with that name will be overwritten.

To get additional information on function fetch, call getHelp:

```
getHelp(fetch)
```

To download the data, simply call the function "fetch". This will establish a connection with the main server and get the data using the parameters listed above. For example:

```
fetch('H2O',1,1,3400,4100)
```

```
BEGIN DOWNLOAD: H2O
  65536 bytes written to data/H2O.data
  65536 bytes written to data/H2O.data
  65536 bytes written to data/H2O.data
...
  65536 bytes written to data/H2O.data
  65536 bytes written to data/H2O.data
  65536 bytes written to data/H2O.data
Header written to data/H2O.header
END DOWNLOAD
                    Lines parsed: 7524
PROCESSED
```

To check the file that you've just downloaded, you can open the local database folder. The new plain text file should have a name "H2O.data" and it should contain line-by-line data in HITRAN format (see Table 1 of Ref. [5] for the HITRAN format).

N.B. If we want several isotopologues in one table, we should use fetch_by_ids instead of just fetch. Fetch_by_ids takes a "global" isotopologue ID number as an input instead of HITRAN's "local" identification.

See getHelp(fetch_by_ids) to get more information on this.

To get a list of tables which are already in the database, use the tableList() function (it takes no arguments):

```
tableList()
```

To learn about the table we just downloaded, let's use a function "describeTable".

```
describeTable('H2O')
```

```
-----------------------------------------
H2O summary:
-----------------------------------------
Comment:
Contains lines for H2(16O)
 in 3400.000-4100.000 wavenumber range
Number of rows: 7524
Table type: column-fixed
-----------------------------------------
            PAR_NAME           PAR_FORMAT

            molec_id                   %2d
        local_iso_id                   %1d
                  nu                %12.6f
                  sw                %10.3E
                   a                %10.3E
           gamma_air                 %5.4f
          gamma_self                 %5.3f
              elower                %10.4f
               n_air                 %4.2f
           delta_air                 %8.6f
 global_upper_quanta                  %15s
 global_lower_quanta                  %15s
  local_upper_quanta                  %15s
  local_lower_quanta                  %15s
                ierr                   %6s
                iref                  %12s
    line_mixing_flag                   %1s
                  gp                 %7.1f
                 gpp                 %7.1f
-----------------------------------------
```

This output tells how many rows are currently in the table H2O and which wavenumber range was used by fetch(). The output also gives basic information about parameters stored in the table.

So having the table downloaded, one can perform different operations on it using the API.

Here is a list of operations currently available with the API:

1) FILTERING
2) OUTPUTTING
3) SORTING
4) GROUPING

3.3. FILTERING AND OUTPUTTING DATA

The table data can be filtered with the help of the select() function.

Use the simple select(...) call to output the table content:

```
select('H2O')
```

```
MI          nu         S         A gair gsel        E_nair    dair  ...
11 1000.288940 1.957E-24 2.335E-02.07100.350 1813.22270.680.008260  ...
11 1000.532321 2.190E-28 1.305E-05.04630.281 2144.04590.39-.011030  ...
...
```

This will display the list of line parameters contained in the table "H2O".

That's the simplest way of using the function select(). Full information on control parameters can be obtained via the getHelp(select) statement.

Suppose that we need lines from a table within some wavenumber range.
That's what filtering is for. Let's apply a simple range filter on a table.

```
select('H2O',Conditions=('between','nu',4000,4100))
```

```
MI          nu         S         A gair gsel        E_nair    dair
 11 4000.188800 1.513E-25 1.105E-02.03340.298 1581.33570.51-.013910 ...
 11 4000.204070 3.482E-24 8.479E-03.08600.454  586.47920.61-.007000 ...
 11 4000.469910 3.268E-23 1.627E+00.05410.375 1255.91150.56-.013050 ...
......
```

As a result of this operation, we see a list of lines from the H_2O table, whose wavenumbers lie between 4000 cm^{-1} and 4100 cm^{-1}. The condition is taken as an input parameter to API function "select".

To specify a subset of columns to display, use another control parameter - ParameterNames:

```
select('H2O',ParameterNames=('nu','sw'),Conditions=('between','nu',4000,4100))
```

```
                nu         S

       4000.188800 1.513E-25
       4000.204070 3.482E-24
       4000.469910 3.268E-23
       4000.722241 1.528E-27
       4000.730660 5.406E-25
       4000.999780 6.975E-29
       4001.281900 9.279E-23
       4001.319998 2.591E-29
       4001.323119 7.773E-29
       4001.325110 2.997E-25
       4001.427670 1.791E-24 ...
```

The usage of ParameterNames is outlined below in the section "Specifying a list of parameters". So far it is worth mentioning that this parameter is a part of a powerful tool for displaying and processing tables from the database.

In the next section we will show how to create queries with more complex conditions.

3.4. FILTERING CONDITIONS

Let's analyze the last example of filtering. Condition input variable is as follows:

('between','nu',4000,4100)

Thus, this is a python list (or tuple), containing logical expressions defined under column names of the table. For example, 'nu' is a name of the column in 'H2O' table, and this column contains a transition wavenumber.
The structure of a simple condition is as follows:

(OPERATION,ARG1,ARG2,...)

where OPERATION must be in a set of predefined operations (see below), and ARG1,ARG2, etc. are the arguments for this operation.

Conditions can be nested, i.e. ARG can itself be a condition (see examples).

The following operations are available in select (case insensitive):

DESCRIPTION	LITERAL	EXAMPLE
Range	'RANGE','BETWEEN'	('BETWEEN','nu',0,1000)
Subset	'IN','SUBSET'	('IN','local_iso_id',[1,2,3,4])
And	'&','&&','AND'	('AND',('<','nu',1000),('>','nu',10))
Or	'|','||','OR'	('OR',('>','nu',1000),('<','nu',10))
Not	'!','NOT'	('NOT',('IN','local_iso_id',[1,2,3]))
Less than	'<','LESS','LT'	('<','nu',1000)
More than	'>','MORE','MT'	('>','sw',1.0e-20)
Less or equal to	'<=','LESSOREQUAL','LTE'	('<=','local_iso_id',10)
Greater or equal to	'>=','MOREOREQUAL','MTE'	('>=','sw',1e-20)
Equal	'=','==','EQ','EQUAL','EQ'	('<=','local_iso_id',10)
Not equal	'!=','<>','~=','NE','NOTE	('!=','local_iso_id',1)
Summation Difference	'+','SUM': '-','DIFF'	('+','v1','v2','v3') ('-','nu','elow')
Multiplication	'*','MUL'	('*','sw',0.98)
Division	'/','DIV'	('/','A',2)
Cast to string	'STR','STRING'	('STR','some_string')
Cast to Python list	'LIST'	('LIST',[1,2,3,4,5])
Match regexp	'MATCH','LIKE'	('MATCH','\w+','some string')
Search single match	'SEARCH'	('SEARCH','\d \d \d','1 2 3 4')
Search all matches	'FINDALL'	('FINDALL','\d','1 2 3 4 5')
Count within group	'COUNT'	('COUNT','local_iso_id')

Let's create a query with a more complex condition. Suppose that we are interested in all lines between 3500 and 4000 with 1e-19 intensity cutoff.

The query will look like this:

```
Cond = ('AND',('BETWEEN','nu',3500,4000),('>=','Sw',1e-19))
select('H2O',Conditions=Cond,DestinationTableName='tmp')
```

Here, apart from other parameters, we have used a new parameter DestinationTableName. This parameter contains a name of the table where we want to put a result of the query. Thus we have

chosen a name “tmp” for a new table. After a database commit (db_commit function), the relevant data is stored in the file '"tmp.data”. All the tables are standard 160-character formatted files by default (in the alpha version).

3.5. ACCESSING COLUMNS IN A TABLE

To get access to a particular table column (or columns) all we need is to get a column from a table and put it to Python variable.

For this purpose, there exist two functions:

getColumn(...)
getColumns(...)

The first one returns just one column at a time. The second one returns a list of columns.

So, here are some examples of how to use both:

```
nu1 = getColumn('H2O','nu')
nu2,sw2 = getColumns('H2O',['nu','sw'])
```

N.B. If you don't remember the exact names of columns in a particular table, use describeTable to get info on its structure!

3.6. SPECIFYING A LIST OF PARAMETERS

Suppose that we want not only to select a set of parameters/columns from a table, but to perform certain transformations on them (for example, multiply a column by a coefficient, or add one column to another etc...).
We can do it in two ways. First, we can extract a column from the table using one of the functions (getColumn or getColumns) and do the rest in Python. The second way is to do it on the level of select. The select function has a control parameter "ParameterNames", which makes it possible to specify parameters we want to be selected, and perform some simple arithmetic expressions with them.

Assume that we need only wavenumber and intensity from the H2O table.
Also we need to scale the intensity to unitary abundance. To do so, we must divide an 'sw' parameter by its natural abundance (0.99731 for the principal isotopologue of water).

Thus, we have to select two columns: wavenumber (nu) and scaled intensity (sw/0.99731)

```
select('H2O',ParameterNames=('nu',('/','sw',0.99731)))
```

```
          nu                          #0
 3400.006750    1.116002045502401E-23
 3400.335198    6.218728379340426E-28
 3400.397711    4.341679116824257E-27
 3400.405850    1.298492946024807E-24
 3400.445191    2.045502401459927E-27
 3400.550910    6.715063520871143E-26
 3400.566080    4.490078310655663E-24
 3400.581360    2.010407997513311E-25 ...
```

3.7. SAVING QUERY TO DISK

To quickly save a result of a query to disk, the user can take advantage of an additional parameter "File". If this parameter is presented in the function call, then the query is saved to a file with the name which was specified in "File".

For example, select all lines from H2O and save the result in file 'H2O.txt':

```
select('H2O',File='H2O.txt')
```

3.8. GETTING INFORMATION ON ISOTOPOLOGUES

HAPI provides the following auxiliary information about isotopologues present in HITRAN. Corresponding functions use the standard HITRAN molecule-isotopologue notation:

1) Natural abundances

```
abundance(mol_id,iso_id)
```

2) Molecular masses

```
molecularMass(mol_id,iso_id)
```

3) Molecule names

```
moleculeName(mol_id,iso_id)
```

4) Isotopologue names

```
isotopologueName(mol_id,iso_id)
```

5) ISO_ID

```
getHelp(ISO_ID)
```

The latter is a dictionary, which contains the summary information about all isotopologues available in HAPI.

IV. CALCULATING SPECTRA

Welcome to the tutorial on calculating a spectra from line-by-line data.
This section will demonstrate how to use different line shapes and partition functions, and how to calculate synthetic spectra with respect to different instruments. It will be shown how to combine different parameters of a spectral calculation to achieve better precision and performance for cross sections.

As it already has been said, HAPI provides a powerful tool to calculate cross-sections based on line-by-line data contained in HITRAN. This features:

1) Python implementation of the HT (Hartmann-Tran [1-3]) profile which is used in spectra simulations. This line shape can also be reduced to a number of conventional line profiles such as Gaussian (Doppler), Lorentzian, Voigt, Rautian, Speed-dependent Voigt and speed-dependent Rautian.
2) Python implementation of total internal partition sums (TIPS-2011 [4]) which is used in spectra simulations.
3) High-resolution spectra simulation accounting for pressure, temperature, and optical path length. The following spectral functions can be calculated:
   a) absorption coefficient
   b) absorption spectrum
   c) transmittance spectrum
   d) radiance spectrum
4) Spectra simulation using a number of apparatus functions.
5) Possibility to extend the user's functionality by adding custom line shapes, partition sums, and apparatus functions.
6) An approach to function code is aimed to be flexible enough, yet hopefully intuitive.

4.1. USING LINE PROFILES

Several line shape (line profile) families are currently available:

1) Gaussian (Doppler) profile
2) Lorentzian profile
3) Voigt profile
4) HT profile (Hartmann-Tran)

Each profile has its own unique set of parameters.
N.B. Normally one should use profiles only with the relevant parameters. However, HAPI provides a possibility to use custom parameters in calculating the cross-section. Note, that this approach can be risky due to misinterpretation of parameters.

Import HAPI and open local folder (you don't have to repeat this step if you have already done so).

```
from hapi import *
db_begin('data')
```

So, let's start exploring the available profiles using getHelp:

```
getHelp(profiles)
```

```
      Profiles available:
        HTP     : PROFILE_HT
        Voigt   : PROFILE_VOIGT
        Lorentz : PROFILE_LORENTZ
        Doppler : PROFILE_DOPPLER
```

The output gives all available profiles. We can get additional info on each of them just by calling getHelp(ProfileName):

```
getHelp(PROFILE_HT)
```

Line profiles, adapted for using with HAPI, are written in Python and heavily use the numerical library "Numpy". This means that the user can calculate multiple values of a particular profile at once having just pasted a numpy array as a wavenumber grid. Let's give a short example of how to calculate the Hartmann-Tran profile using numpy arrays.

```
from numpy import arange
w0 = 1000.
GammaD = 0.005
Gamma0 = 0.2
Gamma2 = 0.01 * Gamma0
Delta0 = 0.002
Delta2 = 0.001 * Delta0
nuVC = 0.2
eta = 0.5
Dw = 1.
ww = arange(w0-Dw, w0+Dw, 0.01)  # GRID WITH THE STEP 0.01
l1 = PROFILE_HT(w0,GammaD,Gamma0,Gamma2,Delta0,Delta2,nuVC,eta,ww)[0]
# now l1 contains values of HT profile calculates on the grid ww
l1 # print calculated values
```

```
      array([ 0.06098146,  0.0621689 ,  0.06339088,  0.06464874,  0.06594385,
              0.06727769,  0.0686518 ,  0.07006778,  0.07152732,  0.07303221,
              0.07458429,  0.07618554,  0.07783802,  0.07954388,  0.08130542,
              0.08312503,  0.08500524,  0.08694872,  0.08895828,  0.09103688,
              ... ]
```

For additional information about parameters see getHelp(PROFILE_HT).

It is worth noting that PROFILE_HT returns 2 entities: the real and imaginary part of the line shape (as is described in Ref. [1]). Apart from HT, all other profiles return just one entity (the real part).

4.2. USING PARTITION SUMS

As mentioned in Section 4.1, the partition sums are taken from the TIPS-2011 [4]. Partition sums are taken for those isotopologues which are present in HITRAN and in TIPS-2011 simultaneously.

N.B. Partition sums are not yet available for the following isotopologues which are in HITRAN at the current time:

Isotopologue ID	Molecule number	Isotopologue number	Isotopologue name
117	12	2	$H^{15}N^{16}O_3$
110	14	2	$D^{19}F$
107	15	3	$D^{35}Cl$
108	15	4	$D^{37}Cl$
111	16	3	$D^{79}Br$
112	16	4	$D^{81}Br$
113	17	2	$D^{127}I$
118	22	2	$^{14}N^{15}N$
119	29	2	$^{13}C^{16}O^{19}F_2$
86	34	1	^{16}O
92	39	1	$^{12}CH_3{}^{16}OH$
114	47	1	$^{32}S^{16}O_3$

The data on these isotopologues are not present in TIPS-2011 but the isotopologues are present in HITRAN. We're planning to add these molecules after a new TIPS program is released.

To calculate a partition sum for most of the isotopologues in HITRAN, we will use a function partitionSum (use getHelp for detailed info).

The syntax is as follows: partitionSum(M,I,T), where M,I - standard HITRAN molecule-isotopologue notation, T - definition of temperature range.

Usecase 1: temperature is defined by a list:

```
Q = partitionSum(1,1,[70,80,90])
Q
```

```
[20.999999542236328, 25.446399765014647, 30.169152160644533]
```

Usecase 2: temperature is defined by bounds and the step:

```
T,Q = partitionSum(1,1,[70,3000],step=1.0)
Q
```

```
array([    20.99999954,     21.43247156,     21.86764758, ...,
       15942.1616    ,  15957.8416    ,  15973.5344    ])
```

In the latter example, we calculate a partition sum on a range of temperatures from 70K to 3000K using a step 1.0 K, and having arrays of temperature (T) and partition sum (Q) as the output.

4.3. CALCULATING ABSORPTION COEFFICIENTS

Currently HAPI can calculate the following spectral function at arbitrary thermodynamic parameters:

1) Absorption coefficient
2) Absorption spectrum
3) Transmittance spectrum
4) Radiance spectrum

All these functions can be calculated with or without accounting of instrument properties (apparatus function, resolution, path length etc...)

As is well known, the spectral functions such as absorption, transmittance, and radiance, are calculated on the basis of the absorption coefficient. For that reason, absorption coefficient is the most important part of simulating a cross section. This part of the tutorial is devoted to a demonstration of how to calculate the absorption coefficient from the HITRAN line-by-line data. Here we give a brief insight on basic parameters of the calculation procedure, and talk about some useful practices and precautions.

To calculate an absorption coefficient, we can use one of the following functions:

-> absorptionCoefficient_HT
-> absorptionCoefficient_Voigt
-> absorptionCoefficient_Lorentz
-> absorptionCoefficient_Doppler

Each of these functions calculates cross sections using different line shapes (the names are quite self-explanatory).

You can get detailed information on using each of these functions by calling getHelp(function_name).

Let's look more closely to the cross sections based on the Lorentz profile. For doing that, let's have a table downloaded from HITRANonline.

Get data on CO2 main isotopologue in the range 2000-2100 cm-1:

```
fetch('CO2',2,1,2000,2100)
```

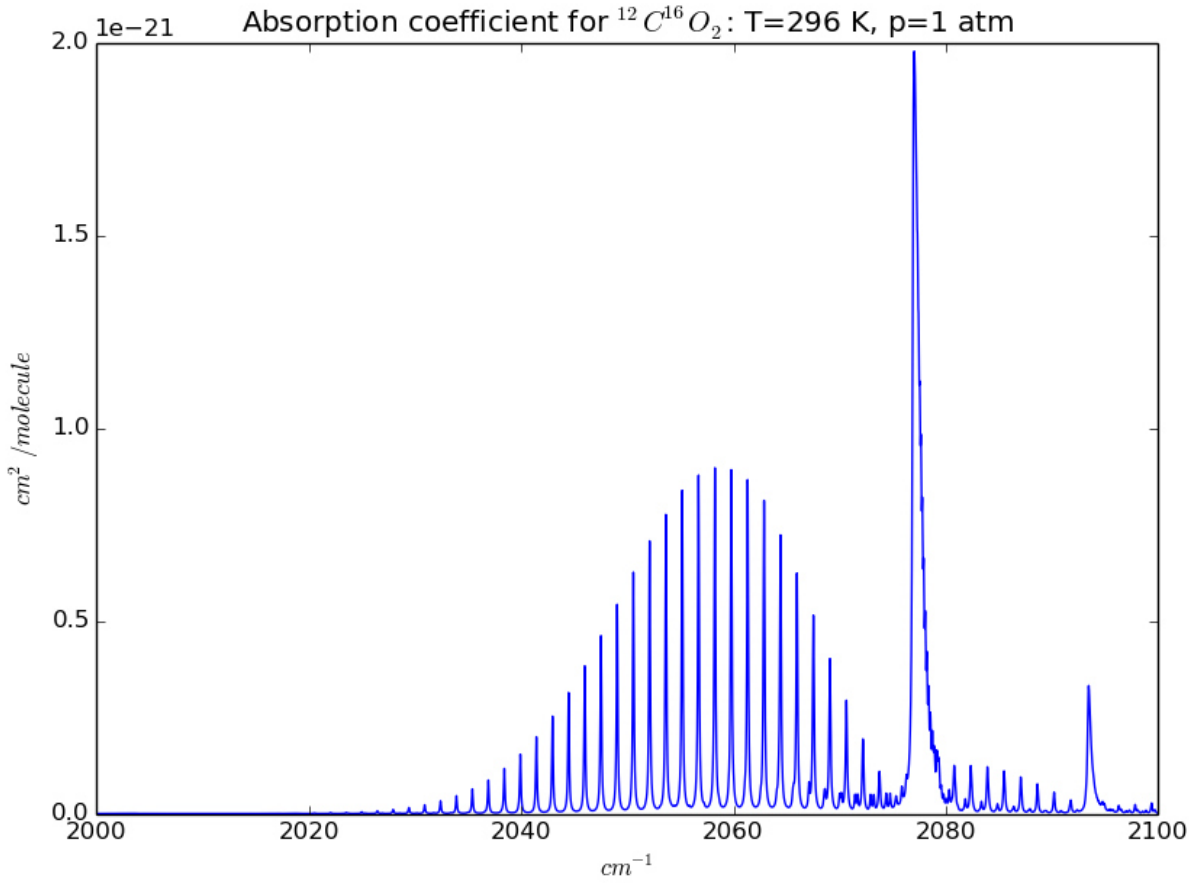
OK, now we're ready to run a fast example of how to calculate an absorption coefficient cross section:

```
nu,coef = absorptionCoefficient_Lorentz(SourceTables='CO2')
```

This example calculates a Lorentz cross section using the whole set of lines in the "CO2" table. This is the simplest possible way to use these functions, because the major part of parameters are constrained to their default values.

If we have Matplotlib installed, then we can visualize it using a plotter:

```
from pylab import plot
plot(nu,coef)
```



More examples on how to use Matplotlib can be found in the Section V. Plotting with Matplotlib.

HAPI provides a flexible control over a calculation procedure. This control can be achieved by using a number of input parameters. So, let's dig into the depth of the settings.

The input parameters of absorptionCoefficient_Lorentz are as follows:

NAME	DEFAULT VALUE
SourceTables	'__BUFFER__'
Components	All isotopologues in SourceTables
partitionFunction	PYTIPS
Environment	{'T':296.,'p':1.}
OmegaRange	depends on Components
OmegaStep	0.01 cm-1
OmegaWing	10 cm-1
OmegaWingHW	50 HWHMs
IntensityThreshold	0 cm/molec
GammaL	'gamma_air'
HITRAN_units	True
File	None
Format	'%e %e'

Now we'll give a brief explanation for each parameter. After each description we'll make some notes about the usage of the corresponding parameter.

SourceTables: (required parameter)

List of source tables to take line-by-line data from.
NOTE: User must provide at least one table in the list.

Components: (optional parameter)

List of tuples (M,I,D) to consider in cross section calculation. M here is a molecule number, I is an isotopologue number, D is an abundance of the component.
NOTE: If this input contains more than one tuple, then the output is an absorption coefficient for a mixture of corresponding gases.
NOTE2: If omitted, then all data from the source tables are involved.

partitionFunction: (optional parameter)

Instance of partition function of the following format:
Func(M,I,T), where Func – name of function, (M,I) - HITRAN numbers for molecule and isotopologue, and T - temperature. Function must return only one output - value of partition sum.
NOTE: Default value is PYTIPS - python version of TIPS-2011

Environment: (optional parameter)

Python dictionary containing value of pressure and temperature.
The format is as follows: Environment = {'p':pval,'T':tval}, where "pval" and "tval" are corresponding values in atm and K respectively.
NOTE: Default value is {'p':1.0,'T':296.0}

OmegaRange: (optional parameter)

List containing minimum and maximum value of wavenumber to consider in cross-section calculation. All lines that are out of these bounds will be skipped.
The format is as follows: OmegaRange=[wn_low,wn_high]
NOTE: If this parameter is skipped, then min and max are taken from the data in SourceTables.

OmegaStep: (optional parameter)

Value for the wavenumber step.
NOTE: Default value is 0.01 cm^{-1}.
NOTE2: Normally the user would want to take the step under 0.001 when calculating absorption coefficient with Doppler profile because of very narrow spectral lines.

OmegaWing: (optional parameter)

Absolute value of the line wing in cm^{-1}, i.e. distance from the center of each line to the farthest point where the profile is considered to be non zero.
NOTE: if omitted, then only OmegaWingHW is taken into account.

OmegaWingHW: (optional parameter)

Relative value of the line wing in halfwidths.
NOTE: The resulting wing is a maximum value from both OmegaWing and OmegaWingHW.

IntensityThreshold: (optional parameter)

Absolute value of minimum intensity in cm^{-1}/ (molec × cm^{-2}) to consider[2].
NOTE: default value is 0.
NOTE2: Setting this parameter to a value above zero is only recommended for very experienced users.

GammaL: (optional parameter)

This is the name of broadening parameter to consider a "Lorentzian" part in the Voigt profile. In the current 160-character format there is a choice between "gamma_air" and "gamma_self".
NOTE: If the table has custom columns with broadening coefficients, the user can specify the name of this column in GammaL. This would let the function calculate an absorption with custom broadening parameter.

[2] In this manual this unit could be also be expressed as cm × molec

HITRAN_units: (optional parameter)

Logical flag for units in which the absorption coefficient should be calculated. Currently, the choices are: cm^2/molec (if True) and cm-1 (if False).
NOTE: to calculate other spectral functions like transmittance, radiance and absorption spectra, the user should set HITRAN_units to False.

File: (optional parameter)

The name of the file to save the calculated absorption coefficient. The file is saved only if this parameter is specified.

Format: (optional parameter)

C-style format for the text data to be saved. Default value is "%e %e".
NOTE: C-style output format specification (which is mostly valid for Python) can be found, for instance, by the link: http://www.gnu.org/software/libc/manual/html_node/Formatted-Output.html

N.B. Other functions such as absorptionCoefficient_Voigt(_HT,_Doppler) have identical parameter sets so the description is the same for each function.

4.4. CALCULATING ABSORPTION, TRANSMITTANCE, AND RADIANCE SPECTRA

Let's calculate an absorption, transmittance, and radiance spectra on the basis of absorption coefficient. In order to be consistent with internal API's units, we need to have an absorption coefficient in cm^{-1}:

```
nu,coef = absorptionCoefficient_Lorentz(SourceTables='CO2',HITRAN_units=False)
```

To calculate absorption spectrum, use the function absorptionSpectrum():

```
nu,absorp = absorptionSpectrum(nu,coef)
```

To calculate transmittance spectrum, use function transmittanceSpectrum():

```
nu,trans = transmittanceSpectrum(nu,coef)
```

To calculate radiance spectrum, use function radianceSpectrum():

```
nu,radi = radianceSpectrum(nu,coef)
```

The last three commands used a default path length (1 m). To see complete info on all three functions, look for the section "calculating spectra" in getHelp()

Generally, all these three functions use a similar set of parameters:

Omegas: (required parameter)

Wavenumber grid for spectrum.

AbsorptionCoefficient: (optional parameter)

Absorption coefficient as input.

Environment: (optional parameter)

Environmental parameters for calculating spectrum. This parameter is a bit specific for each of the functions. For absorptionSpectrum(...) and transmittanceSpectrum(...) the default value is as follows: Environment={'l': 100.0}. For transmittanceSpectrum() the default value, besides path length, contains a temperature: Environment={'T': 296.0, 'l': 100.0}
NOTE: temperature must be equal to that which was used in the absorptionCoefficient_(...) routine!

File: (optional parameter)

Filename of output file for calculated spectrum. If omitted, then the file is not created.

Format: (optional parameter)

C-style format for spectra output file.
NOTE: Default value is as follows: Format='%e %e'

4.5. APPLYING INSTRUMENTAL FUNCTIONS

For comparison of the theoretical spectra with the real-world instrument output, it's necessary to take into account instrumental resolution. For this purpose, HAPI has a function convolveSpectrum(...) which can calculate spectra with variable resolution using custom instrumental functions.

The following instrumental functions are available:

1) Rectangular
2) Triangular
3) Gaussian
4) Diffraction
5) Michelson
6) Dispersion (Lorentz)

To get a description of each instrumental function we can use getHelp():

```
getHelp(slit_functions)
```

```
        RECTANGULAR : SLIT_RECTANGULAR
        TRIANGULAR  : SLIT_TRIANGULAR
        GAUSSIAN    : SLIT_GAUSSIAN
        DIFFRACTION : SLIT_DIFFRACTION
        MICHELSON   : SLIT_MICHELSON
        DISPERSION/LORENTZ : SLIT_DISPERSION
```

For instance,

```
getHelp(SLIT_MICHELSON)
```

... will give detailed info about the Michelson instrumental function.

The function convolveSpectrum() convolves a high-resolution spectrum with one of the supplied instrumental (slit) functions. The following parameters of this function are provided:

Omega: (required parameter)

Array of wavenumbers in high-resolution input spectrum.

CrossSection: (required parameter)

Values of high-resolution input spectrum.

Resolution: (optional parameter)

This parameter is passed to the slit function. It represents the resolution of the corresponding instrument.
NOTE: default value is 0.1 cm-1

AF_wing: (optional parameter)

Width of an instrument function where it is considered non-zero.
NOTE: default value is 10.0 cm-1

SlitFunction: (optional parameter)

Custom instrumental function to convolve with spectrum. Format of the instrumental function must be
as follows: Func(x,g), where Func - function name, x - wavenumber, g - resolution.
NOTE: if omitted, then the default value is SLIT_RECTANGULAR

Before using the convolution procedure it is worth giving some practical advice and remarks:

1) The quality of a convolution depends of many things: quality of calculated spectra, width of AF_wing and OmegaRange, Resolution, OmegaStep etc… Most of these factors are taken from previous stages of the spectral calculation. The right choice of all these factors is crucial for the correct computation.
2) Dispersion, Diffraction and Michelson apparatus functions don't work well in a narrow wavenumber range because of their broad wings.
3) Generally one must consider OmegaRange and AF_wing as wide as possible.
4) After applying a convolution, the resulting spectral range for the convolved spectra is reduced by the doubled value of AF_wing. For this reason, try to make an initial spectral range for high-resolution spectrum (absorption, transmittance, radiance) sufficiently broad.

The following command will calculate a convolved spectra from the CO_2 transmittance, which was calculated in a previous section.

The spectral resolution is 0.1 cm^{-1} by default.

```
nu_,trans_,i1,i2,slit = convolveSpectrum(nu,trans)
```

The outputs in this case are:

nu_, trans_ – wavenumbers and transmittance for the resulting convolved spectrum.

i1,i2 – indexes for initial nu,trans spectrum denoting the part of wavenumber range which was taken for convolved spectrum. Thus, the resulting spectrum is calculated on nu[i1:i2]

slit – array of slit function values calculated on grid "nu"

Note, in order to achieve more flexibility, one has to specify most of the optional parameters. For instance, a more complete call is as follows:

```
nu_,trans_,i1,i2,slit =
convolveSpectrum(nu,trans,SlitFunction=SLIT_MICHELSON,Resolution=1.0,AF_wing=20.0)
```

V. PLOTTING WITH MATPLOTLIB

This section briefly explains how to make plots using the Matplotlib - Python library for plotting.

Let's generate a plot using the basic entities which are provided by HAPI.
To do so, we will do all necessary steps to download, filter and calculate cross sections "from scratch".
To demonstrate the different possibilities of matplotlib, we will mostly use Pylab - a part of Matplotlib with an interface similar to Matlab. Please note that it's not the only way to use Matplotlib. More information can be found on its site.

The next part is a step-by-step guide, demonstrating basic possibilities of HAPI in conjunction with Matplotlib.

First, do some preliminary imports:

```
from hapi import *
from pylab import show,plot,subplot,xlim,ylim,title,legend,xlabel,ylabel,hold
```

Start the local database in folder 'data':

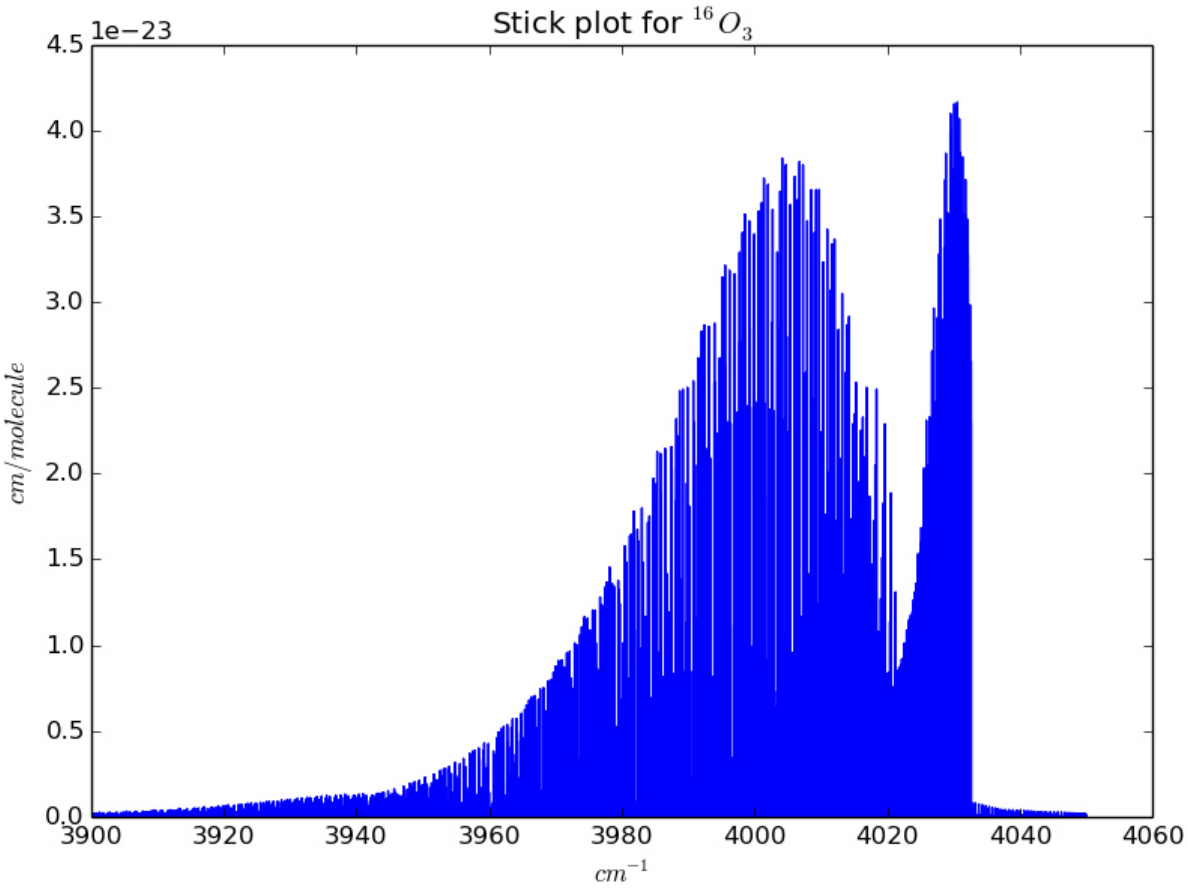
```
db_begin('data')
```

Download lines for the main isotopologue of ozone in the [3900,4050] range:

```
fetch('O3',3,1,3900,4050)
```

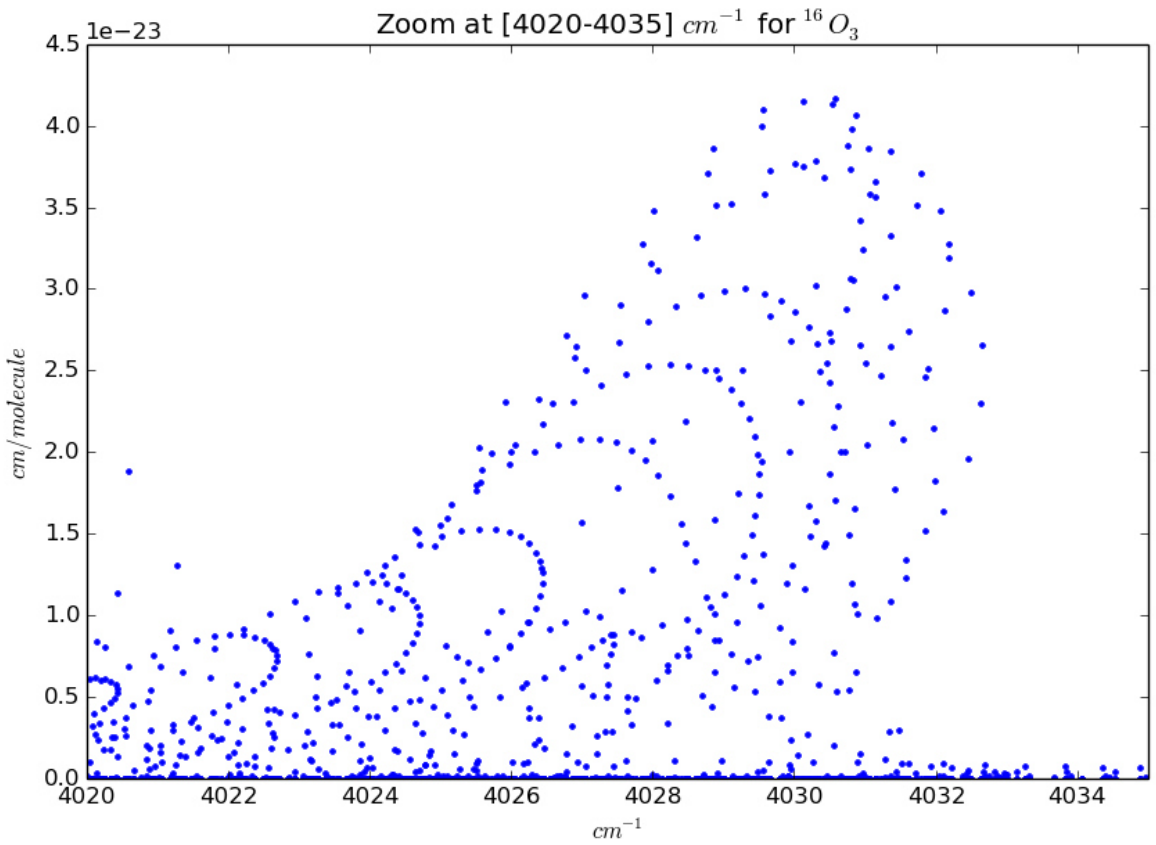
Plot a stick spectrum using the function getStickXY(...):

```
x,y = getStickXY('O3')
plot(x,y); show()
```



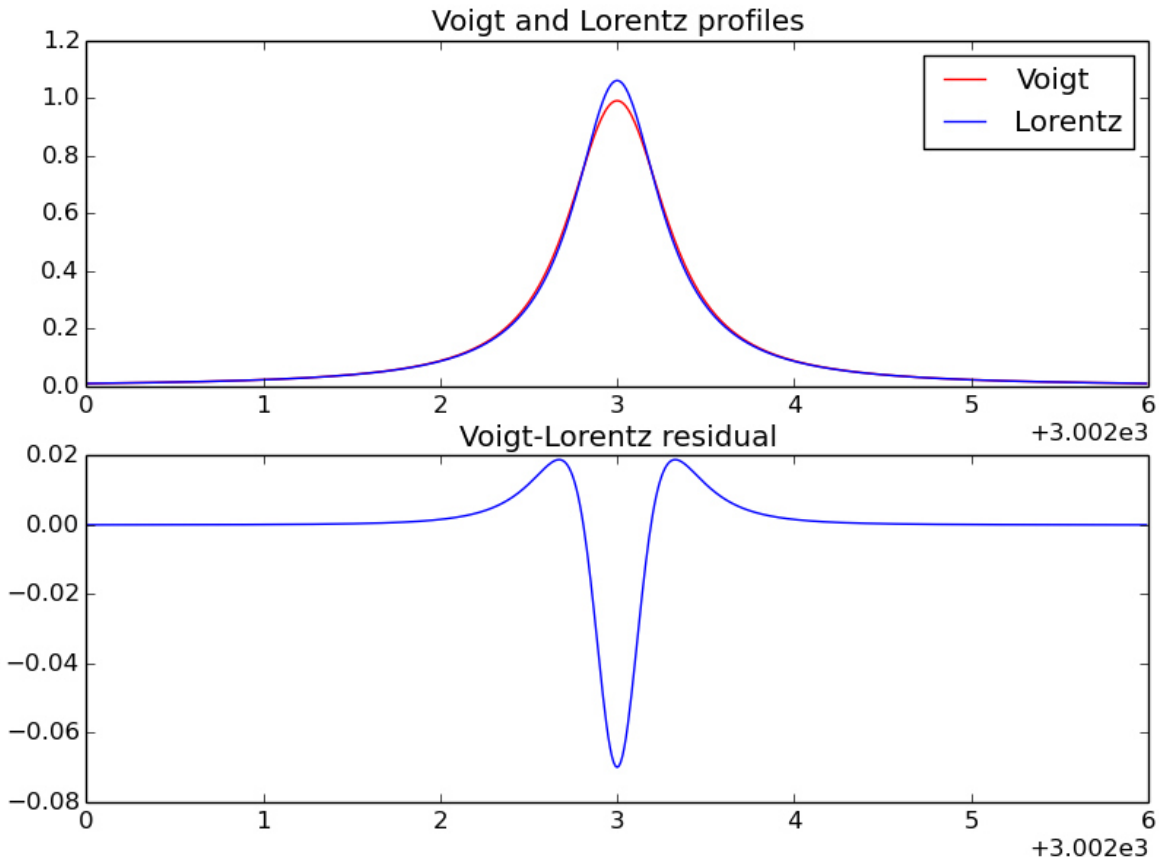
Zoom in spectral region [4020,4035] cm-1:

```
plot(x,y,'.'); xlim([4020,4035]); show()
```



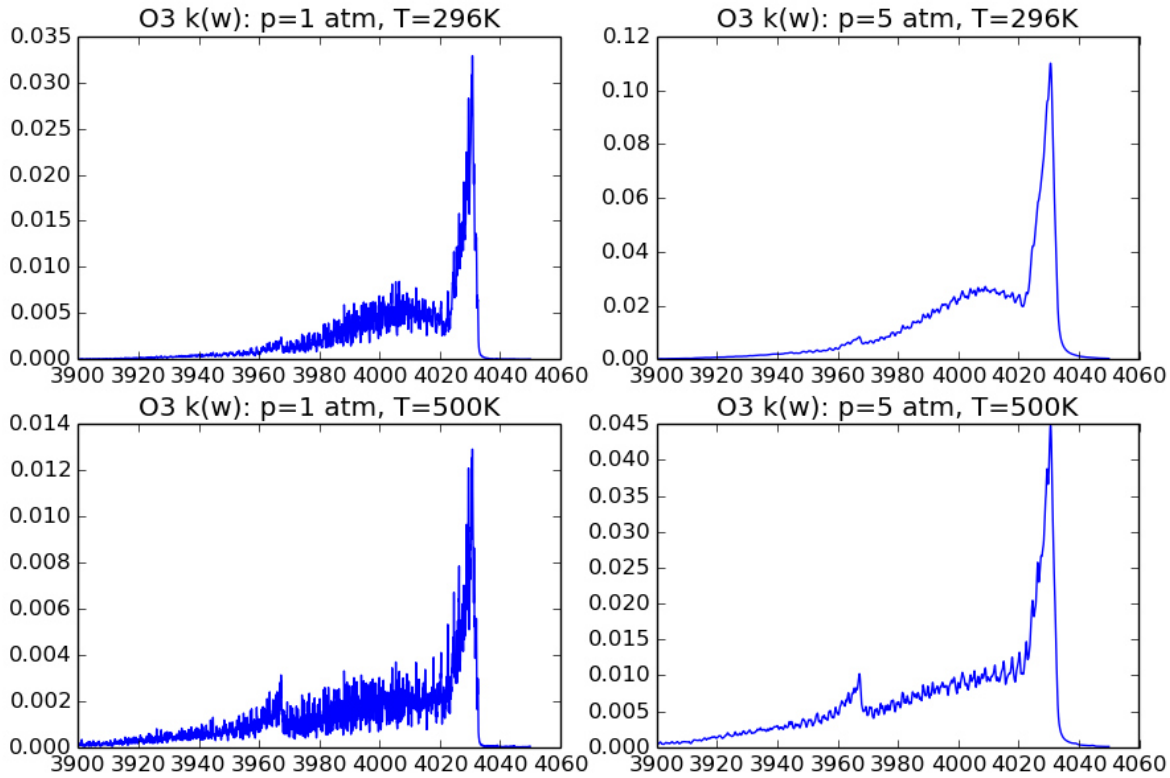
Calculate and plot difference between Voigt and Lorentzian lineshape:

```
wn = arange(3002,3008,0.01) # get wavenumber range of interest
voi = PROFILE_VOIGT(3005,0.1,0.3,wn)[0] # calc Voigt
lor = PROFILE_LORENTZ(3005,0.3,wn) # calc Lorentz
diff = voi-lor  # calc difference
subplot(2,1,1) # upper panel
plot(wn,voi,'red',wn,lor,'blue') # plot both profiles
legend(['Voigt','Lorentz']) # show legend
title('Voigt and Lorentz profiles') # show title
subplot(2,1,2) # lower panel
plot(wn,diff) # plot difference
title('Voigt-Lorentz residual') # show title
show() # show all figures
```



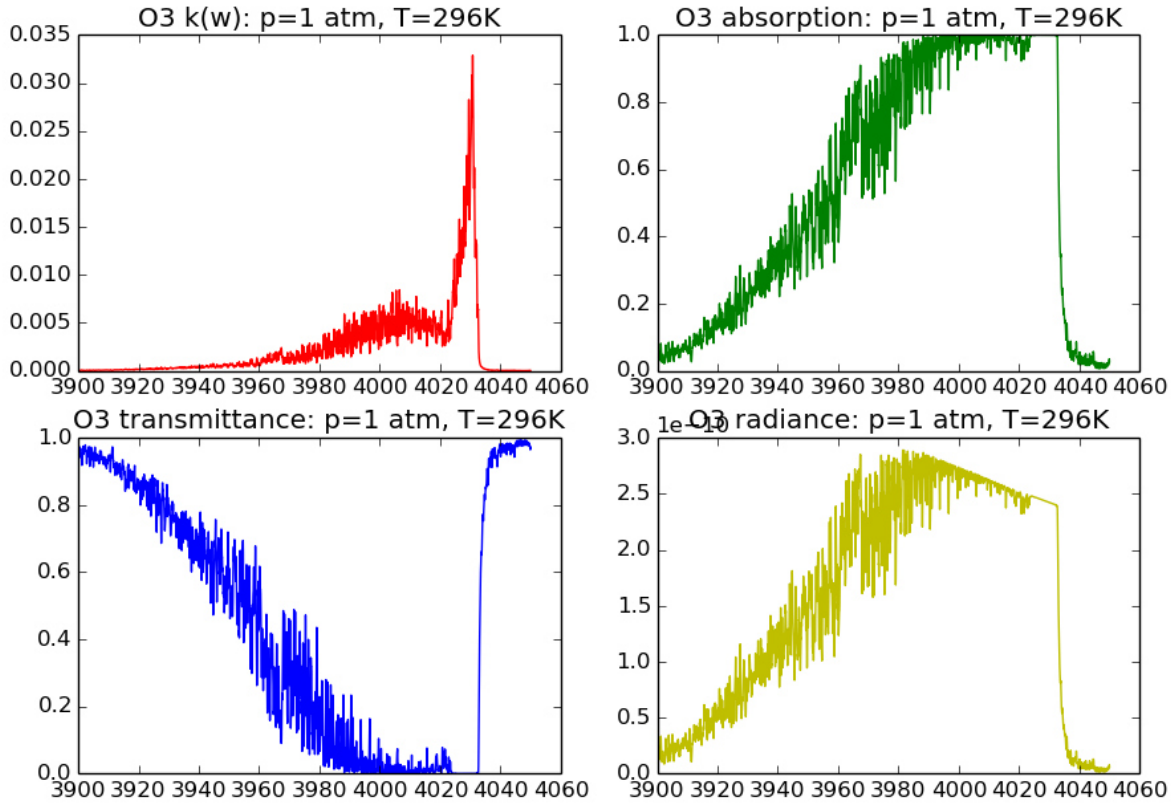
Calculate and plot absorption coefficients for ozone using Voigt profile. Spectra are calculated for 4 cases of thermodynamic parameters:
(1 atm, 296 K), (5 atm, 296 K), (1 atm, 500 K), and (5 atm, 500 K)

```
nu1,coef1 = absorptionCoefficient_Voigt(((3,1),),'O3',
        OmegaStep=0.01,HITRAN_units=False,GammaL='gamma_self',
        Environment={'p':1,'T':296.})
nu2,coef2 = absorptionCoefficient_Voigt(((3,1),),'O3',
        OmegaStep=0.01,HITRAN_units=False,GammaL='gamma_self',
        Environment={'p':5,'T':296.})
nu3,coef3 = absorptionCoefficient_Voigt(((3,1),),'O3',
        OmegaStep=0.01,HITRAN_units=False,GammaL='gamma_self',
        Environment={'p':1,'T':500.})
nu4,coef4 = absorptionCoefficient_Voigt(((3,1),),'O3',
        OmegaStep=0.01,HITRAN_units=False,GammaL='gamma_self',
        Environment={'p':5,'T':500.})

subplot(2,2,1); plot(nu1,coef1); title('O3 k(w): p=1 atm, T=296K')
subplot(2,2,2); plot(nu2,coef2); title('O3 k(w): p=5 atm, T=296K')
subplot(2,2,3); plot(nu3,coef3); title('O3 k(w): p=1 atm, T=500K')
subplot(2,2,4); plot(nu4,coef4); title('O3 k(w): p=5 atm, T=500K')
show()
```



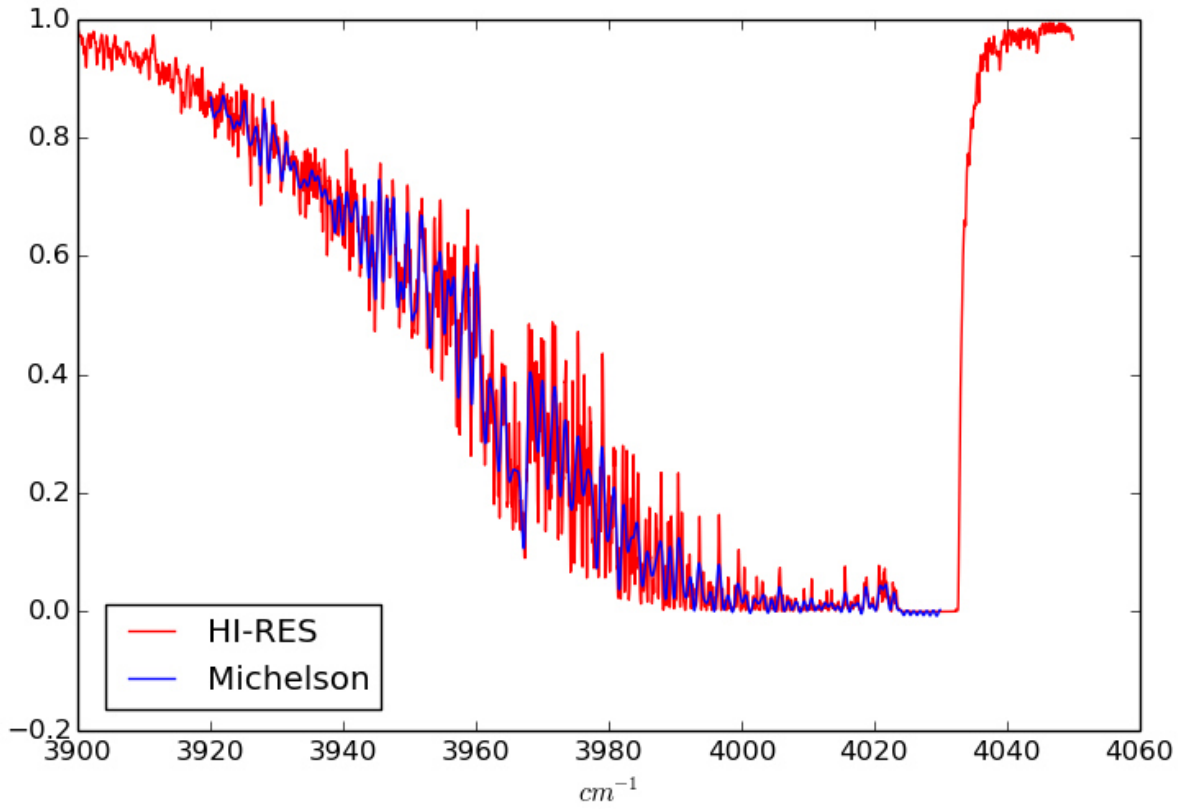
Calculate and plot absorption, transmittance, and radiance spectra for 1 atm and 296K. Path length is set to 10 m.

```
nu,absorp = absorptionSpectrum(nu1,coef1,Environment={'l':1000.})
nu,transm = transmittanceSpectrum(nu1,coef1,Environment={'l':1000.})
nu,radian = radianceSpectrum(nu1,coef1,Environment={'l':1000.,'T':296.})

subplot(2,2,1); plot(nu1,coef1,'r'); title('O3 k(w): p=1 atm, T=296K')
subplot(2,2,2); plot(nu,absorp,'g'); title('O3 absorption: p=1 atm, T=296K')
subplot(2,2,3); plot(nu,transm,'b'); title('O3 transmittance: p=1 atm, T=296K')
subplot(2,2,4); plot(nu,radian,'y'); title('O3 radiance: p=1 atm, T=296K')
show()
```



Calculate and compare high-resolution spectrum for O_3 with lower resolution spectrum convoluted with an instrumental function of an ideal Michelson interferometer.

```
nu_,trans_,i1,i2,slit = convolveSpectrum(nu,transm,SlitFunction=SLIT_MICHELSON,
                                         Resolution=1.0,AF_wing=20.0)
plot(nu,transm,'red',nu_,trans_,'blue');
legend(['HI-RES','Michelson']);
show()
```



VI. KEY FUNCTIONS: EXAMPLES

6.1. Help system

HAPI has an interactive help system which is provided by the function getHelp().

To get an access to it, run getHelp() in your console and it will give options which you can provide to getHelp() as in input:

```
getHelp()
```

For example, getHelp(tutorials) provides tutorials on data filtering, spectra calculation, Python language etc…

```
getHelp(tutorials)
```

Calling getHelp(name_of_the_function) gives separate help on each principal function of HAPI:

```
getHelp(PROFILE_HT)
```

The next sub-sections contain document strings for each principal function of HAPI.

6.2. Fetching data

```
fetch(TableName, M, I, numin, numax)
    INPUT PARAMETERS:
        TableName:   local table name to fetch in (required)
        M:           HITRAN molecule number       (required)
        I:           HITRAN isotopologue number   (required)
        numin:       lower wavenumber bound       (required)
        numax:       upper wavenumber bound       (required)
    OUTPUT PARAMETERS:
        none
    ---
    DESCRIPTION:
        Download line-by-line data from HITRANonline server
        and save it to local table.  The input parameters M and I
        are the HITRAN molecule and isotopologue numbers.
        This function results in a table containing single
        isotopologue specie.  To have multiple species in a
```

```
        single table use fetch_by_ids instead.
    ---
    EXAMPLE OF USAGE:
        fetch('HOH',1,1,4000,4100)
    ---
```

```
fetch_by_ids(TableName, iso_id_list, numin, numax)
    INPUT PARAMETERS:
        TableName:   local table name to fetch in (required)
        iso_id_list: list of isotopologue id's    (required)
        numin:       lower wavenumber bound       (required)
        numax:       upper wavenumber bound       (required)
    OUTPUT PARAMETERS:
        none
    ---
    DESCRIPTION:
        Download line-by-line data from HITRANonline server
        and save it to local table.  The input parameter iso_id_list
        contains list of "global" isotopologue Ids (see help on ISO_ID).
        Note: this function is required if user wants to download
        multiple species into single table.
    ---
    EXAMPLE OF USAGE:
        fetch_by_ids('water',[1,2,3,4],4000,4100)
```

6.3. Working with data

```
db_begin(db=None)
    INPUT PARAMETERS:
        db: database name (optional)
    OUTPUT PARAMETERS:
        none
    ---
    DESCRIPTION:
        Open a database connection.  A database is stored
        in a folder given in db input parameter.
        Default=data
    ---
    EXAMPLE OF USAGE:
        db_begin('bar')
    ---
```

```
db_commit()
    INPUT PARAMETERS:
        none
    OUTPUT PARAMETERS:
        none
```

```
    ---
    DESCRIPTION:
        Commit all changes made to opened database.
        All tables will be saved in corresponding files.
    ---
    EXAMPLE OF USAGE:
        db_commit()
    ---
```

```
tableList()
    INPUT PARAMETERS:
        none
    OUTPUT PARAMETERS:
        TableList: a list of available tables
    ---
    DESCRIPTION:
        Return a list of tables present in database.
    ---
    EXAMPLE OF USAGE:
        lst = tableList()
    ---
```

```
describeTable(TableName)
    INPUT PARAMETERS:
        TableName: name of the table to describe
    OUTPUT PARAMETERS:
        none
    ---
    DESCRIPTION:
        Print information about table, including
        parameter names, formats and wavenumber range.
    ---
    EXAMPLE OF USAGE:
        describe('sampletab')
    ---
```

```
select(TableName, DestinationTableName='__BUFFER__', ParameterNames=None, Conditions=None,
Output=True, File=None)
    INPUT PARAMETERS:
        TableName:            name of source table              (required)
        DestinationTableName: name of resulting table           (optional)
        ParameterNames:       list of parameters or expressions (optional)
        Conditions:           list of logical expressions       (optional)
        Output:   enable (True) or suppress (False) text output (optional)
        File:     enable (True) or suppress (False) file output (optional)
    OUTPUT PARAMETERS:
        none
    ---
    DESCRIPTION:
        Select or filter the data in some table
        either to standard output or to file (if specified)
    ---
    EXAMPLE OF USAGE:
        select('sampletab',DestinationTableName='outtab',ParameterNames=(p1,p2),
```

```
                Conditions=(('and',('>=','p1',1),('<',('*','p1','p2'),20))))
        Conditions means (p1>=1 and p1*p2<20)
    ---
```

```
sort(TableName, DestinationTableName=None, ParameterNames=None, Accending=True,
Output=False, File=None)
    INPUT PARAMETERS:
        TableName:                name of source table          (required)
        DestinationTableName:     name of resulting table       (optional)
        ParameterNames:       list of parameters or expressions to sort by    (optional)
        Accending:       sort in ascending (True) or descending (False) order (optional)
        Output:   enable (True) or suppress (False) text output (optional)
        File:     enable (True) or suppress (False) file output (optional)
    OUTPUT PARAMETERS:
        none
    ---
    DESCRIPTION:
        Sort a table by a list of its parameters or expressions.
        The sorted table is saved in DestinationTableName (if specified).
    ---
    EXAMPLE OF USAGE:
        sort('sampletab',ParameterNames=(p1,('+','p1','p2')))
    ---
```

```
group(TableName, DestinationTableName='__BUFFER__', ParameterNames=None,
GroupParameterNames=None, Output=True)
    INPUT PARAMETERS:
        TableName:                name of source table          (required)
        DestinationTableName:     name of resulting table       (optional)
        ParameterNames:       list of parameters or expressions to take       (optional)
        GroupParameterNames:  list of parameters or expressions to group by   (optional)
        Accending:       sort in ascending (True) or descending (False) order (optional)
        Output:   enable (True) or suppress (False) text output (optional)
    OUTPUT PARAMETERS:
        none
    ---
    DESCRIPTION:
        none
    ---
    EXAMPLE OF USAGE:
        group('sampletab',ParameterNames=('p1',('sum','p2')),GroupParameterNames=('p1'))
        ... makes grouping by p1,p2.  For each group it calculates sum of p2 values.
    ---
```

```
extractColumns(TableName, SourceParameterName, ParameterFormats, ParameterNames=None,
FixCol=False)
    INPUT PARAMETERS:
        TableName:             name of source table              (required)
        SourceParameterName:   name of source column to process  (required)
        ParameterFormats:      c formats of unpacked parameters  (required)
        ParameterNames:        list of resulting parameter names (optional)
        FixCol:      column-fixed (True) format of source column (optional)
    OUTPUT PARAMETERS:
        none
```

```
    ---
    DESCRIPTION:
        Note, that this function is aimed to do some extra job on
        interpreting string parameters which is normally supposed
        to be done by the user.
    ---
    EXAMPLE OF USAGE:
        extractColumns('sampletab',SourceParameterName='p5',
                       ParameterFormats=('%d','%d','%d'),
                       ParameterNames=('p5_1','p5_2','p5_3'))
        This example extracts three integer parameters from
        a source column 'p5' and puts results in ('p5_1','p5_2','p5_3').
    ---
```

```
getColumn(TableName, ParameterName)
    INPUT PARAMETERS:
        TableName:      source table name     (required)
        ParameterName:  name of column to get (required)
    OUTPUT PARAMETERS:
        ColumnData:     list of values from specified column
    ---
    DESCRIPTION:
        Returns a column with a name ParameterName from
        table TableName. Column is returned as a list of values.
    ---
    EXAMPLE OF USAGE:
        p1 = getColumn('sampletab','p1')
    ---
```

```
getColumns(TableName, ParameterNames)
    INPUT PARAMETERS:
        TableName:       source table name           (required)
        ParameterNames:  list of column names to get (required)
    OUTPUT PARAMETERS:
        ListColumnData:   tuple of lists of values from specified column
    ---
    DESCRIPTION:
        Returns columns with a name in ParameterNames from
        table TableName.  Columns are returned as a tuple of lists.
    ---
    EXAMPLE OF USAGE:
        p1,p2,p3 = getColumns('sampletab',('p1','p2','p3'))
    ---
```

```
dropTable(TableName)
    INPUT PARAMETERS:
        TableName:  name of the table to delete
    OUTPUT PARAMETERS:
        none
    ---
    DESCRIPTION:
        Deletes a table from local database.
    ---
    EXAMPLE OF USAGE:
```

```
        dropTable('some_dummy_table')
    ---
```

6.4. Calculating spectra

LINE PROFILES:

```
Profiles available:
  HT      : PROFILE_HT
  Voigt   : PROFILE_VOIGT
  Lorentz : PROFILE_LORENTZ
  Doppler : PROFILE_DOPPLER
```

```
PROFILE_HT(sg0, GamD, Gam0, Gam2, Shift0, Shift2, anuVC, eta, sg)
     ----------------------------------------------------------------------------
           "pCqSDHC": partially-Correlated quadratic-Speed-Dependent Hard-Collision
           Subroutine to Compute the complex normalized spectral shape of an
           isolated line by the pCqSDHC model

           References:

           1) N.H. Ngo, D. Lisak, H. Tran, J.-M. Hartmann.
              An isolated line-shape model to go beyond the Voigt profile in
              spectroscopic databases and radiative-transfer codes.
              JQSRT, Volume 129, November 2013, Pages 89-100
              http://dx.doi.org/10.1016/j.jqsrt.2013.05.034

           2) H. Tran, N.H. Ngo, J.-M. Hartmann.
              Efficient computation of some speed-dependent isolated line profiles.
              JQSRT, Volume 129, November 2013, Pages 199-203
              http://dx.doi.org/10.1016/j.jqsrt.2013.06.015

           3) H. Tran, N.H. Ngo, J.-M. Hartmann.
              Erratum to “Efficient computation of some speed-dependent isolated line
              profiles”.
              JQSRT, Volume 134, February 2014, Pages 104
              http://dx.doi.org/10.1016/j.jqsrt.2013.10.015

           Input/Output Parameters of Routine (Arguments or Common)
           --------------------------------
           T       : Temperature in Kelvin (Input).
           amM1    : Molar mass of the absorber in g/mol (Input).
           sg0     : Unperturbed line position in cm-1 (Input).
           GamD    : Doppler HWHM in cm-1 (Input)
           Gam0    : Speed-averaged line-width in cm-1 (Input).
           Gam2    : Speed dependence of the line-width in cm-1 (Input).
           anuVC   : Velocity-changing frequency in cm-1 (Input).
           eta     : Correlation parameter, No unit (Input).
           Shift0  : Speed-averaged line-shift in cm-1 (Input).
           Shift2  : Speed dependence of the line-shift in cm-1 (Input)
```

```
          sg      : Current WaveNumber of the Computation in cm-1 (Input).

          The function has two outputs:
          -----------------
          (1): Real part of the normalized spectral shape (cm)
          (2): Imaginary part of the normalized spectral shape (cm)

          Called Routines: 'CPF'       (Complex Probability Function)
          ---------------  'CPF3'      (Complex Probability Function for the region 3)

          Based on a double precision Fortran version
```

```
PROFILE_VOIGT(sg0, GamD, Gam0, sg)
     Voigt profile based on HTP.
     Input parameters:
       sg0: Unperturbed line position in cm-1 (Input).
       GamD: Doppler HWHM in cm-1 (Input)
       Gam0: Speed-averaged line-width in cm-1 (Input).
       sg: Current WaveNumber of the Computation in cm-1 (Input).
```

```
PROFILE_LORENTZ(sg0, Gam0, sg)
     Lorentz profile.
     Input parameters:
       sg0: Unperturbed line position in cm-1 (Input).
       Gam0: Speed-averaged line-width in cm-1 (Input).
       sg: Current WaveNumber of the Computation in cm-1 (Input).
```

```
PROFILE_DOPPLER(sg0, GamD, sg)
     Doppler profile.
     Input parameters:
       sg0: Unperturbed line position in cm-1 (Input).
       GamD: Doppler HWHM in cm-1 (Input)
       sg: Current WaveNumber of the Computation in cm-1 (Input).
```

PARTITION SUM:

```
partitionSum(M, I, T, step=None)
    INPUT PARAMETERS:
        M: HITRAN molecule number              (required)
        I: HITRAN isotopologue number          (required)
        T: temperature conditions              (required)
        step:  step to calculate temperatures  (optional)
    OUTPUT PARAMETERS:
        TT: list of temperatures (present only if T is a list)
        PartSum: partition sums calculated on a list of temperatures
    ---
    DESCRIPTION:
        Calculate a range of partition sums at different temperatures.
        This function uses a python implementation of TIPS-2011 code:
```

```
    Reference:
        A. L. Laraia, R. R. Gamache, J. Lamouroux, I. E. Gordon, L. S. Rothman.
        Total internal partition sums to support planetary remote sensing.
        Icarus, Volume 215, Issue 1, September 2011, Pages 391-400
        http://dx.doi.org/10.1016/j.icarus.2011.06.004

    Output depends on a structure of input parameter T so that:
        1) If T is a scalar/list and step IS NOT provided,
            then calculate partition sums over each value of T.
        2) If T is a list and step parameter IS provided,
            then calculate partition sums between T[0] and T[1]
            with a given step.
---
EXAMPLE OF USAGE:
    PartSum = partitionSum(1,1,[296,1000])
    TT,PartSum = partitionSum(1,1,[296,1000],step=0.1)
---
```

ABSORPTION COEFFICIENTS:

```
absorptionCoefficient_HT(Components=None, SourceTables=None, partitionFunction=<function
<lambda>>, Environment=None, OmegaRange=None, OmegaStep=None, OmegaWing=None,
IntensityThreshold=0.0, OmegaWingHW=50.0, ParameterBindings={},
EnvironmentDependencyBindings={}, GammaL='gamma_air', HITRAN_units=True, File=None,
Format='%e %e')
    INPUT PARAMETERS:
        Components:  list of tuples [(M,I,D)], where
                       M - HITRAN molecule number,
                       I - HITRAN isotopologue number,
                       D - abundance (optional)
        SourceTables:  list of tables from which to calculate cross-section   (optional)
        partitionFunction:  pointer to partition function (default is PYTIPS) (optional)
        Environment:  dictionary containing thermodynamic parameters.
                       'p' - pressure in atmospheres,
                       'T' - temperature in Kelvin
                       Default={'p':1.,'T':296.}
        OmegaRange:  wavenumber range to consider.
        OmegaStep:   wavenumber step to consider.
        OmegaWing:   absolute wing for calculating a lineshape (in cm-1)
        IntensityThreshold:  threshold for intensities
        OmegaWingHW:  relative wing for calculating a lineshape (in halfwidths)
        GammaL:  specifies broadening parameter ('gamma_air' or 'gamma_self')
        HITRAN_units:  use cm2/molecule (True) or cm-1 (False) for absorption coefficient
        File:   write output to file (if specified)
        Format:  c format of file output ('%e %e' by default)
    OUTPUT PARAMETERS:
        Omegas: wavenumber grid with respect to parameters OmegaRange and OmegaStep
        Xsect: absorption coefficient calculated on the grid.
               Units are switched by HITRAN_units
    ---
    DESCRIPTION:
        Calculate absorption coefficient using HT (Hartmann-Tran) profile.
        Absorption coefficient is calculated at arbitrary temperature and pressure.
        User can vary a wide range of parameters to control a process of calculation
        (such as OmegaRange, OmegaStep, OmegaWing, OmegaWingHW, IntensityThreshold).
        The choice of these parameters depends on properties of a particular linelist.
        Default values are a sort of guess which gives a decent precision (on average)
        for a reasonable amount of cpu time.  To increase calculation accuracy,
```

```
    user should use a trial and error method.
---
EXAMPLE OF USAGE:
    nu,coef = absorptionCoefficient_HT(((2,1),),'co2',OmegaStep=0.01,
                                       HITRAN_units=False,GammaL='gamma_self')
---
```

```
absorptionCoefficient_Voigt(Components=None, SourceTables=None, partitionFunction=<function
<lambda>>, Environment=None, OmegaRange=None, OmegaStep=None, OmegaWing=None,
IntensityThreshold=0.0, OmegaWingHW=50.0, ParameterBindings={},
EnvironmentDependencyBindings={}, GammaL='gamma_air', HITRAN_units=True, File=None,
Format='%e %e')
    INPUT PARAMETERS:
        Components:  list of tuples [(M,I,D)], where
                       M - HITRAN molecule number,
                       I - HITRAN isotopologue number,
                       D - abundance (optional)
        SourceTables:  list of tables from which to calculate cross-section   (optional)
        partitionFunction:  pointer to partition function (default is PYTIPS) (optional)
        Environment:  dictionary containing thermodynamic parameters.
                       'p' - pressure in atmospheres,
                       'T' - temperature in Kelvin
                       Default={'p':1.,'T':296.}
        OmegaRange:  wavenumber range to consider.
        OmegaStep:   wavenumber step to consider.
        OmegaWing:   absolute wing for calculating a lineshape (in cm-1)
        IntensityThreshold:  threshold for intencities
        OmegaWingHW:  relative wing for calculating a lineshape (in halfwidths)
        GammaL:  specifies broadening parameter ('gamma_air' or 'gamma_self')
        HITRAN_units:  use cm2/molecule (True) or cm-1 (False) for absorption coefficient
        File:   write output to file (if specified)
        Format:  c format of file output ('%e %e' by default)
    OUTPUT PARAMETERS:
        Omegas: wavenumber grid with respect to parameters OmegaRange and OmegaStep
        Xsect: absorption coefficient calculated on the grid
    ---
    DESCRIPTION:
        Calculate absorption coefficient using Voigt profile.
        Absorption coefficient is calculated at arbitrary temperature and pressure.
        User can vary a wide range of parameters to control a process of calculation
        (such as OmegaRange, OmegaStep, OmegaWing, OmegaWingHW, IntensityThreshold).
        The choice of these parameters depends on properties of a particular linelist.
        Default values are a sort of guess which gives a decent precision (on average)
        for a reasonable amount of cpu time.  To increase calculation accuracy,
        user should use a trial and error method.
    ---
    EXAMPLE OF USAGE:
        nu,coef = absorptionCoefficient_Voigt(((2,1),),'co2',OmegaStep=0.01,
                                              HITRAN_units=False,GammaL='gamma_self')
    ---
```

```
absorptionCoefficient_Lorentz(Components=None, SourceTables=None,
partitionFunction=<function <lambda>>, Environment=None, OmegaRange=None, OmegaStep=None,
OmegaWing=None, IntensityThreshold=0.0, OmegaWingHW=50.0, ParameterBindings={},
EnvironmentDependencyBindings={}, GammaL='gamma_air', HITRAN_units=True, File=None,
Format='%e %e')
    INPUT PARAMETERS:
        Components:  list of tuples [(M,I,D)], where
```

```
                    M - HITRAN molecule number,
                    I - HITRAN isotopologue number,
                    D - abundance (optional)
    SourceTables:  list of tables from which to calculate cross-section   (optional)
    partitionFunction:  pointer to partition function (default is PYTIPS) (optional)
    Environment:  dictionary containing thermodynamic parameters.
                    'p' - pressure in atmospheres,
                    'T' - temperature in Kelvin
                    Default={'p':1.,'T':296.}
    OmegaRange:  wavenumber range to consider.
    OmegaStep:   wavenumber step to consider.
    OmegaWing:   absolute wing for calculating a lineshape (in cm-1)
    IntensityThreshold:  threshold for intensities
    OmegaWingHW:  relative wing for calculating a lineshape (in halfwidths)
    GammaL:  specifies broadening parameter ('gamma_air' or 'gamma_self')
    HITRAN_units:  use cm2/molecule (True) or cm-1 (False) for absorption coefficient
    File:   write output to file (if specified)
    Format:  c format of file output ('%e %e' by default)
OUTPUT PARAMETERS:
    Omegas: wavenumber grid with respect to parameters OmegaRange and OmegaStep
    Xsect: absorption coefficient calculated on the grid
---
DESCRIPTION:
    Calculate absorption coefficient using Lorentz profile.
    Absorption coefficient is calculated at arbitrary temperature and pressure.
    User can vary a wide range of parameters to control a process of calculation
    (such as OmegaRange, OmegaStep, OmegaWing, OmegaWingHW, IntensityThreshold).
    The choice of these parameters depends on properties of a particular linelist.
    Default values are a sort of guess which gives a decent precision (on average)
    for a reasonable amount of cpu time.  To increase calculation accuracy,
    user should use a trial and error method.
---
EXAMPLE OF USAGE:
    nu,coef = absorptionCoefficient_Lorentz(((2,1),),'co2',OmegaStep=0.01,
                                            HITRAN_units=False,GammaL='gamma_self')
---
```

```
absorptionCoefficient_Doppler(Components=None, SourceTables=None,
partitionFunction=<function <lambda>>, Environment=None, OmegaRange=None, OmegaStep=None,
OmegaWing=None, IntensityThreshold=0.0, OmegaWingHW=50.0, ParameterBindings={},
EnvironmentDependencyBindings={}, GammaL='dummy', HITRAN_units=True, File=None, Format='%e
%e')
    INPUT PARAMETERS:
        Components:  list of tuples [(M,I,D)], where
                        M - HITRAN molecule number,
                        I - HITRAN isotopologue number,
                        D - abundance (optional)
        SourceTables:  list of tables from which to calculate cross-section   (optional)
        partitionFunction:  pointer to partition function (default is PYTIPS) (optional)
        Environment:  dictionary containing thermodynamic parameters.
                        'p' - pressure in atmospheres,
                        'T' - temperature in Kelvin
                        Default={'p':1.,'T':296.}
        OmegaRange:  wavenumber range to consider.
        OmegaStep:   wavenumber step to consider.
        OmegaWing:   absolute wing for calculating a lineshape (in cm-1)
        IntensityThreshold:  threshold for intensities
        OmegaWingHW:  relative wing for calculating a lineshape (in halfwidths)
        GammaL:  specifies broadening parameter ('gamma_air' or 'gamma_self')
        HITRAN_units:  use cm2/molecule (True) or cm-1 (False) for absorption coefficient
        File:   write output to file (if specified)
        Format:  c format of file output ('%e %e' by default)
```

```
    OUTPUT PARAMETERS:
        Omegas: wavenumber grid with respect to parameters OmegaRange and OmegaStep
        Xsect: absorption coefficient calculated on the grid
    ---
    DESCRIPTION:
        Calculate absorption coefficient using Doppler (Gauss) profile.
        Absorption coefficient is calculated at arbitrary temperature and pressure.
        User can vary a wide range of parameters to control a process of calculation
        (such as OmegaRange, OmegaStep, OmegaWing, OmegaWingHW, IntensityThreshold).
        The choice of these parameters depends on properties of a particular linelist.
        Default values are a sort of guess which gives a decent precision (on average)
        for a reasonable amount of cpu time.  To increase calculation accuracy,
        user should use a trial and error method.
    ---
    EXAMPLE OF USAGE:
        nu,coef = absorptionCoefficient_Doppler(((2,1),),'co2',OmegaStep=0.01,
                                                HITRAN_units=False,GammaL='gamma_self')
    ---
```

TRANSMITTANCE SPECTRUM

```
transmittanceSpectrum(Omegas, AbsorptionCoefficient, Environment={'l': 100.0}, File=None,
Format='%e %e')
    INPUT PARAMETERS:
        Omegas:       wavenumber grid                          (required)
        AbsorptionCoefficient:  absorption coefficient on grid  (required)
        Environment:  dictionary containing path length in cm.
                      Default={'l':100.}
        File:         name of the output file                 (optional)
        Format: c format used in file output, default '%e %e' (optional)
    OUTPUT PARAMETERS:
        Omegas: wavenumber grid
        Xsect:  transmittance spectrum calculated on the grid
    ---
    DESCRIPTION:
        Calculate a transmittance spectrum (dimensionless) based
        on previously calculated absorption coefficient.
        Transmittance spectrum is calculated at an arbitrary
        optical path length 'l' (1 m by default)
    ---
    EXAMPLE OF USAGE:
        nu,trans = transmittanceSpectrum(nu,coef)
    ---
```

ABSORPTION SPECTRUM

```
absorptionSpectrum(Omegas, AbsorptionCoefficient, Environment={'l': 100.0}, File=None,
Format='%e %e')
    INPUT PARAMETERS:
        Omegas:       wavenumber grid                          (required)
        AbsorptionCoefficient:  absorption coefficient on grid  (required)
        Environment:  dictionary containing path length in cm.
                      Default={'l':100.}
        File:         name of the output file                 (optional)
        Format: c format used in file output, default '%e %e' (optional)
    OUTPUT PARAMETERS:
```

```
        Omegas: wavenumber grid
        Xsect:  transmittance spectrum calculated on the grid
    ---
    DESCRIPTION:
        Calculate an absorption spectrum (dimensionless) based
        on previously calculated absorption coefficient.
        Absorption spectrum is calculated at an arbitrary
        optical path length 'l' (1 m by default)
    ---
    EXAMPLE OF USAGE:
        nu,absorp = absorptionSpectrum(nu,coef)
    ---
```

RADIANCE SPECTRUM

```
radianceSpectrum(Omegas, AbsorptionCoefficient, Environment={'T': 296.0, 'l': 100.0},
File=None, Format='%e %e')
    INPUT PARAMETERS:
        Omegas:       wavenumber grid                          (required)
        AbsorptionCoefficient:  absorption coefficient on grid (required)
        Environment:  dictionary containing path length in cm.
                      and temperature in Kelvin.
                      Default={'l':100.,'T':296.}
        File:         name of the output file                  (optional)
        Format: c format used in file output, default '%e %e' (optional)
    OUTPUT PARAMETERS:
        Omegas: wavenumber grid
        Xsect:  radiance spectrum calculated on the grid
    ---
    DESCRIPTION:
        Calculate a radiance spectrum (in W/sr/cm^2/cm-1) based
        on previously calculated absorption coefficient.
        Radiance spectrum is calculated at an arbitrary
        optical path length 'l' (1 m by default) and
        temperature 'T' (296 K by default).  For obtaining a
        physically meaningful result 'T' must be the same
        as a temperature which was used in absorption coefficient.
    ---
    EXAMPLE OF USAGE:
        nu,radi = radianceSpectrum(nu,coef)
    ---
```

6.5. Convolving spectra

SLIT FUNCTIONS:

```
  RECTANGULAR : SLIT_RECTANGULAR

  TRIANGULAR  : SLIT_TRIANGULAR

  GAUSSIAN    : SLIT_GAUSSIAN
```

```
  DIFFRACTION : SLIT_DIFFRACTION
  MICHELSON   : SLIT_MICHELSON
  DISPERSION/LORENTZ : SLIT_DISPERSION
```

```
SLIT_RECTANGULAR(x, g)
    Instrumental (slit) function.
    B(x) = 1/γ , if |x| ≤ γ/2 & B(x) = 0, if |x| > γ/2,
    where γ is a slit width or the instrumental resolution.
```

```
SLIT_TRIANGULAR(x, g)
    Instrumental (slit) function.
    B(x) = 1/γ*(1-|x|/γ), if |x| ≤ γ & B(x) = 0, if |x| > γ,
    where γ is the line width equal to the half base of the triangle.
```

```
SLIT_GAUSSIAN(x, g)
    Instrumental (slit) function.
    B(x) = sqrt(ln(2)/pi)/γ*exp(-ln(2)*(x/γ)**2),
    where γ is a gaussian halfwidth within 3-sigma rule.
```

```
SLIT_DISPERSION(x, g)
    Instrumental (slit) function.
    B(x) = 1/pi * γ/2/(x**2 + (γ/2)**2),
    where γ is a halfwidth of a Lorentz profile.
```

```
SLIT_MICHELSON(x, g)
    Instrumental (slit) function.
    B(x) = 2/γ*sin(2pi*x/γ)/(2pi*x/γ) if x!=0 else 1,
    where 1/γ is the maximum optical path difference.
```

CONVOLVE SPECTRUM:

```
convolveSpectrum(Omega, CrossSection, Resolution=0.1, AF_wing=10.0, SlitFunction=<function
SLIT_RECTANGULAR>)
    INPUT PARAMETERS:
        Omega:         wavenumber grid                          (required)
        CrossSection:  high-res cross section calculated on grid (required)
        Resolution:    instrumental resolution γ                (optional)
        AF_wing:       instrumental function wing               (optional)
        SlitFunction:  instrumental function for low-res spectra calculation (optional)
    OUTPUT PARAMETERS:
        Omega: wavenumber grid
```

```
    CrossSection: low-res cross section calculated on grid
    i1: lower index in Omega input
    i2: higher index in Omega input
    slit: slit function calculated over grid [-AF_wing; AF_wing]
            with the step equal to instrumental resolution.
---
DESCRIPTION:
    Produce a simulation of experimental spectrum via the convolution
    of a "dry" spectrum with an instrumental function.
    Instrumental function is provided as a parameter and
    is calculated in a grid with the width=AF_wing and step=Resolution.
---
EXAMPLE OF USAGE:
    nu_,radi_,i,j,slit = convolveSpectrum(nu,radi,Resolution=2.0,AF_wing=10.0,
                                          SlitFunction=SLIT_MICHELSON)
---
```

6.6. Information on isotopologues

ISO_ID:

id		M	I	iso_name	abundance	mass	mol_name
1	:	1	1	H2(16O)	0.9973170000	18.010565	H2O
2	:	1	2	H2(18O)	0.0019998300	20.014811	H2O
3	:	1	3	H2(17O)	0.0003720000	19.014780	H2O
4	:	1	4	HD(16O)	0.0003106900	19.016740	H2O
5	:	1	5	HD(18O)	0.0000006230	21.020985	H2O
6	:	1	6	HD(17O)	0.0000001160	20.020956	H2O
7	:	2	1	(12C)(16O)2	0.9842000000	43.989830	CO2
8	:	2	2	(13C)(16O)2	0.0110600000	44.993185	CO2
9	:	2	3	(16O)(12C)(18O)	0.0039471000	45.994076	CO2
10	:	2	4	(16O)(12C)(17O)	0.0007340000	44.994045	CO2
11	:	2	5	(16O)(13C)(18O)	0.0000443400	46.997431	CO2
12	:	2	6	(16O)(13C)(17O)	0.0000082500	45.997400	CO2
13	:	2	7	(12C)(18O)2	0.0000039573	47.998322	CO2
14	:	2	8	(17O)(12C)(18O)	0.0000014700	46.998291	CO2
15	:	2	0	(13C)(18O)2	0.0000000450	49.001675	CO2
16	:	3	1	(16O)3	0.9929010000	47.984745	O3
17	:	3	2	(16O)(16O)(18O)	0.0039819400	49.988991	O3
18	:	3	3	(16O)(18O)(16O)	0.0019909700	49.988991	O3
19	:	3	4	(16O)(16O)(17O)	0.0007400000	48.988960	O3
20	:	3	5	(16O)(17O)(16O)	0.0003700000	48.988960	O3
21	:	4	1	(14N)2(16O)	0.9903330000	44.001062	N2O
22	:	4	2	(14N)(15N)(16O)	0.0036409000	44.998096	N2O
23	:	4	3	(15N)(14N)(16O)	0.0036409000	44.998096	N2O
24	:	4	4	(14N)2(18O)	0.0019858200	46.005308	N2O
25	:	4	5	(14N)2(17O)	0.0003690000	45.005278	N2O
26	:	5	1	(12C)(16O)	0.9865400000	27.994915	CO
27	:	5	2	(13C)(16O)	0.0110800000	28.998270	CO
28	:	5	3	(12C)(18O)	0.0019782000	29.999161	CO
29	:	5	4	(12C)(17O)	0.0003680000	28.999130	CO
30	:	5	5	(13C)(18O)	0.0000222200	31.002516	CO
31	:	5	6	(13C)(17O)	0.0000041300	30.002485	CO
32	:	6	1	(12C)H4	0.9882700000	16.031300	CH4
33	:	6	2	(13C)H4	0.0111000000	17.034655	CH4
34	:	6	3	(12C)H3D	0.0006157500	17.037475	CH4
35	:	6	4	(13C)H3D	0.0000049203	18.040830	CH4
36	:	7	1	(16O)2	0.9952620000	31.989830	O2
37	:	7	2	(16O)(18O)	0.0039914100	33.994076	O2
38	:	7	3	(16O)(17O)	0.0007420000	32.994045	O2
39	:	8	1	(14N)(16O)	0.9939740000	29.997989	NO

40	:	8	2	(15N)(16O)	0.0036543000	30.995023	NO
41	:	8	3	(14N)(18O)	0.0019931200	32.002234	NO
42	:	9	1	(32S)(16O)2	0.9456800000	63.961901	SO2
43	:	9	2	(34S)(16O)2	0.0419500000	65.957695	SO2
44	:	10	1	(14N)(16O)2	0.9916160000	45.992904	NO2
45	:	11	1	(14N)H3	0.9958715000	17.026549	NH3
46	:	11	2	(15N)H3	0.0036613000	18.023583	NH3
47	:	12	1	H(14N)(16O)3	0.9891100000	62.995644	HNO3
48	:	13	1	(16O)H	0.9974730000	17.002740	OH
49	:	13	2	(18O)H	0.0020001400	19.006986	OH
50	:	13	3	(16O)D	0.0001553700	18.008915	OH
51	:	14	1	H(19F)	0.9998442500	20.006229	HF
52	:	15	1	H(35Cl)	0.7575870000	35.976678	HCl
53	:	15	2	H(37Cl)	0.2422570000	37.973729	HCl
54	:	16	1	H(79Br)	0.5067800000	79.926160	HBr
55	:	16	2	H(81Br)	0.4930600000	81.924115	HBr
56	:	17	1	H(127I)	0.9998442500	127.912297	HI
57	:	18	1	(35Cl)(16O)	0.7559100000	50.963768	ClO
58	:	18	2	(37Cl)(16O)	0.2417200000	52.960819	ClO
59	:	19	1	(16O)(12C)(32S)	0.9373900000	59.966986	OCS
60	:	19	2	(16O)(12C)(34S)	0.0415800000	61.962780	OCS
61	:	19	3	(16O)(13C)(32S)	0.0105300000	60.970341	OCS
62	:	19	4	(16O)(12C)(33S)	0.0105300000	60.966371	OCS
63	:	19	5	(18O)(12C)(32S)	0.0018800000	61.971231	OCS
64	:	20	1	H2(12C)(16O)	0.9862400000	30.010565	H2CO
65	:	20	2	H2(13C)(16O)	0.0110800000	31.013920	H2CO
66	:	20	3	H2(12C)(18O)	0.0019776000	32.014811	H2CO
67	:	21	1	H(16O)(35Cl)	0.7557900000	51.971593	HOCl
68	:	21	2	H(16O)(37Cl)	0.2416800000	53.968644	HOCl
69	:	22	1	(14N)2	0.9926874000	28.006147	N2
70	:	23	1	H(12C)(14N)	0.9851100000	27.010899	HCN
71	:	23	2	H(13C)(14N)	0.0110700000	28.014254	HCN
72	:	23	3	H(12C)(15N)	0.0036217000	28.007933	HCN
73	:	24	1	(12C)H3(35Cl)	0.7489400000	49.992328	CH3Cl
74	:	24	2	(12C)H3(37Cl)	0.2394900000	51.989379	CH3Cl
75	:	25	1	H2(16O)2	0.9949520000	34.005480	H2O2
76	:	26	1	(12C)2H2	0.9776000000	26.015650	C2H2
77	:	26	2	(12C)(13C)H2	0.0219700000	27.019005	C2H2
78	:	27	1	(12C)2H6	0.9769900000	30.046950	C2H6
79	:	28	1	(31P)H3	0.9995328300	33.997238	PH3
80	:	29	1	(12C)(16O)(19F)2	0.9865400000	65.991722	COF2
81	:	31	1	H2(32S)	0.9498800000	33.987721	H2S
82	:	31	2	H2(34S)	0.0421400000	35.983515	H2S
83	:	31	3	H2(33S)	0.0074980000	34.987105	H2S
84	:	32	1	H(12C)(16O)(16O)H	0.9838980000	46.005480	HCOOH
85	:	33	1	H(16O)2	0.9951070000	32.997655	HO2
86	:	34	1	(16O)	0.9976280000	15.994915	O
87	:	36	1	(14N)(16O)+	0.9939740000	29.997989	NOp
88	:	37	1	H(16O)(79Br)	0.5056000000	95.921076	HOBr
89	:	37	2	H(16O)(81Br)	0.4919000000	97.919027	HOBr
90	:	38	1	(12C)2H4	0.9773000000	28.031300	C2H4
91	:	38	2	(12C)H2(13C)H2	0.0219600000	29.034655	C2H4
92	:	39	1	(12C)H3(16O)H	0.9859300000	32.026215	CH3OH
93	:	40	1	(12C)H3(79Br)	0.5013000000	93.941811	CH3Br
94	:	40	2	(12C)H3(81Br)	0.4876600000	95.939764	CH3Br
95	:	41	1	(12C)H3(12C)(14N)	0.9748200000	41.026549	CH3CN
96	:	42	1	(12C)(19F)4	0.9893000000	87.993616	CF4
97	:	46	1	(12C)(32S)	0.9396240000	43.971036	CS
98	:	46	2	(12C)(34S)	0.0416817000	45.966787	CS
99	:	46	3	(13C)(32S)	0.0105565000	44.974368	CS
100	:	46	4	(12C)(33S)	0.0074166800	44.970399	CS
101	:	1001	1	H	-1.0000000000	-1.000000	H
102	:	1002	1	He	-1.0000000000	-1.000000	He
103	:	45	1	H2	0.9996880000	2.015650	H2
104	:	1018	1	Ar	-1.0000000000	-1.000000	Ar
105	:	26	3	(12C)2HD	0.0003045500	27.021825	C2H2
106	:	27	2	(12C)H3(13C)H3	0.0219526110	31.050305	C2H6
107	:	15	3	D(35Cl)	0.0001180050	36.982954	HCl
108	:	15	4	D(37Cl)	0.0000377350	38.980004	HCl
109	:	44	1	H(12C)3(14N)	0.9646069000	51.010899	HC3N
110	:	14	2	D(19F)	0.0001150000	21.012505	HF
111	:	16	3	D(79Br)	0.0000582935	80.932439	HBr
112	:	16	4	D(81Br)	0.0000567065	82.930392	HBr
113	:	17	2	D(127I)	0.0001150000	128.918575	HI

```
  114     :     47    1                (32S)(16O)3    0.9423964000  79.956820            SO3
  115     :     45    2                        HD     0.0002299700   3.021825             H2
  116     :     43    1                   (12C)4H2    0.9559980000  50.015650           C4H2
  117     :     12    2               H(15N)(16O)3    0.0036360000  63.992680           HNO3
  118     :     22    2                 (14N)(15N)    0.0072535000  29.997989             N2
  119     :     29    2           (13C)(16O)(19F)2    0.0110834000  66.995083           COF2
  120     :      2   11            (18O)(13C)(17O)    0.0000000165  48.001650            CO2
  121     :      2    9                (12C)(17O)2    0.0000001368  45.998262            CO2
```

ABUNDANCE:

```
abundance(M, I)
    INPUT PARAMETERS:
        M: HITRAN molecule number
        I: HITRAN isotopologue number
    OUTPUT PARAMETERS:
        Abbundance: natural abundance
    ---
    DESCRIPTION:
        Return natural (Earth) abundance of HITRAN isotolopogue.
    ---
    EXAMPLE OF USAGE:
        ab = abundance(1,1) # H2O
    ---
```

MOLECULAR MASS:

```
molecularMass(M, I)
    INPUT PARAMETERS:
        M: HITRAN molecule number
        I: HITRAN isotopologue number
    OUTPUT PARAMETERS:
        MolMass: molecular mass
    ---
    DESCRIPTION:
        Return molecular mass of HITRAN isotolopogue.
    ---
    EXAMPLE OF USAGE:
        mass = molecularMass(1,1) # H2O
    ---
```

MOLECULE NAME:

```
moleculeName(M)
    INPUT PARAMETERS:
        M: HITRAN molecule number
    OUTPUT PARAMETERS:
        MolName: molecular name
    ---
    DESCRIPTION:
```

```
        Return name of HITRAN molecule.
    ---
    EXAMPLE OF USAGE:
        molname = moleculeName(1) # H2O
    ---
```

ISOTOPOLOGUE NAME:

```
isotopologueName(M, I)
    INPUT PARAMETERS:
        M: HITRAN molecule number
        I: HITRAN isotopologue number
    OUTPUT PARAMETERS:
        IsoMass: isotopologue mass
    ---
    DESCRIPTION:
        Return name of HITRAN isotolopogue.
    ---
    EXAMPLE OF USAGE:
        isoname = isotopologueName(1,1) # H2O
    ---
```

6.7. Miscellaneous

GET X AND Y FOR A STICK SPECTRUM:

```
getStickXY(TableName)
    Get X and Y for fine plotting of a stick spectrum.
    Usage: x,y = getStickXY(TableName); plot(x,y) # stick spectrum
```

```
COMPATIBILITY WITH HITRAN ON THE WEB (http://hitran.iao.ru)

read_hotw(filename)

    Read datafile fetched from HITRAN-on-the-Web.
```

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