

SFIT4 – Quickstart HOWTO

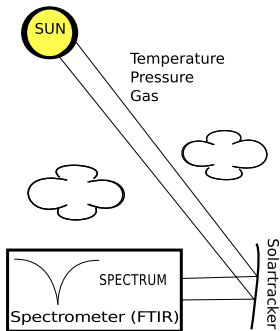
Mathias Palm

Bremen, 2020



Introduction

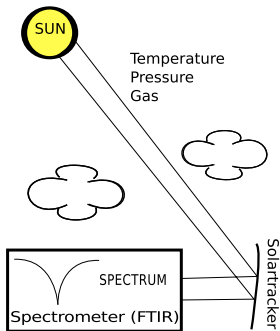
Absorption spectroscopy



Measurements in solar or lunar
absorption and emission
possible

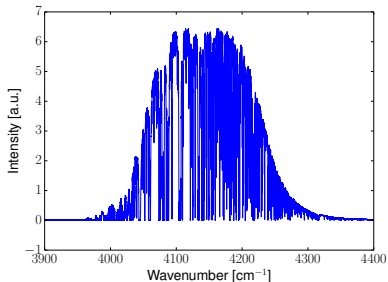
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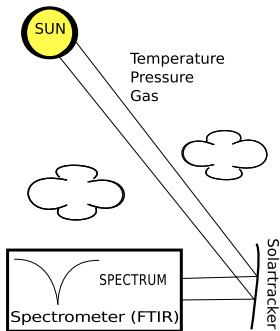
Received spectrum given by the sum of all absorption along the path of sight.



Envelope defined by band filter 3900 - 4400 cm^{-1}

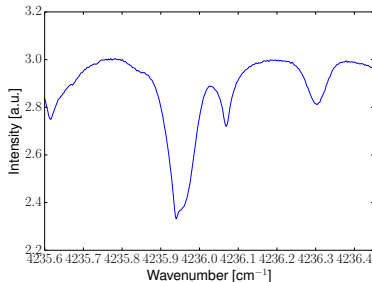
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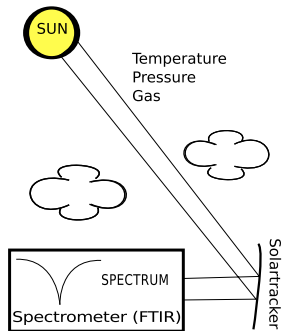
Received spectrum given by the sum of all absorption along the path of sight.



Microwindow containing a CO-line

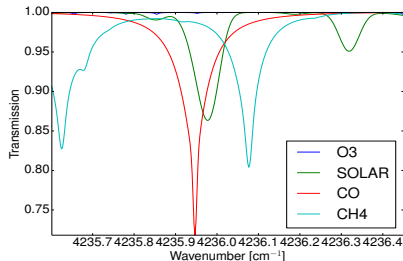
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Absorption spectroscopy



Measurements in solar or lunar absorption and emission possible

Received spectrum given by the sum of all absorption along the path of sight.

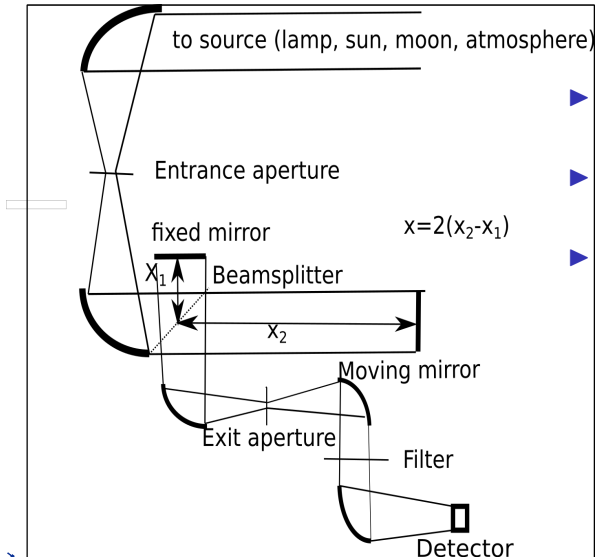


Contribution of gases and solar lines not calculated for this particular spectrum



Introduction

Principle of a Fourier transform spectrometer



- ▶ apertures define and restrict field of view
- ▶ aperture influences resolution
- ▶ filter restricts wavelength sensitivity

Contents

- ▶ Other documentation files and what they contain
- ▶ Files needed and where to get them
- ▶ How to modify `sfit4.cti`
- ▶ Create the spectral file `LLLLL.IIIII-HHHHH.hhhhhh.hbin`
- ▶ Run SFIT4



Contents

[sfit4_init/sfit4_init.pdf](#) The tentative description of the keys in the sfit4.ctl file and their interdependencies

[hbin/sfit4-hbin_ctl.docx](#) describes the structure of the hbin.ctl file (input file of hbin) to create the file
LLLLL.IIIII-HHHHH.hhhhhh.hbin

[Linelist/sfit4-isotope_descrip.docx](#) contains the structure of the file.in.isotope file

[Workshop2019-Palm-sfit4-fwdmodel-params.pdf](#) contains many descriptions of forward model parameters. Is referred to as FWDMODEL-PARAMS.



Files needed and where to get them

Files always necessary

The section file.in contains the names of the input files. The structure of the files is described on extra slides later on.

file.in.spectrum The measured spectrum. This file is created using pspec or any other tool. Is also needed for calculating a synthetic spectrum, because it defines the spectral grid, SFIT4 is working on.

file.in.stalayers The file containing the altitude bins for the forward model and the retrieval. This file defines the altitude grid which is used in SFIT4.

file.in.refprofile Contains the atmosphere and is created by the processing environment or elsewhere. The atmosphere used in SFIT4 is interpolated to the altitudes given in file.in.stalayers, i.e. its range has to be equal or larger

LLLLL.IIIII-HHHHH.hhhhhh.hbin Contains the spectral data and is created by hbin (part of the sfrit4 package, check sfrit4-hbin_ctl.docx)



Files needed and where to get them

Files needed for certain optional calculations

file.in.solarlines needed if `fw.solarspectrum = T`. Is a linelist of solar lines and part of the spectroscopy which comes with SFIT4

file.in.modulation_fcn needed if `fw.apod_fcn = T`. Parameters of the empirical apodisation function. See file FWDMODEL_PARAMS slide 3ff.

file.in.phase_fcn needed if `fw.phase_fcn = T`, Parameters of empirical phase function. See file FWDMODEL_PARAMS slide 3ff.

file.in.isotope needed if `fw.isotope_separation = T`. Contains definitions necessary for treating isotopes separately from the main isotope of the retrieved gas. Check the file `sfit4-isotope_descrip.docx` for its structure and contents. Files for the most common isotopes are part of the spectroscopy which comes with SFIT4.



Download and build SFIT4, HBIN and PSPEC

From <<https://wiki.ucar.edu/display/sfit4/>->SFIT 4 Version 1.0.+ (Pre) Release> download the following files:

[sfit4_v1.0.zip](#) contains the sfit4, hbin and pspec programs

[linelist-core-20200706.tar.gz](#) contains the linelist which are used with SFIT4

1. unpack both archives
2. in the directory sfit-core-code/src: type
make clean
make

SFIT4 has been tested with gfortran version 9.3.0. Most of the gfortran builds work, but we would recommend to use at least gfortran version 8.0.

3. go into directory sfit-core-code/sfit4_testbed, modify test.cfg and run
python2.7 script/run_testcases.py

If test.cfg is still filled in with the place-holders it will ask for the directories. Details are found in the README file.



Download and build SFIT4, HBIN and PSPEC (cont'd)

4. After it finishes it compares the results to the results stored in `sfitt4_testbed/results_v1.0` and prints out the differences if they are any. The differences should be small (fractions of a percent) if not, use another compiler.
5. in the `hbin.ctl` set the key `file.in.linelist` to your linelist directory.
6. run some or all of the testcases in `test_cases_NDACC`. It is better you start modifying testcases rather than building up a new one from scratch.



Getting help

1. make sure you have the latest SFIT4 version (check on <https://wiki.ucar.edu/display/sfit4/>)
2. Pack a full testcase, i.e.
 - 2.1 sfit4.ctf
 - 2.2 hbin.ctf
 - 2.3 all files the section file.in. point to
 - 2.4 sfit4.dtl if it exists.
 - 2.5 a screenshot of the output.
3. sent them to one or all people listed in the CONTACT section of <https://wiki.ucar.edu/display/sfit4/>.
4. We rely on bug reports to improve the program further. Many bugs tend to be subtle and turn up only in very special circumstances.

