	HIFI FM Gas-cell measurements	Hifi no.: SRON-G/HIFI/TR/2008-002 Inst.no.: n Issue: Draft 1.0 Date: :16-04-08 Category: 2.
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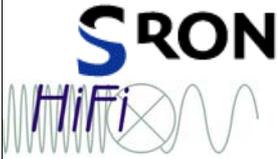
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0.Introduction

This document describes the test campaigns and associated results of the pre-launch calibration activity dedicated to gas-cell measurements with the HIFI Flight Model. This report provides a detailed overview of the measurement objectives, the strategy implemented, and of the data analysis and its inputs into the calibration equation.

0. References

a. Applicable Documents

AD1	SRON-G/HIFI/PL/1999-001	AIV plan for HIFI	Issue 1.0
AD2	LRM-ENS/HIFI/PL/2000-001	Calibration Plan for HIFI	Issue 1
AD3	SRON-G/HIFI/PL/2001-001	Detailed test plan of HIFI Instrument Tests	Draft 0.3
AD4	ICC/2001-005	HIFI calibration use cases	Draft 0.3

b. Reference Documents

RD1	SRON-U/HIFI/SP/2001-009	Test-equipment interface URD	Issue 1.1
RD2	Alma memo 442	The intensity calibration for HIFI	Issue 1.0
RD3	SRON-G/HIFI/TN/2004-xxx	Hot-Cold switch for HIFI AIV/ILT	Issue 0.1
RD4	IAS-LERMA/HIFI/AIV/2002-01	Technical report: realisation of a gas cell for tests of Herschel/HIFI	Issue 1.0
RD5	SRON-G/HIFI/ILT/2007-01200	HIFI System stability	Issue 1.0
RD6	SWAS/TM-4027	SWAS report on gas cell measurements	
RD7	IAS-LERMA/HIFI/TN/2006-01	HIFI Gas Cell Manual	Issue 0.2
RD8	SRON-G/HIFI/PR/2007-101	FM ILT Spurious Test Report	Issue 1.0

c. Information repository

The gas-cell working group has a wiki page gathering all the relevant information and some details that will not be repeated in this report. Please visit:

<http://www.sron.rug.nl/~wikiman/wikis/HifiIlt/GasCellTeamPages>

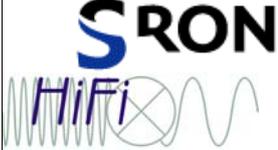
d. Acronyms

HK	HouseKeeping
IF	Intermediate Frequency
LO	Local Oscillator
LOU	Local Oscillator Unit
LSU	Local oscillator Source Unit
SBR	Side-Band Ratio
TEI	Test Equipment Interface

0.Test set-up and measurement principles

3.1 Objectives

Following AD4, the goal of these measurements is twofold:

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- using saturated isolated lines, it provides a measure of the mixer side-band gain ratio (SBR)
- using un-biased surveys of rich spectra of molecular species, it offers a representative data-set for the development of de-convolution tools. As a side-product, it is a very useful source of information for standing wave, spurious signal and spurious response analysis.

Ideally, the SBR needs to be surveyed over the full HIFI frequency range. The granularity obtained is totally dependent of the availability of adequate molecular lines absorbing sufficiently at the frequencies of interest.

3.2 The Gas-cell and associated set-up

Details about the gas-cell specification and design can be found in RD4 and RD7. The main characteristics of the HIFI gas-cell, in particular compared to previous ones used e.g. for the SWAS satellite (see RD6), is its full under-vacuum optical path, as well as its optical set-up allowing to keep the beam within a 4w criteria on all optics along the line-of-sight.

The gas-cell makes use of the thermal radiation from a Hot-Cold switch (see RD3) fed at its input port and folded towards the gas cavity containing the absorbing gas. The output port is connected to a re-imager tank allowing to couple each of the HIFI 7 beams to a single waist size and position at the gas-cell interface. This re-imager is located on top of the HIFI FM test cryostat, and feeds the gas-cell emission onto M3, and therefore down to the mixer.

A dedicated pump system has been designed for these measurements, allowing a totally autonomous use of the gas-cell (see RD7). Although temperatures and pressure should have been permanently monitored during the campaigns, some TEI shortages made these parameters sometimes un-available. The pressure in the cell is however believed to have been monitored accurately during the bulk of the campaigns.

Figure 1 shows a picture of the gas-cell set-up in combination with the above-mentioned re-imager and Hot-cold switch.

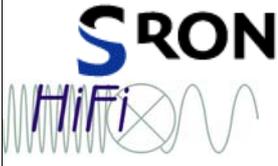
	<p style="text-align: center;">HIFI FM Gas-cell measurements</p>	<p>Hifi no.: SRON-G/HIFI/TR/2008-002 Inst.no.: n Issue: Draft 1.0 Date: :16-04-08 Category: 2.</p>
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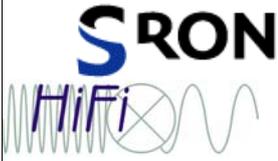


Fig. 1: Gas-cell set-up. The big tank at the back is the re-imager, located on top of the HIFI FM test-cryostat, hosting the FPU. The gas-cell is connected to the Hot-cold switch (golden cryostat), and controlled by the pump circuit shown at the bottom.

3.3 Measurement principles

In a given LO and mixer bias-setting, the side-band ratio measurement is based on the comparison of two signals taken successively through a filled and an empty cell. The measurements are performed against hot and cold loads, and the differential signal, if done fast enough, should be free from system noise contribution. The frequency range is chosen such that an absorption line affects only one of the side-bands and can be compared to the absolute continuum level. In that sense, the absorption level of the line seen in one single side-band provides a direct measurement of the mixer gain applying to this band. The equation used to retrieve this gain ratio will be given in section 6.1.

3.4 Side-band ratio in the calibration equation, and its impact

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Following RD2, the calibrated data will be obtained following:

$$J_{source} - J_{OFF} = \frac{1}{G_{ssb} \eta_l + \omega_{ssb}} \frac{\eta_{hot} + \eta_{cold} - 1}{\eta_{sf}} \times [...]$$

where G_{ssb} corresponds to the side-band ratio. The relation between this parameter and the numbers directly derived from the gas-cell measurements is given in section 6.1. The contribution of this parameter to the calibration error budget is directly proportional to the error on the gain. In other words, an error of 1% on the SBR translates into a contribution of 1% on the error in the overall calibration.

0. Overview of the measurements

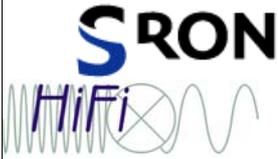
Gas-cell measurements have been performed over 3 dedicated campaigns: January 2007, May 2007 and June 2007. In between these campaigns, several instrument configuration changes have occurred, the main one being the insertion of attenuators between in the LOU and the FPU before the May campaign. Therefore, the full set of data has been unequally affected by the caveats of the test environment.

The following table summarizes the configuration applying to the data acquired. Further details can be found on the wiki pages. The figure below illustrates the molecule distribution with obsid.

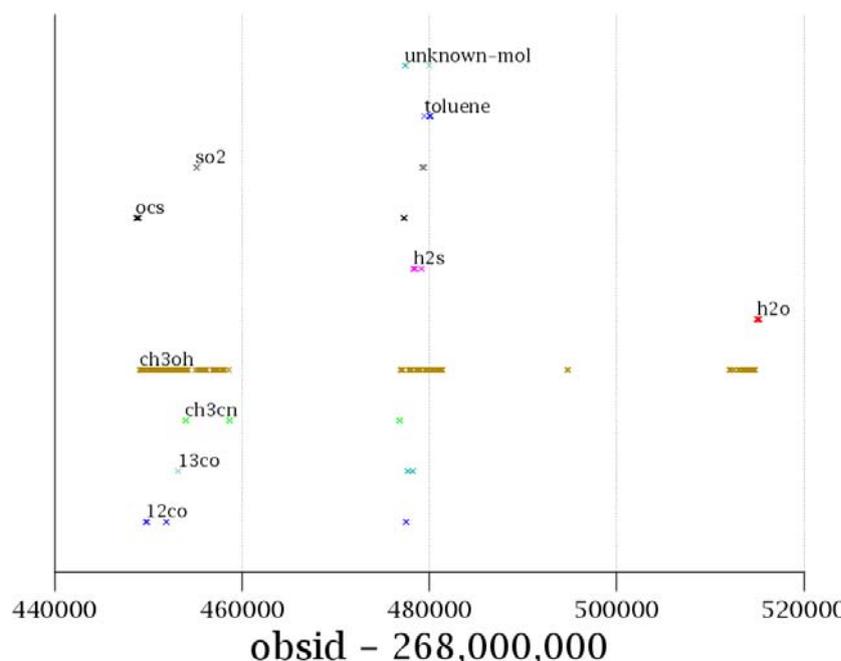
Test campaign	February 07	May 07	June 07
Bands covered	1,2,4,5,6	2b,3,4,6,7	2, 4, 5 6, 7
Molecules	OCS, CH ₃ OH, CH ₃ CN, SO ₂ , ¹² CO, ¹³ CO	CH ₃ OH, H ₂ S, toluene, ¹² CO, ¹³ CO	CH ₃ OH, H ₂ O
Database	fm_ilt_2 and fm_ilt_3	fm_ilt_4	fm_ilt_5
Obsid's	268448707 - 268454314 in fm_ilt_2 268455008 - 268458850 in fm_ilt_3	26847678 to 268494855	268511942 to 268515312
H/W config	No LOU attenuators	LOU attenuators, but not yet on LO baffle	LOU attenuators on LO baffle
Remarks	Very poor stability in bands 2, 4, 6.	Bands 6 and 7 still have poor baselines	All measurements in fast-chop

Tale 1: summary table for the gas-cell measurement campaigns

Beside these campaigns, the gas-cell was used as a laboratory spectral source to simulate some of the observing modes and check the baseline quality. These tests are reported somewhere else.

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Molecules observed during the gascell campaign



0. Data processing and data repository

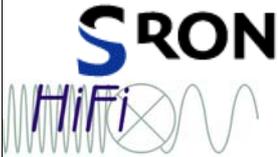
5.1 Detailed pipeline

Raw data from the database have been processed using the standard instruments pipelines. Although data have been obtained simultaneously by both back-ends (and in both polarizations), this report only concentrates on the WBS data. Frequency scales have been calibrated in the WBS pipeline using the COMB measurements.

The gas-cell data has been acquired without dedicated AOT's. Therefore, the generic pipeline which is supposed to take place after the instrument pipeline can not process them. As a consequence, we wrote our own gas-cell pipeline. Following the philosophy of pipeline development, the gas-cell pipeline falls down into several tasks which can be executed or not, in a more or less independent order.

Despite this theoretical freedom, there is one 'normal' way of applying the gas-cell pipeline, one 'normal' sequence of tasks with 'normal' input parameters. Depending on the needs and desire of the calibration scientist interested in the gas-cell data, we stop this 'normal' gas-cell pipeline either just after a few tasks, or at the middle, or at the very end. Those different needs lead to the development of higher-level tasks grouping elementary tasks together. We have now a *Gascell Pipeline Minimal*, followed by a *Gascell Pipeline Standard*, then a *Gascell Pipeline Extended*. The *Gascell Pipeline Quality-Analysis* is still being an on-going development.

The Gascell Pipeline Minimal starts when the instrument pipeline ends. It gathers the gas-cell-specific housekeeping parameters values and stores them in the data Product. It also corrects the bad assignment of BbTypes to data-frames (some onboard software issue) using the knowledge we have of what the data should look like. No calibration or information lost at this step: we just transform the simple Hifi Product in a *Hifi Gascell Product*, by adding gas-cell information to it.

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Comes then the Gascell Pipeline Standard, which results in a Product we thought most useful for the majority of the people looking at gas-cell data. Non-scientific spectra (like comb measurements, attenuators scans) are removed from the product. Integrations on a same source (such as Hot-Black-Body-behind-Empty-Gascell) are averaged. Datasets within the product are re-organized and renamed to make the product more user-friendly. Still, no hot-cold or on-off calibration is done at this level. That is with Products getting out of the Gascell Pipeline Standard that we populated the Gascell Standard Pool (see next section).

The Gascell Pipeline Extended can be applied to Products produced by the Gascell Pipeline Standard (either directly or read back from the Gascell Standard Pool). This third area of the Gascell Pipeline takes care of the absorption calibration (provides several calibration formulae), the sub-bands stitching (with removal of the WBS sub-band overlap), the re-sampling on a regular sky-frequency grid (strong requirement for the de-convolution, regardless of whether the de-convolution is performed with HCSS or CLASS).

The Gascell Pipeline Quality-Analysis aims at detecting and flagging bad data. There are multiple reasons for an observation to have poor scientific value: low stability, LO wrongly tuned, bad attenuators settings, strong standing waves, plus things which are still to be determined. The Gascell Pipeline Quality-Analysis aims at automatizing this analysis. So far, it provides tools to detect ripples, filter-out some features, check some HK parameters. This is still under design and development. Most of what is being developed here could be used later for flight data.

All those tasks have been written in Jython and are available in the HCSS HIFI builds along with their documentation.

5.2 Data format and repository

A data pool has been created. This pool is our answer to several wishes and requirements from the astronomers and calibration scientists wanting to work on gas-cell data:

- it shall be fast, faster than an access to a remote versant database
- it shall work offline,
- it shall fit on a laptop's hard drive,
- it shall contain everything most people need,
- it shall be fully HCSS-compliant,
- it shall be the same for everyone.

We designed a SimplePool which we populated with products of the Gascell Pipeline Standard (see previous section). ~ 6,500 Obsids have been acquired during the gas-cell campaigns. This number should multiplied by 2 back-ends, 2 polarizations: in total ~ 26,000 products. The high number of meta-data added to these products by the Gascell Pipeline Minimal make the products easily retrievable with proper metadata-queries. The pool also contains tables summarizing its content and allowing to access the products using navigation rather than queries (which is faster and easier in most cases).

The pool is hosted at SRON Groningen, and whoever has an account on the SRON computer network can link this pool to his HCSS environment and access the gas-cell data. Hosted next to it is a compressed version of this pool (tar.gz) which can be downloaded on one's laptop via SFTP. The size of the compressed archive is expected to be 12 Gb.

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So far, only WBS bands 1 to 5 has been exported to the pool (3.3 Gb compressed, 4.4 Gb uncompressed). Issues with the HRS pipeline and with the data processing of spectra taken with LO bands 6 and 7 prevented us to populate the pool with those data. SPR's about these issues have been raised and are followed-up.

A more complete documentation of the pool, content and structure can be found on the ILT wiki:

<http://www.sron.rug.nl/~wikiman/wikis/Hifillt/GascellStandardPool>

A script defining convenient functions for accessing the pool, the products within the pool and the spectra within the products has been written, included in the HIFI build. It is also available on the ILT wiki:

<http://www.sron.rug.nl/~wikiman/wikis/Hifillt/GascellPoolToolsPy>

0. Side-band ratio determination

6.1 Definition of the side-band ratio

The following equations illustrate the basics for the ratio derivation and allow assessing the accuracy of a measurement. We assume that an absorption line (of opacity τ) is seen in the lower side-band, while the spectra in the upper side-band are not affected by any spectral feature. The differential measurements are then respectively:

$$S_{filled} = G_u(J_{hot} - J_{cold}) + G_l(J_{hot} - J_{cold})e^{-\tau}$$

and

$$S_{empty} = G_u(J_{hot} - J_{cold}) + G_l(J_{hot} - J_{cold})$$

where G_u and G_l stand for the upper and lower side-band gains respectively, including all transmission elements along the optical path, and J_{hot} and J_{cold} are the effective (Rayleigh-Jeans) hot and cold load temperatures of a black body of temperature T and frequency ν .

Using the measurements described above, the side-band ratio is finally given by:

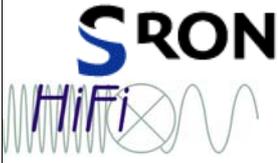
$$R_G = \frac{G_l}{G_u} = \frac{1 - S_{filled} / S_{empty}}{S_{filled} / S_{empty} - e^{-\tau}}$$

The opacity needs to be accurately known, unless the line is saturated (high τ), in which case R_G simply writes $S_{empty}/S_{filled} - 1$. Typically, a gain ratio of unity would be observed for $S_{empty}/S_{filled} = 0.5$ at the line peak position, i.e. an absorption line of half the continuum level in a normalized spectra.

The relation between the SBR as introduced in the equation above, and the respective side-band gains used in section 3.3 is as follows:

$$G_{ssb} = \frac{G_u}{G_l + G_u} = \frac{1}{1 + R_G}$$

In this document, we will call SBR the value as introduced in the equation above, i.e. the one entering the HIFI calibration equation of section 3.4. In this convention, a gain ratio of 1 thus

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translates into a SBR of 0.5. Note that this value applies to the calibration of line located in the USB. For a line located in the LSB, the number to be used should be $1-G_{ssb}$.

6.2 Hardware and environment limitations

6.2.1 Instrument tuning capabilities

Because of the high dynamic in the LOU output power, not all sky frequencies can be effectively. Indeed, in some LO frequency area, the mixer cannot be pumped to a level providing a decent sensitivity. This ends up as gaps in the coverage.

6.2.2 LO purity

It was only discovered very late during the ILT campaign that some of the LSU would not be as pure as originally believed. This means that in some areas, other frequencies than the requested one will enter in the mixing product, and thus be down-converted in the IF. It has been shown that such spurs have occurred in bands 3b (above 930 GHz), 5b (above 1200 GHz) and in band 7b (above 1830 GHz). Sometimes, the spurious LO frequencies can be even stronger than the main carrier, implying an apparent very low or very high side-band ratio. This effect is illustrated in Fig. 2

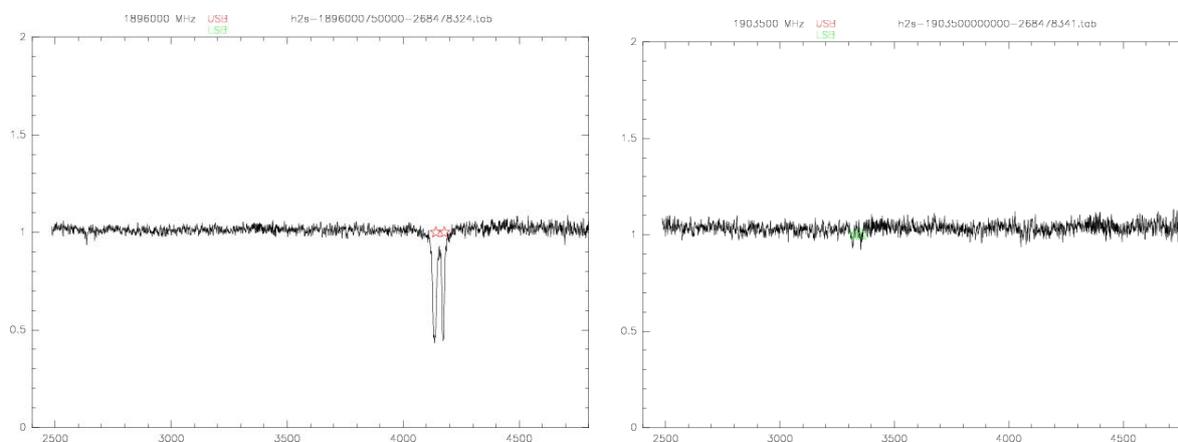
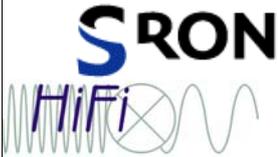


Fig 2: Gas-cell measurement of the H₂S line doublet expected at a rest frequency of 1900.15 GHz. *Left:* measurement in the USB (LO at 1896 GHz). Both lines appear saturated, at the expected level of 50% of the normalized continuum. *Right:* measurement in the LSB (LO at 1903 GHz). Here the line absorption is very low compared to the expected one, suggesting that the mixer is pumped at multiple LO frequencies.

6.2.3 Instrument stability

Because the source coupling determination makes use of measurements taken at different times, the final result is sensitive to gain drifts. During the HIFI FM campaign, it has been shown that operations of the LOU without attenuators would lead to quite poor Allan time, resulting in relatively strong drifts and poor baselines (see RD5).

These potential baseline distortions are mostly present in bands 2b, 4a, 4b, and all HEB bands. They are clearly affecting the data of the February and May campaigns. In June, measurements

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performed with the attenuators in place showed an improvement in the SIS bands, but HEB bands are still suffering from drifts. They mostly show up as slopes and 0-order shifts on the normalized continuum level, making it sometimes complex to derive an accurate line absorption level.

Finally, spurious signals can show up at sporadic places in the IF spectrum, esp. in the CCD1 of the WBS. Further details can be found in RD8.

Such effects are illustrated at several places in sections 6.2.4, 6.3 and 6.4.

6.2.3 Instrument standing waves

A special section is dedicated here to the standing waves affecting the gas-cell data. The distortion due to these effects is indeed of up-most importance when retrieving the side-band ratio as it is obtained from the comparison of the line absorption level with the total continuum. Obviously, the assessment of the line absorption is strongly affected by fast spectral features of period similar to the typical line width of the lines.

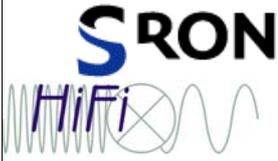
Although a dedicated report on standing waves can be found elsewhere, we summarize here the main effects seen on the gas-cell baselines:

- In all SIS bands, baselines are affected by optical standing waves originating from the cavity formed between the mixer horn and the LO window. This standing wave has period of ~170 MHz. Some weaker standing waves can be seen in bands 1 and 2 (because of the high sensitivity of those mixers) at shorter periods, representative of reflection taking place in the gas-cell, i.e. due to the test equipment in general.
- In HEB bands, the main baseline distortion appears to be due to an electrical standing wave, finding its origin in between the IF1 circuitry and the mixers. Contrary to the SIS bands indeed, there is no isolator in this circuitry for the HEB bands.

At a fundamental level, electrical and optical standing waves behave the same. Electrical standing waves are however more complex since the reflecting surfaces properties are highly frequency dependent. The medium of travel is also different, electrical through co-axial cable and optical through air (or vacuum). The speed of light in co-axial cable is an important parameter in the modelling of electrical standing wave as it varies with co-axial cable. From a HIFI perspective, one distinct difference between the optical and the IF standing wave is that the latter is independent of LO frequency. Since electrical standing waves occur after the mixer their phase does not change with LO frequency.

The complexity of the electrical standing basically resides in its dependence on the mixer impedance. The impedance of the HEB is a function of the LO power and bias current across it. Additionally recent research has shown evidence of a phase component in the impedance. Evidence of a complex component in the HEB is also seen in the standing wave. The standing wave is seen to change period across the IF frequency, if this was an optical standing wave one would think that the optical path was changing length for different frequencies, see figure 3 below. This stretching of the standing wave across the IF bandwidth makes a fitting solution difficult.

At the time of writing this report, there is still no efficient method to fit and remove this standing wave.

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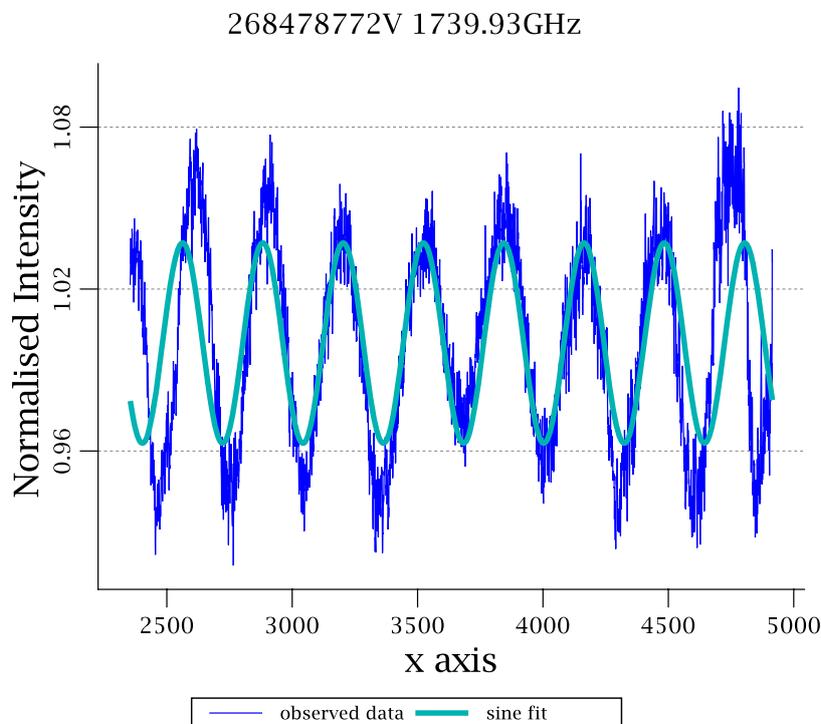


Fig 3: Example of an electrical standing wave in band 7a.

6.3 Zero-order assessment of the side-band ratio

In order to get a first overview of how the side-band ratio would be distributed over the mixer bands, and over the molecules probed, we performed a preliminary estimate of the SBR through an automatic inspection of the line absorption level. For this very crude estimate, we relied only on lines which were isolated enough so that the line density would not confuse the absorption level assignment.

The SBR estimate is based on an automatic measurement of the minimum of the line absorption dip. At a given LO frequency, the expected position of the transition of interest allows to restrict the domain in which the minimum is expected. This position is also used in order to define a blanking window to perform a 1-order baseline fitting and removal. The level of this baseline is then divided to the gas-cell spectrum. This crude estimate has the following caveats:

- The exact continuum level (to which the line absorption is compared) can be inaccurate (baseline distortion, spikes, slopes, etc)
- Standing waves are not corrected, so they can affect strongly the value of the line minimum
- The noise in the data can significantly lower the value of the minimum (there is not fit performed over the line profile)
- The opacity of the line is assumed to be infinite

This latter point has a very significant effect on molecules like OCS, where lines will not saturate any longer above ~ 800 GHz. The following plot is an illustration of the line strengths for the transitions probed in this survey.

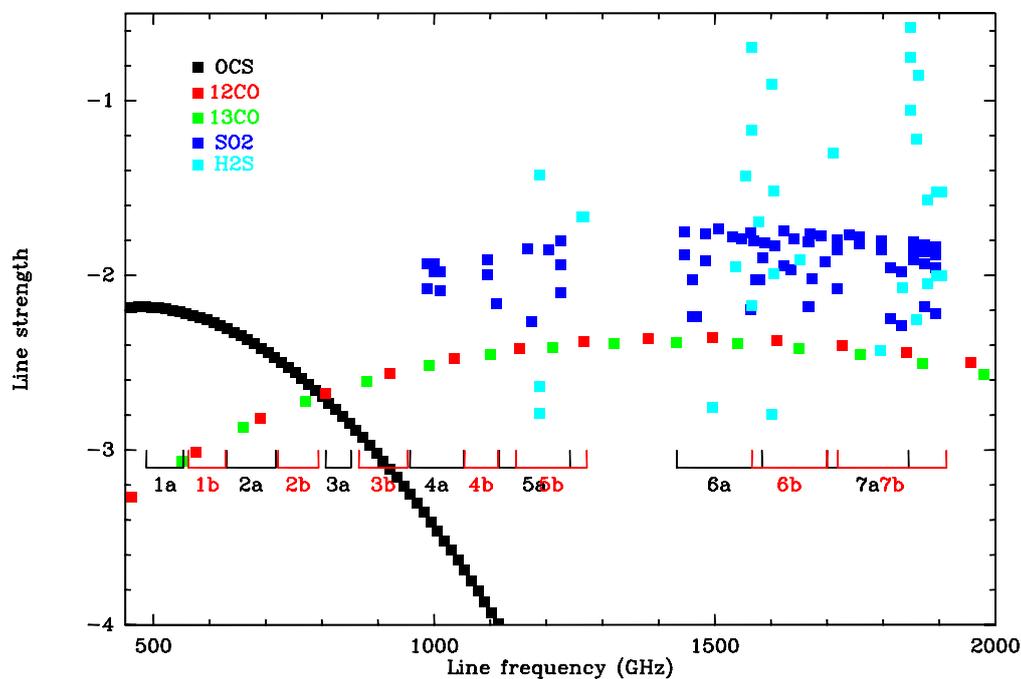


Fig 4: Illustration of the line strength for the main molecules probed during the gas-cell measurement. As can be seen, CO will only saturate above ~ 1 THz, while OCS will no longer saturate after ~ 800 GHz (these limits are linked to the length of the cell)

The SBR obtained via this crude method are shown in the following plot. The opacity effect on OCS is clearly seen. We also note that large scatters can be observed for SBR measured either several times at the same frequency, or at nearby frequency, indicative of stability issues. The SBR are only shown here for the H-mixer, but the numbers obtained for the V-mixer are very similar.

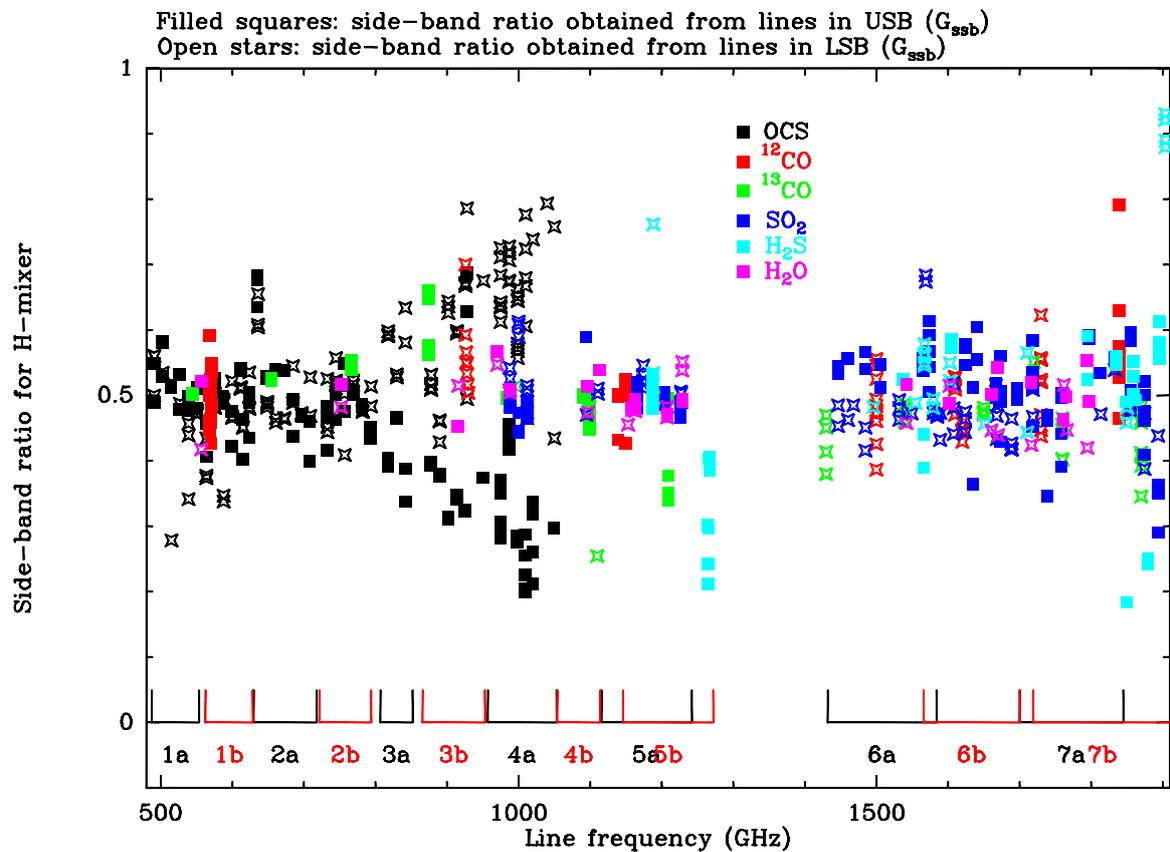


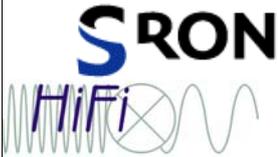
Fig 5: SBR ($G_u/(G_u+G_l)$) obtained from the crude method described in section 6.3 for the H-mixer. The frequency scale corresponds to the line frequency (i.e. not the LO frequency)

6.4 SBR determination from LTE model line fitting

6.4.1 Theoretical principles

The information concerning the physical conditions in the environment can be deduced from the shape of the observed lines. There are several causes of line broadening, the main being:

- Natural broadening: The Uncertainty principle relates the life of an excited state with the precision of the energy, so the same excited level will have slightly different energies in different atoms. This broadening effect is described by a Lorentzian profile.
- Thermal Doppler broadening: Atoms will have different thermal velocities, so they will see the photons red or blue shifted, absorbing photons of different energies in the frame of reference of the observer. The higher the temperature of the gas, the larger the velocity differences (and velocities), and the broader the line. This broadening effect is described by a Doppler profile.
- Pressure broadening: the collision of other particles with the emitting particle interrupts the emission process. The duration of the collision is much shorter than the lifetime of the emission process. This effect depends on the density of the gas. The broadening effect is described by a Lorentzian profile.

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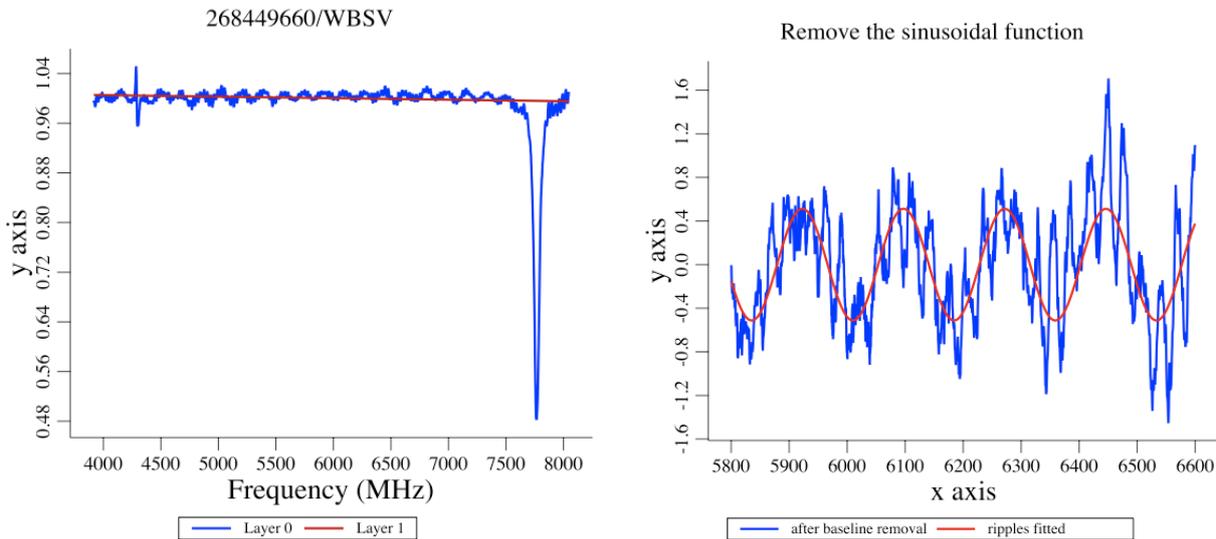
- Opacity broadening: considerable re-absorption of emission line photons, an effect known as opacity, often causes line broadening. The line is broadened since photons at the line wings have a smaller re-absorption probability than photons at the line center.

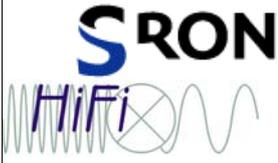
The combined line profile will be the convolution of the line profiles of each mechanism. For example, a combination of thermal Doppler broadening and pressure broadening will yield a Voigt profile. The natural broadening is usually too small to be taken into account.

The detailed equations used in order to model the full profile of the absorption lines are given in Appendix A.

6.4.2 The fitting procedure and its limitations

We used the calibrated data generated according to the data processing described in section 5. We first remove the baseline and potential ripples using a Jide routine. The subsequent data reduction is described in the following via an example. The ^{12}CO line has been observed with HIFI-WBS V polarization (see upper left in figure 3). A 1-order baseline has been fitted and removed. In order to remove the ripples we select a short wavelength range in the spectrum (usually the closest where the line is). Here we define a wavelength range in the middle of the spectrum (upper right in figure 3) in order to illustrate the importance of this wavelength selection. We fit the ripples giving initial guesses for the amplitude and the phase. We then fit the whole spectrum from the best-guess parameters obtained in the reduced range (bottom left). In the bottom right of figure 3, we remove the fitted baseline and find that the fitted spectrum diverges on the edges.



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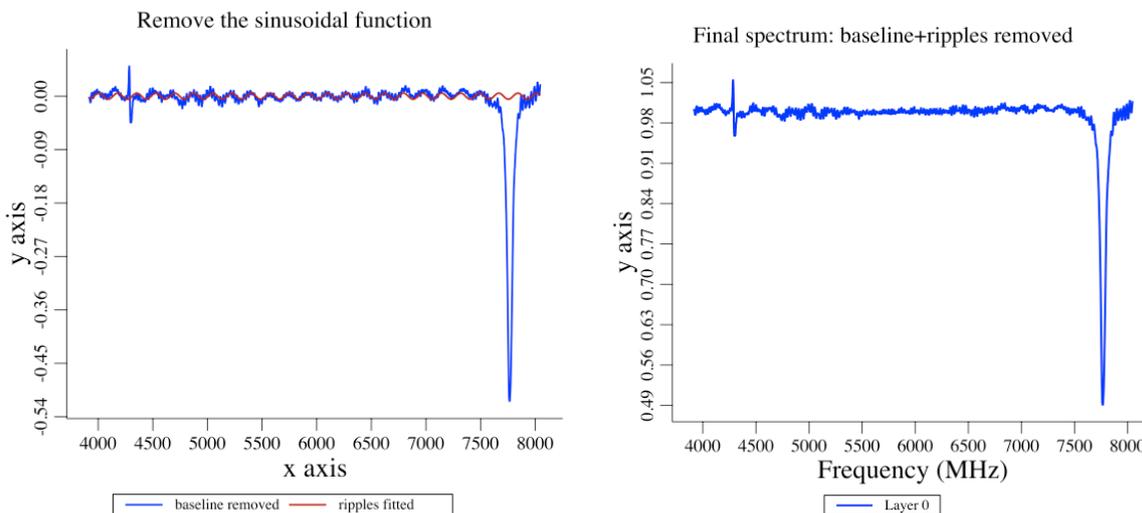
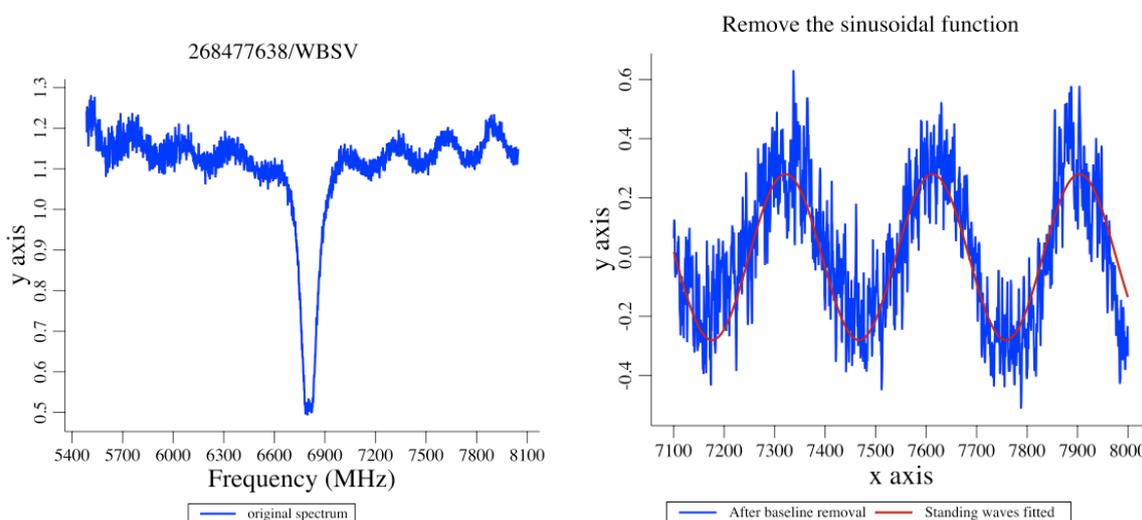
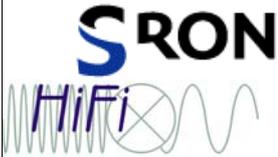


Fig 6 Example of a fitted spectrum through removal of a baseline and standing waves. The standing wave observed here is an optical one (see section 6.2).

A case of electrical standing wave (on a ^{13}CO line) is illustrated in the following figure, where the ripple cannot be properly fitted:



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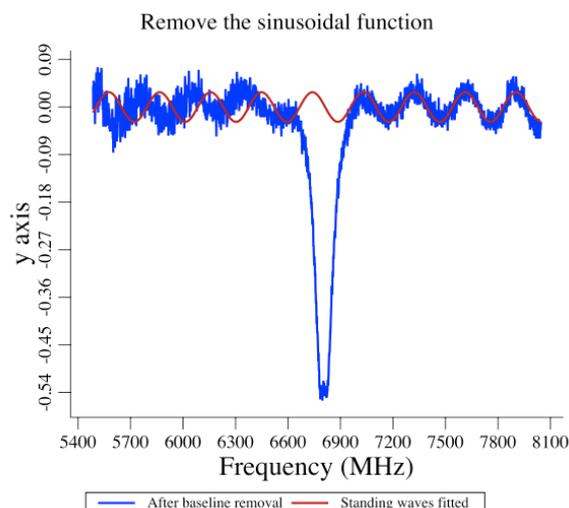


Fig 7 Example of a fitted spectrum through removal of a baseline and electrical standing waves.

From all the data, we carefully flagged the spectra where:

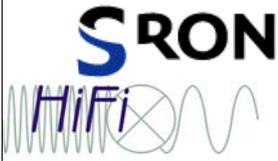
- 1) the baseline cannot be fitted
- 2) the ripples cannot be removed
- 3) the spectrum is too noisy
- 4) a strong emission line appears at the line center of the absorption
- 5) many spikes affect the spectrum.

These comments are listed in the summary files (see Section 6.5).

The program aiming to determine the sideband ratio is written in IDL. The user is asked to enter the Obsid of interest as well as the polarization (H or V). The program then reads the housekeeping data containing important information concerning the way the observations were performed: the Obsid, the polarization of the WBS, the gas in the cell (^{12}CO , ^{13}CO , OCS, H_2S , CH_3OH , SO_2), the LO frequency, the LO band (band 1-7, a/b), and the pressure as measured during the observation. Because the pressure is polled every second, the values actually filled in correspond to the median of the HK sampled during the empty of filled cell phases. It could sometimes happen that this value was not correctly recorded by the TEI so that interpolation from the nearest bracketing measurements was necessary. In some cases, the user has to enter a best guess for this pressure by hand during the fitting process. As such the pressure read in the housekeeping will be a first guess to start our best fit routine.

The program then explores the CDMS or JPL databases within the frequency range of the observation in order to find the potential lines associated with the observed molecule in the upper and/or lower sideband. The CDMS database has been used for the ^{12}CO , ^{13}CO and SO_2 molecules, while the JPL database has been used for the H_2S molecule.

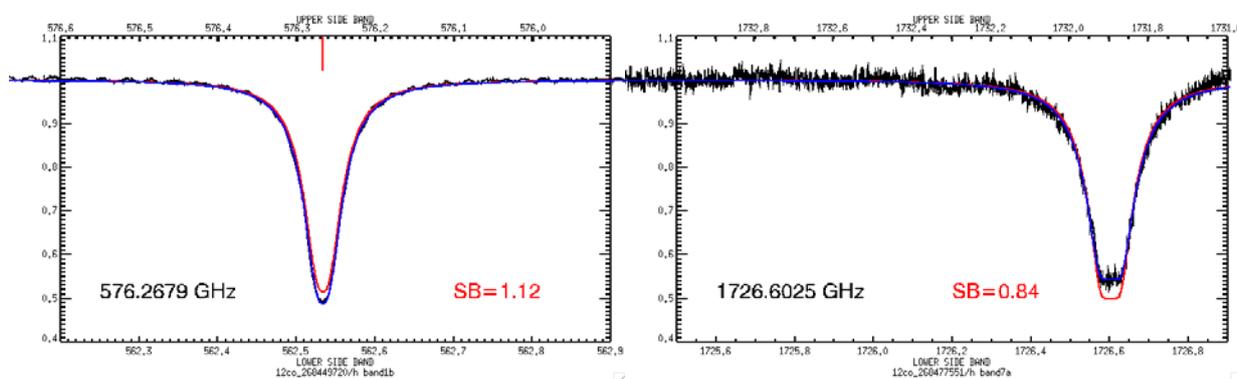
Another crucial parameter is the pressure broadening (γ_{self}). It is extracted from the HITRAN database by the program identifying the lines by comparison with the CDMS or JPL frequencies as well as the quantum numbers. Since the CDMS/JPL catalogs are more suited for high frequency measurements than the HITRAN database, the program uses the Einstein coefficient and

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frequencies from the former. This analysis can be performed for the ^{12}CO , ^{13}CO , CH_3OH and H_2S lines where trustful HITRAN parameters can be used. For SO_2 and OCS the broadening coefficients are null. Appendix B compiles the current HITRAN entries for the self-broadening coefficients of the molecules in use in our study.

Based on the frequencies, Einstein coefficients, γ_{self} , temperature of the gas cell (room temperature at 296 K), the length of the gas cell (102.54 cm), the program then performs a best fit of the observed lines varying the sideband ratio (starting at unity) and the pressure (starting at the value read from the housekeeping).

The following 2 plots show the resulting fits in two cases: the left one moderately optically thick while the right one is strongly optically thick.



The observed spectrum is represented in back while the simulated spectrum, where a sideband ratio of unity and the pressure as read in the housekeeping data have been used, is shown in red. Our final Voigt fitted spectrum is plotted in blue, varying the sideband ratio AND the pressure. On the left figure (band 1b), the sideband ratio is about 1.12 with an adjusted pressure of about 6.1 compared to the house keeping data of 6.0. On the right figure (band 7a consequently more noisy), the sideband ratio is about 0.84 with an adjusted pressure of about 8.3 mbar compared to the housekeeping data of 7.5 mbar.

The uncertainty of the adjustment is difficult to quantify and an rms has been defined around the line as:

$$rms = \frac{1}{N} \sqrt{\sum_{i=1}^N (obs_i - fit_i)^2}$$

The following sections present the detailed results for each molecule.

6.4.3 ^{12}CO and ^{13}CO

The SBR retrieved from the ^{12}CO and ^{13}CO analysis are shown in the following plots:

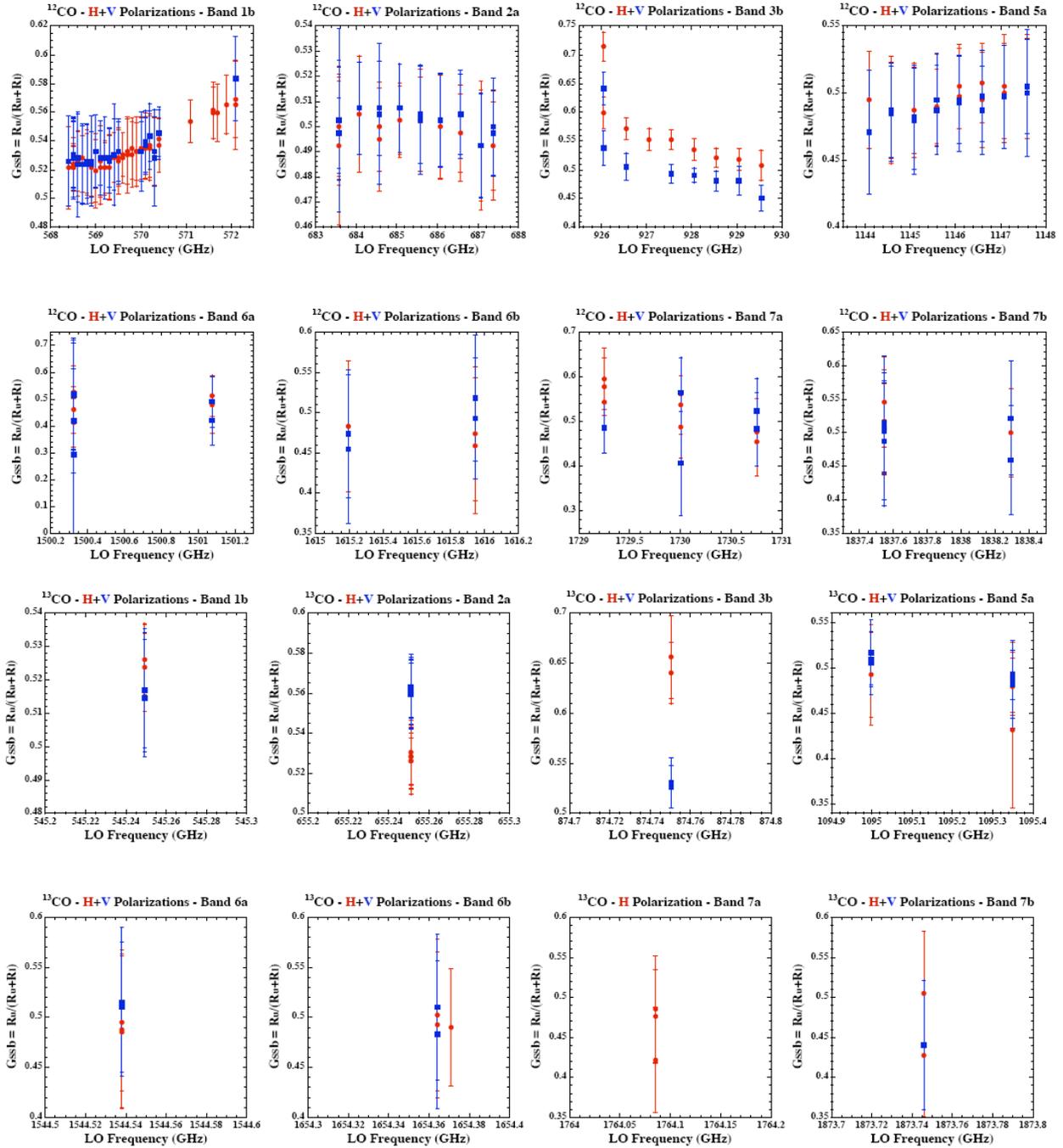
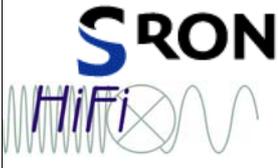


Fig 8: SBR obtained from the ^{12}CO and ^{13}CO analysis

As can be seen, there is a clear trend over the IF range of 4 GHz for those bands where it could be measured. Also, as we go to higher frequencies, in-stabilities are starting to harm seriously and the reproducibility of a measurement at a given frequency is degrading.

6.4.4 H_2S

The H_2S analysis is currently on hold due to a problem observed in frequency scale of the processed data. It appears that one of the polarisation is shifted by $\sim 10\text{MHz}$ with respect to the

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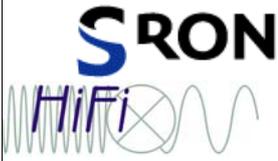
other one. The V-mixer seems to be found at the expected frequency. In some other cases, both polarizations seem to be off by this amount with respect to the frequency given in the JPL database. The analysis of this bug is still on-going.

6.4.5 SO₂

As is mentioned in the appendix B, the analysis of SO₂ still awaits the availability of pressure broadening coefficient. An experiment has been planned at JPL for that purpose.

6.4.6 OCS

As is mentioned in the appendix B, the analysis of OCS still awaits the availability of pressure broadening coefficient. An experiment has been planned at JPL for that purpose.

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6.4.7 CH₃CN

CH₃CN is a symmetric top molecule, with two degenerate moments of inertia, with the total angular momentum of the molecule (J) and the other quantum number (K) associated with the angular momentum of the axis which has different moment of inertia. In addition, it displays an hyperfine structure due to the nitrogen atom further splitting each level. The rotational transitions originating from the same ΔJ and with different initial K (with $\Delta K=0$) arise in a relatively narrow frequency range. The spectrum is then dominated by accumulations of transitions separated by approximately 18 Ghz.

To model the spectra, we make use of the JPL line catalogue (<http://spec.jpl.nasa.gov/>) list for the CH₃CN ($v_8=0,1$), CH₃¹³CN and CH₃C¹⁵N, assuming terrestrial abundances for the isotopomers.

With the pressures used, the broadening in our Gas cell tests are generally dominated by pressure broadening. Nevertheless, we use a Voigt profile as template profile in the SBR determination.

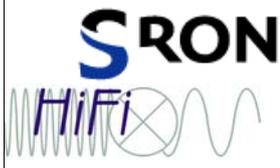
Dedicated data processing steps for CH₃CN:

We first make a pre-selection of the data to throw away (detect the “bad” data). To do so we make use of the individual subsets of the experimental sequence. We expect the sequence *check_baseline = (hot filled-cold empty)/(hot empty-cold empty)* to give us to first order a straight line as we should see almost no temperature difference between the hot gas and the hot load. It allows us to estimate the instability during each four subset of the sequence except the cold filled one. If the baseline obtained is good, it gives us a strong hint that the overall sequence was performed with a stable environment. Putting a threshold on the baseline obtained allows us to reject bad spectra, but also to estimate what kind of confidence we can have in the baseline to perform SBR estimates. ***A deviation from unity, even with a flat spectrum tells us that gain changes occurred during a subset of the sequence and a corresponding uncertainty will affect the SBR determination.***

CH₃CN SBR fitting: the assumptions:

Once selected, the spectra are modelled using a four parameter model described below:

- A **Baseline gain (G) correction**, i.e. a proportional factor to compensate for first order deviations is applied. The consequence on “true” gain determination, given the operational sequence, is that it assumes the input power variation during the four steps measurements affects evenly the two first measurements and the two last ones. Any deviation from this assumption changes the determined SBR. In particular, if the origin of this deviation occurs from the input power variation into an individual subset of the sequence, then the gain determination will be affected.
- The **Side Band Ratio (SBR)**, defined as upper side band (USB) over the sum of the upper and lower side band (USB+LSB), is the parameter we are searching for.
- The **Intensity factor (I)**, defined as a multiplicative factor to the intrinsic intensity of each considered line of the catalogue, i.e. defining the column density of molecules in the experiment.
- The **Damping factor (D)**, defined as the damping parameter for the Voigt profile i.e. the ratio of the natural + collisional widths to the Doppler width.

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We make no assumption on the measured pressure, use a single SBR across each side-band and take the pipeline frequency axis calibration.

The model spectra, produced on the same axis as the ones provided by the pipeline product, are prepared for the USB and ISB, and are subsequently folded. We start with an initial guess for G, SBR, I and D. A four dimension downhill simplex minimisation under IDL, using reasonable initial guesses, is performed. Once converged, the minimisation is started again and extending the parameter space to check the validity of the result.

We describe below some examples of the spectra measured.

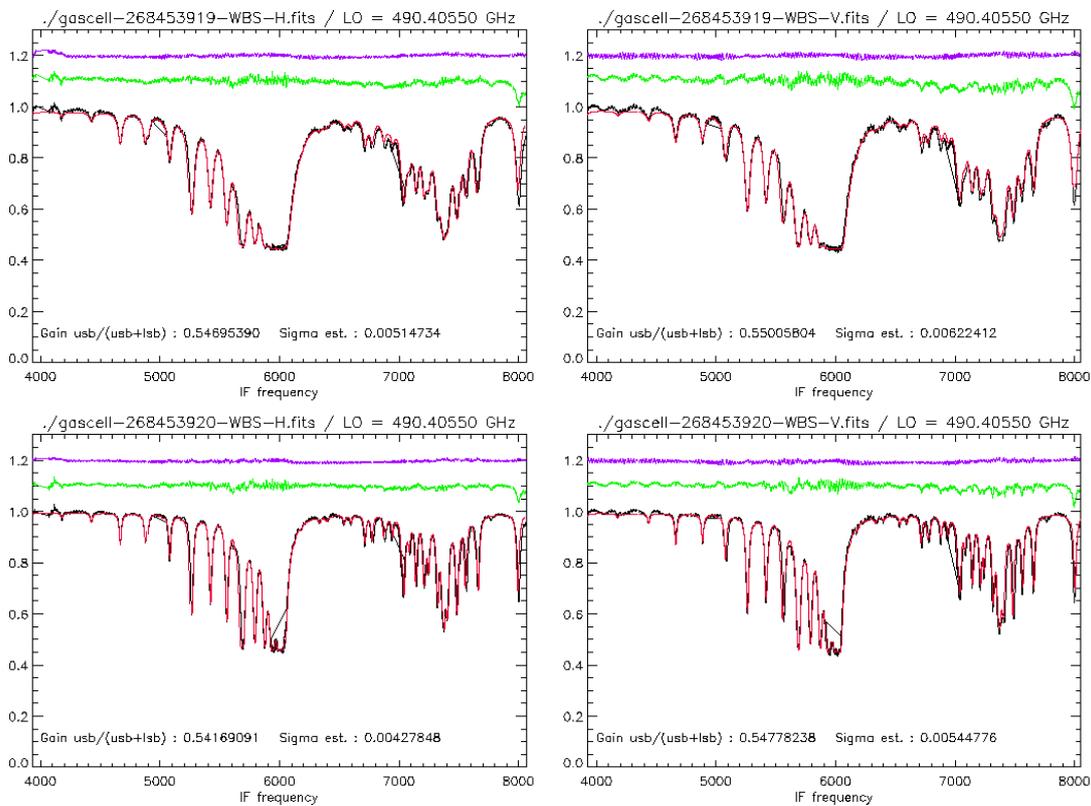


Fig 9: illustration of the results in band 1 around 490 GHz. The upper purple line curve is the combination discussed above giving a hint to the instabilities during the sequential measurements, shifted by 0.2 for clarity. The green curve is the result of the division between the measured and modelled spectrum, shifted by 0.1 for clarity. The black line is the measured spectrum and the red one the best modelled one. No attempt was made to merge individual observed sub-bands of the WBS which explains some straight line linking the end of a sub-band to the beginning of the next one like in the Obsid 268453920-H around 6 GHz in the IF. One can see that in this specific case, the green curve displays some ripples appearing in the division of the Obsid 268453919, vertical polarization, whereas they are almost absent from the horizontal one.

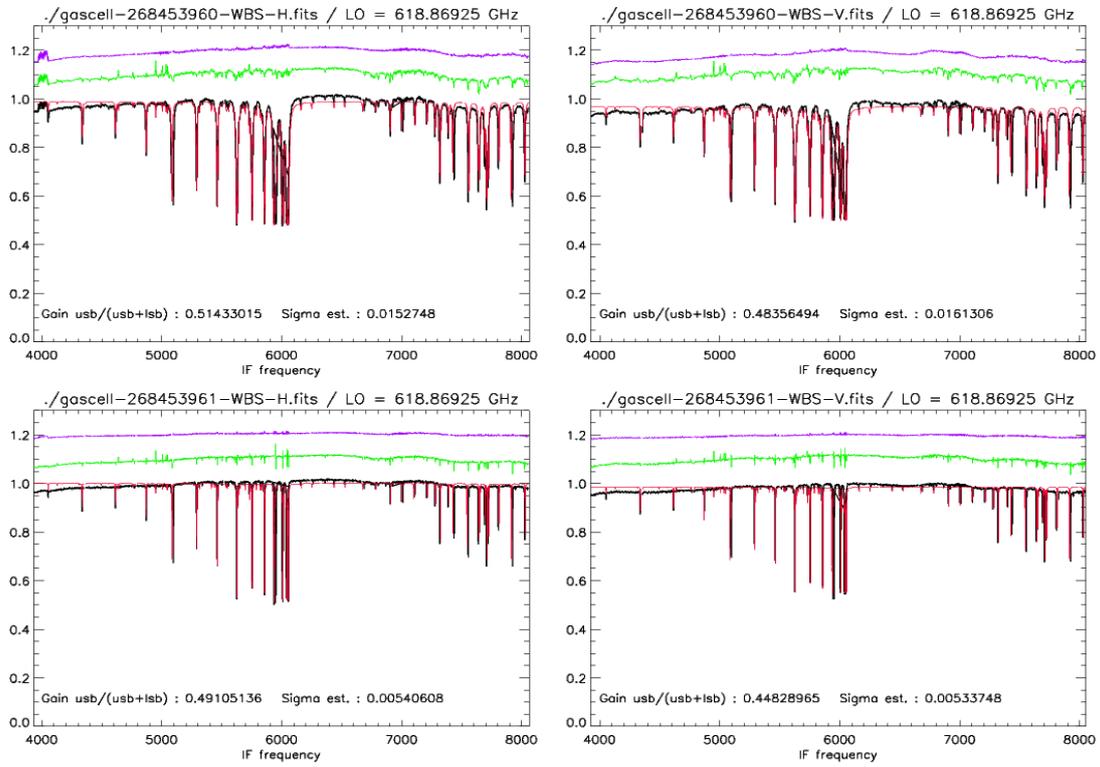


Fig 10: Examples of unstable baselines during measurements for obsid 268453960. One can see that the *check_sequence* described above already shows a clear deviation from flat unity.

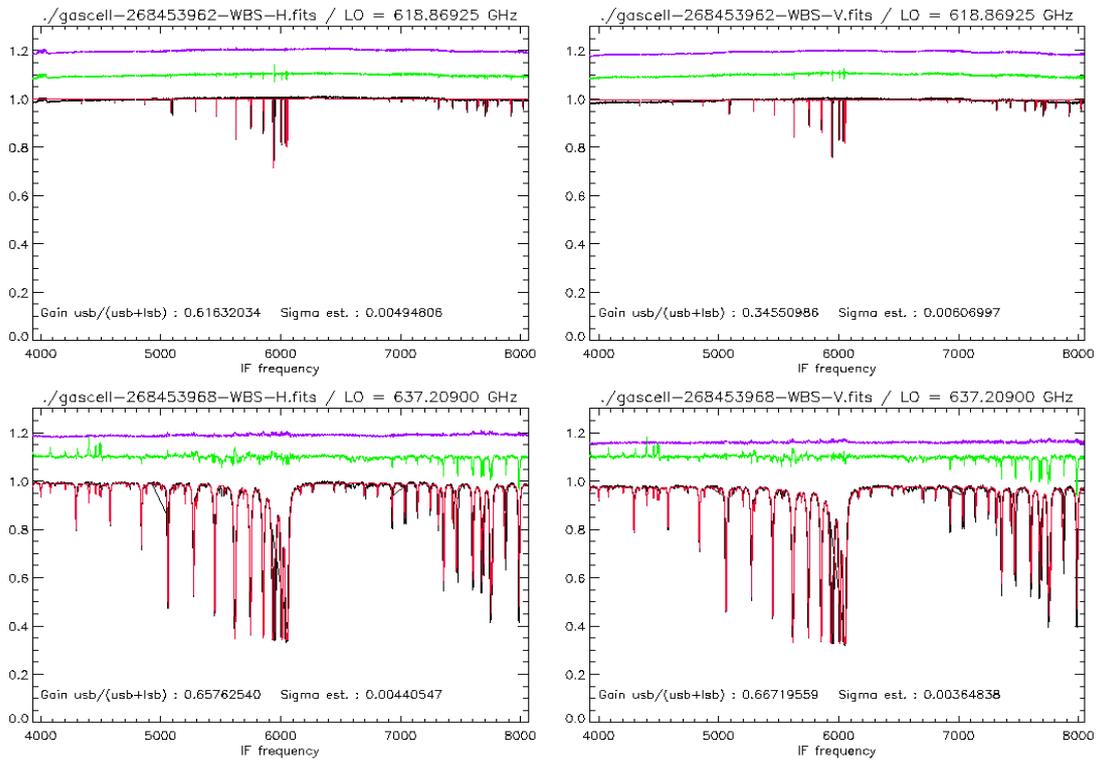
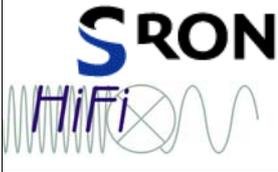


Fig.11: illustration of cases where the model deviates from the observed lines, see e.g. Obsid 268453968 at IF frequencies around 4000 MHz.

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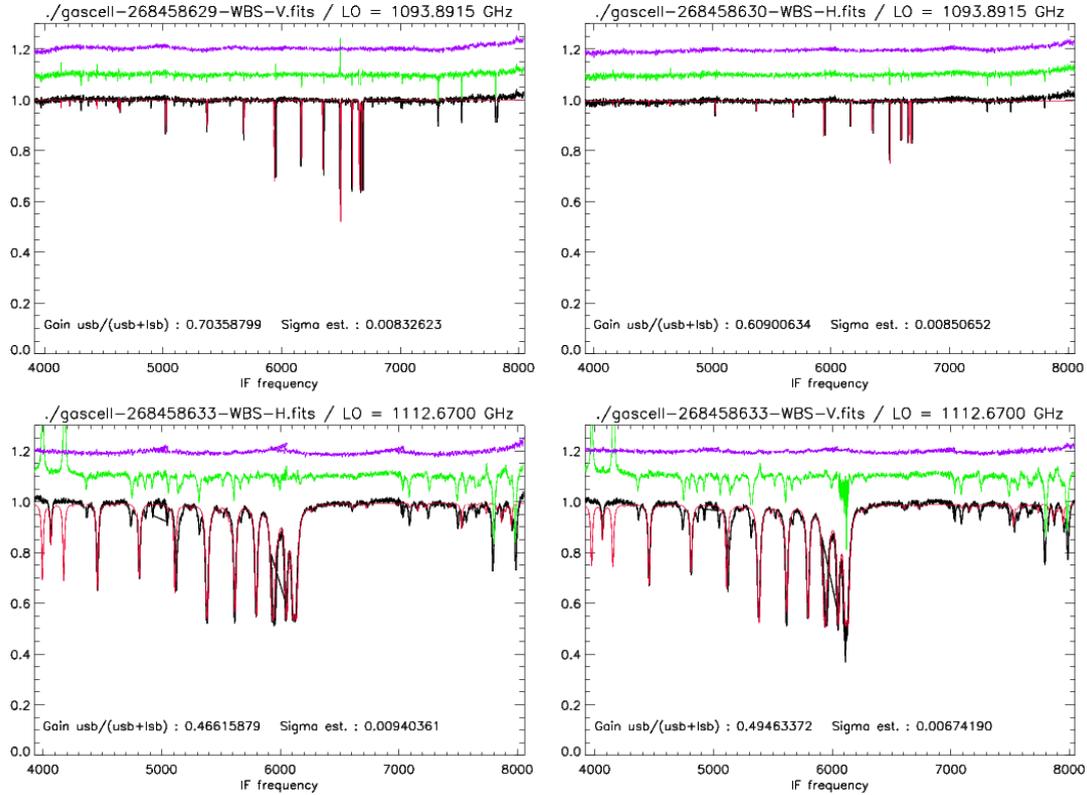
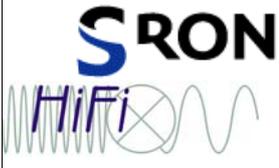


Fig.12: illustration of plat-forming and/or skewed sub-bands, like in Obsids 268458633.

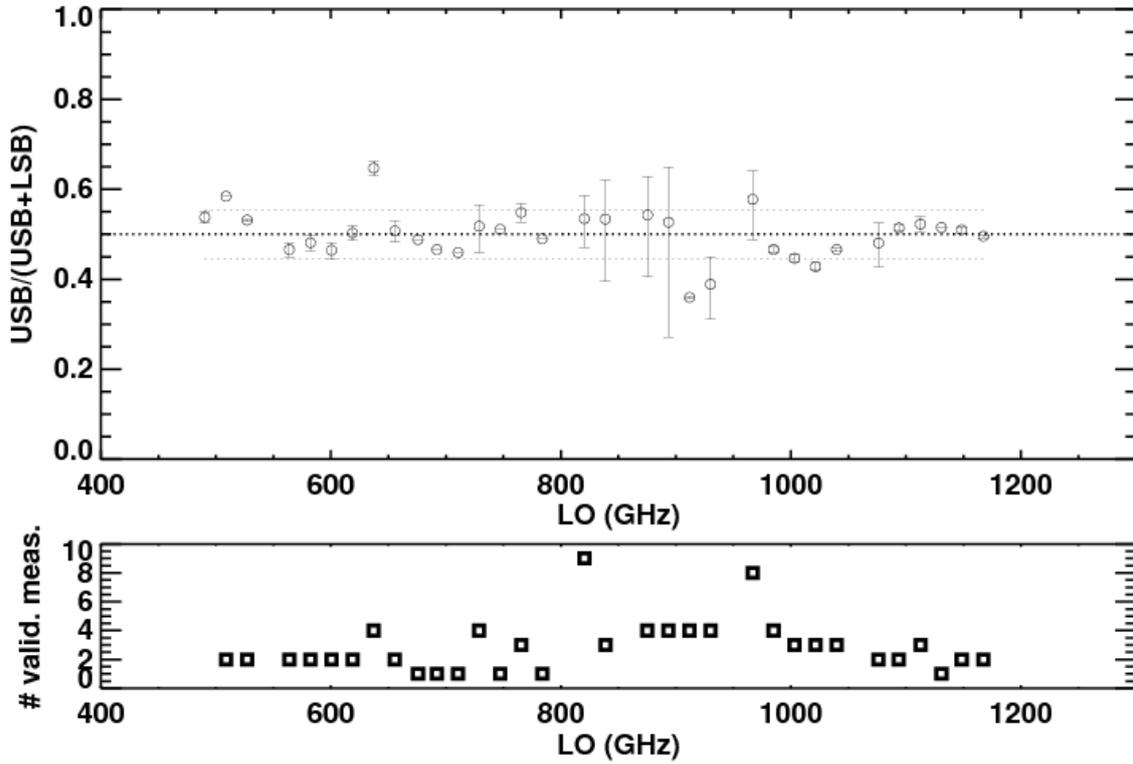
Once the « good » spectra have been analysed, one can form the frequency-dependent SBR. An assumption-free way to estimate the confidence in the SBR is to use the redundancy of spectra taken at the same tuning frequency, when available. We therefore display the results in a two window display for each polarisation. The upper panel gives the determined SBR as a function of tuned frequency, the lower one the number of individual measurements available for the determination. The SBR error bars are therefore a conservative r.m.s on the retrieved SBR. The equal gain line is drawn and the global plus or minus one sigma are also displayed.



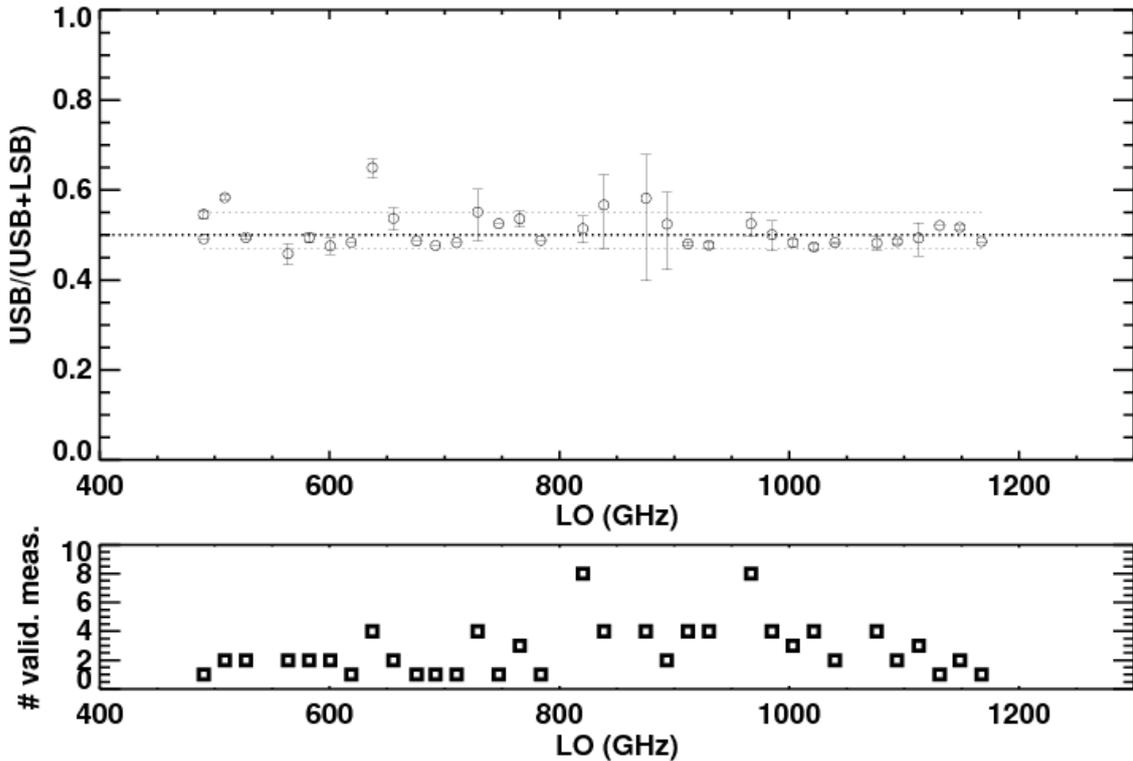
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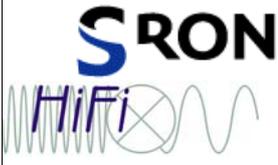
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CH3CN / Polarisation H



CH3CN / Polarisation V



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6.4.8 CH₃OH

The use of methanol data is very promising, but also very complex due to the richness of the methanol spectrum. Very recent measurements from J. Pearson et al. have allowed to build a new line catalogue covering the full HIFI range (the JPL on-line catalogue currently stops at 1THz). Line intensities are however still believed to be too inaccurate to embark onto a similar line fitting approach, but this is only a question of months before we get to the required accuracy.

TBD

6.5 Overview of line fitting results and preliminary conclusions

Although many of the molecules still need to be processed, the available results show that the initial accuracy goal of 1% will very unlikely be met. Instabilities have affected the data more than we expected and we can only rely on the statistic obtained over the various measurements. This effect is especially strong in the HEB bands and further work on the standing wave characterisation and removal is a must if we want to recover some accuracy in those bands.

The high signal-to-noise ratio measurements of CO in the low frequency band tend to show a significant slope over the 4 GHz IF bandwidth. Whether this really reflects the SBR behaviour is still to be assessed but if this is the case, this is clearly an effect that we will not be able to characterise very extensively over the HIFI operational range.

0.The side-band ratio as a calibration product

7.1 Description of the deliverable format

TBD

7.2 Error budget

TBD

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0. Appendix A: detailed equations for the absorption line profile fitting

The Voigt profile must be evaluated by numerical integration. Let us consider a Lorentzian profile f_L and a Gaussian profile f_G . The resulting line shape will result in a Voigt profile f_V , which can be expressed as the convolution of the first two:

$$f_V(\nu - \nu_0, \delta\nu_L, \delta\nu_D) = f_L \otimes f_G = \frac{\sqrt{\ln 2} a}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{[-(\ln 2)(\nu' - \nu_0)^2 / \delta\nu_D^2]}{(\nu - \nu')^2 + \delta\nu_L^2} d\nu'$$

where $\delta\nu_L$ and $\delta\nu_D$ are half-widths of the Lorentzian and Gaussian profiles respectively, $\delta\nu$ is the source frequency, $\delta\nu_0$ is the frequency of the line center and a is the ratio of the profiles width ($\delta\nu_L / \delta\nu_D$).

We used the Liu et al. (2001) empirical analytical approximation to determine the Voigt profile:

$$\begin{aligned} f_V(\nu - \nu_0, \delta\nu_V) &= c_L f_L(\nu - \nu_0, \delta\nu_V) + c_G f_G(\nu - \nu_0, \delta\nu_V) \\ &= c_L \frac{1}{\pi} \frac{\delta\nu_V}{(\nu - \nu_0)^2 + \delta\nu_V^2} + c_G \frac{\sqrt{\ln 2}}{\sqrt{\pi} \delta\nu_V} \exp\left(-\frac{(\ln 2)(\nu - \nu_0)^2}{\delta\nu_V^2}\right) \end{aligned}$$

From Olivero and Longbothom (1977, J. Quant. Spectrosc. Radiati. Transfer), one gets:

$$\delta\nu_V = 0.5346\delta\nu_L + \sqrt{0.2166\delta\nu_L^2 + \delta\nu_D^2}$$

Introducing a dimensionless parameter, $d = (\delta\nu_L - \delta\nu_D) / (\delta\nu_L + \delta\nu_D)$, the weight coefficients are given by:

$$c_L = f_1(d), \quad c_G = f_2(d)$$

where d is the profile parameter. If $d=1$ (-1 respectively), we obtain a pure Lorentzian profile (Gaussian respectively).

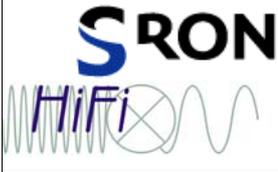
Olivero and Longbothom (1977) found from the fitting on 2 molecules that:

$$c_L = 0.68188(17) + 0.61293(31) \times d - 0.18384(39) \times d^2 - 0.11568(44) \times d^3$$

$$c_G = 0.32460(17) + 0.61825(31) \times d - 0.17681(39) \times d^2 - 0.12109(44) \times d^3$$

The pressure broadening can be obtained from the HITRAN database (<http://cfa-www.harvard.edu/hitran/>). The γ_{self} parameter (in $\text{cm}^{-1} \cdot \text{atm}^{-1}$ at 296 K) is extracted from this database and converted for the needed pressure P .

$$\delta\nu_L = \gamma_{self} \times \frac{P(\text{mbar})}{1013.25} \times 299792.45810^5$$

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The probability that a molecule in a gas at temperature T has a velocity v in a particular direction is proportional to $\exp(-mv^2/2kT)$, where m is the molecular mass. Consequently the line is symmetric and has a half width at half maximum of:

$$\delta\nu_D = \frac{\nu_0}{c} \sqrt{\frac{2(\ln 2)kT}{m}}$$

Determining the line profile, the absorption coefficient α_{max} (in units of cm^{-1}) can be obtained from I_{ba} (Base 10 logarithm of the integrated intensity in units of $\text{nm}^2 \text{ MHz}$ at 300 K quoted in the JPL and CDMS catalogs):

$$\alpha_{max}[L^{-1}] = H[L^2] \times n[L^{-3}]$$

where H is the line strength, L is the length of the gas cell and n is the density in the gas cell ($=P/kT$). H can be expressed as a function of I_{ba} (in $\text{nm}^2.\text{MHz}$; based on the integral of the absorption cross-section over the spectral line shape (see figure 1):

$$I_{ba} = H \times \left[\pi\delta\nu_L + \sqrt{\frac{\pi}{\ln 2}}\delta\nu_D \right]$$

We then get:

$$\alpha_{max} = H \times n = \frac{I_{ba}}{\pi\delta\nu_L + \sqrt{\frac{\pi}{\ln 2}}\delta\nu_D} \times \frac{P}{kT}$$

The power transmission through a uniform medium of length L at the peak of the line is $\exp(-\alpha_{max}L)$. The opacity can be computed as $\alpha_{max}L$.

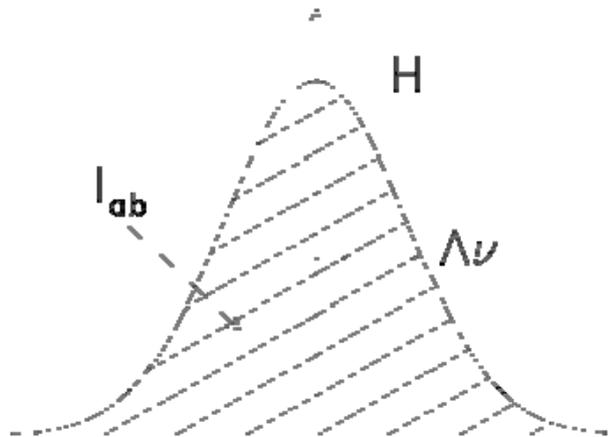
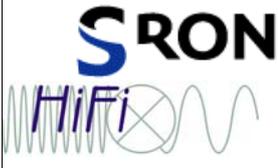


Fig 4: Gaussian line profile, with height H, and half width at half maximum $\Delta\nu$ and the integrated profile represented by the I_{ab} parameter (in $\text{nm}^2.\text{MHz}$) found in the JPL and CDMS catalogues.

	<p style="text-align: center;">HIFI FM Gas-cell measurements</p>	<p>Hifi no.: SRON-G/HIFI/TR/2008-002 Inst.no.: n Issue: Draft 1.0 Date: :16-04-08 Category: 2.</p>
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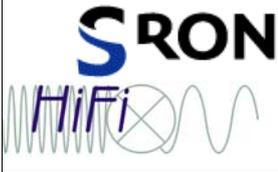
Example: ^{12}CO (4-3) transition at 461040.7682 MHz, in our 102.54 cm length cell, at T=300 K, and P=3.3 mB

(Note: 1 bar = 10^6 baryes, 1 mmHg = 0.00133 bar, 1 Torr = 1mm Hg, 760 mm Hg = 101325 Pa=1 atm=1013.25 mbar. The cgs unit for pressure is barye - 1 mB = 10^3 barye).

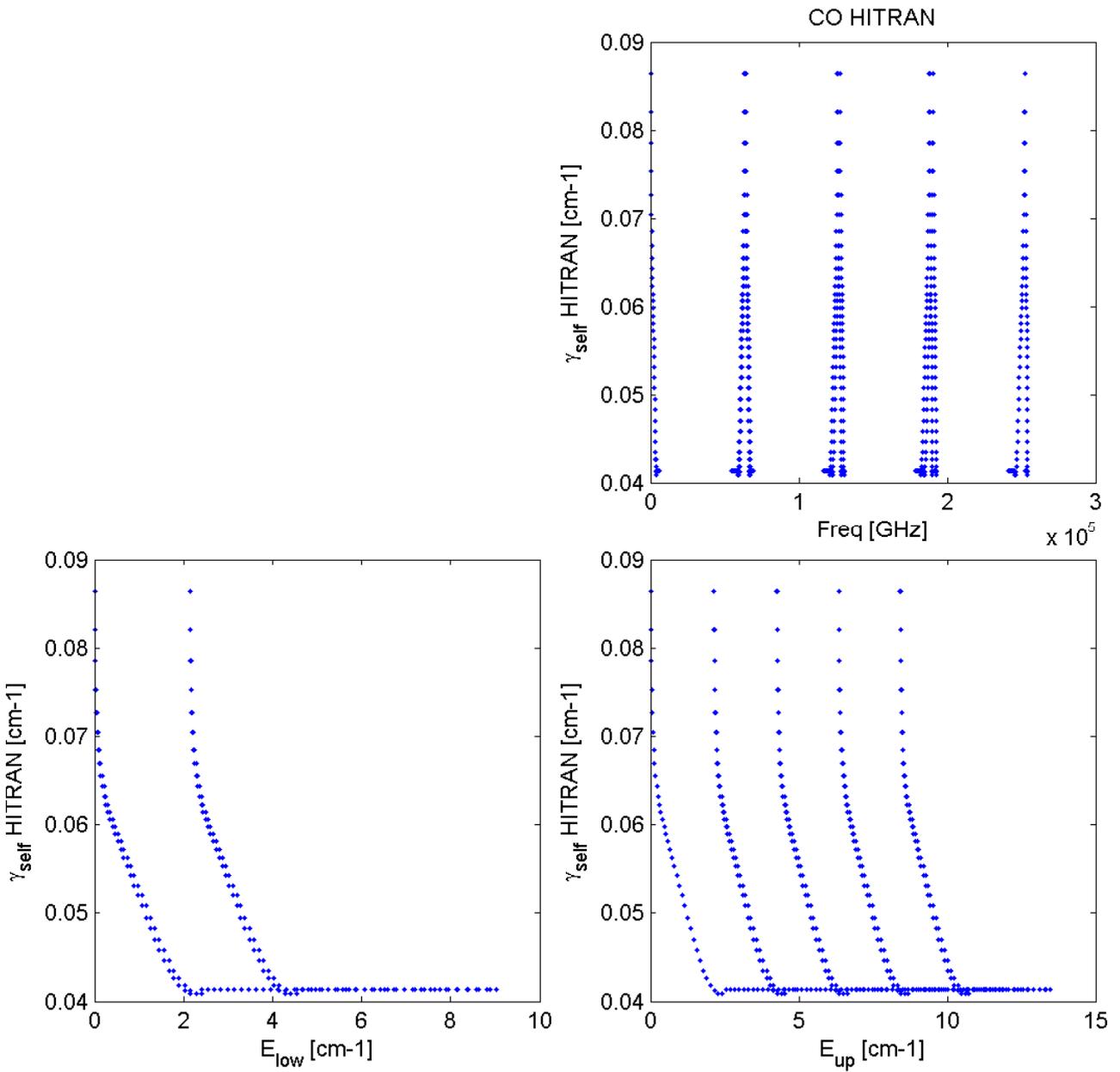
From the HITRAN database $\delta v_L = 7451480.17$ Hz. At T=300K $\delta v_D = 1076200.38$ Hz.

$$\alpha_{max} = \frac{10^{-3.2657}}{(\pi\delta_L + \sqrt{\frac{\pi}{\ln 2}}\delta_D) \times 3.02284} \times \frac{3.310^3}{1.3810^{-16} \times 300} \times 10^{-18} \times 10^{-2}$$

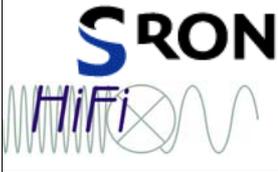
The opacity is then about $0.018 \text{ cm}^{-1} \times 102.54 \text{ cm} = 1.83$.

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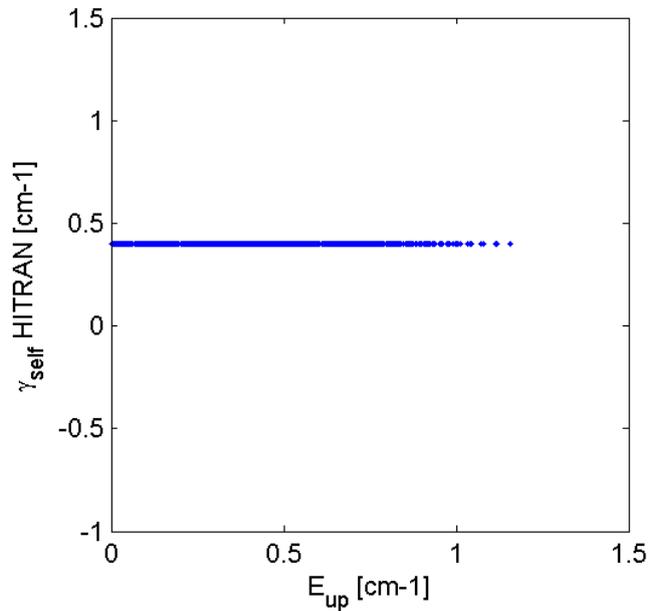
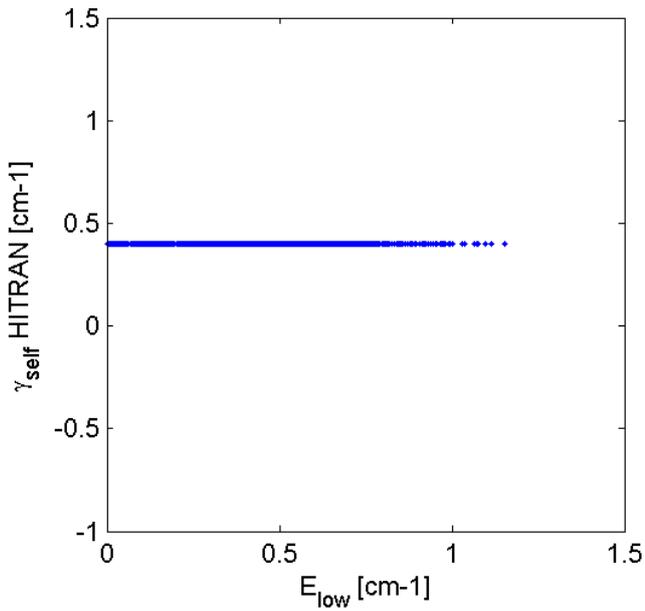
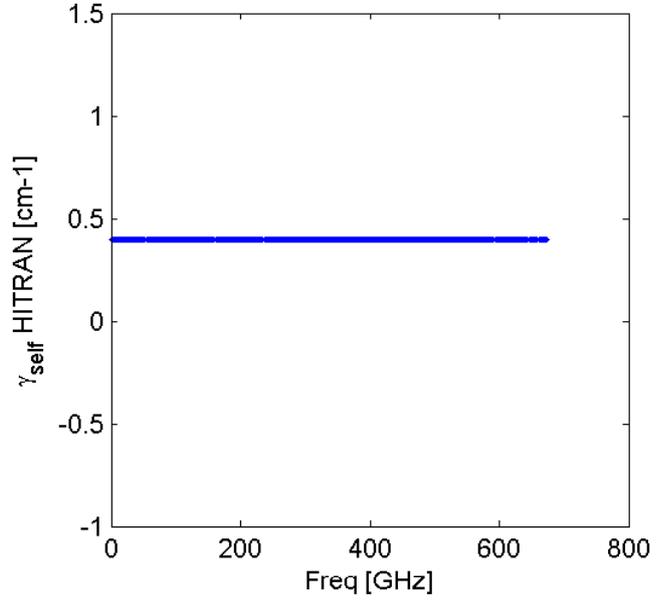
0. Appendix B: HITRAN self-broadening coefficients



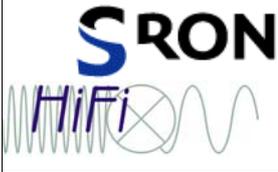
CO molecule in the HITRAN database

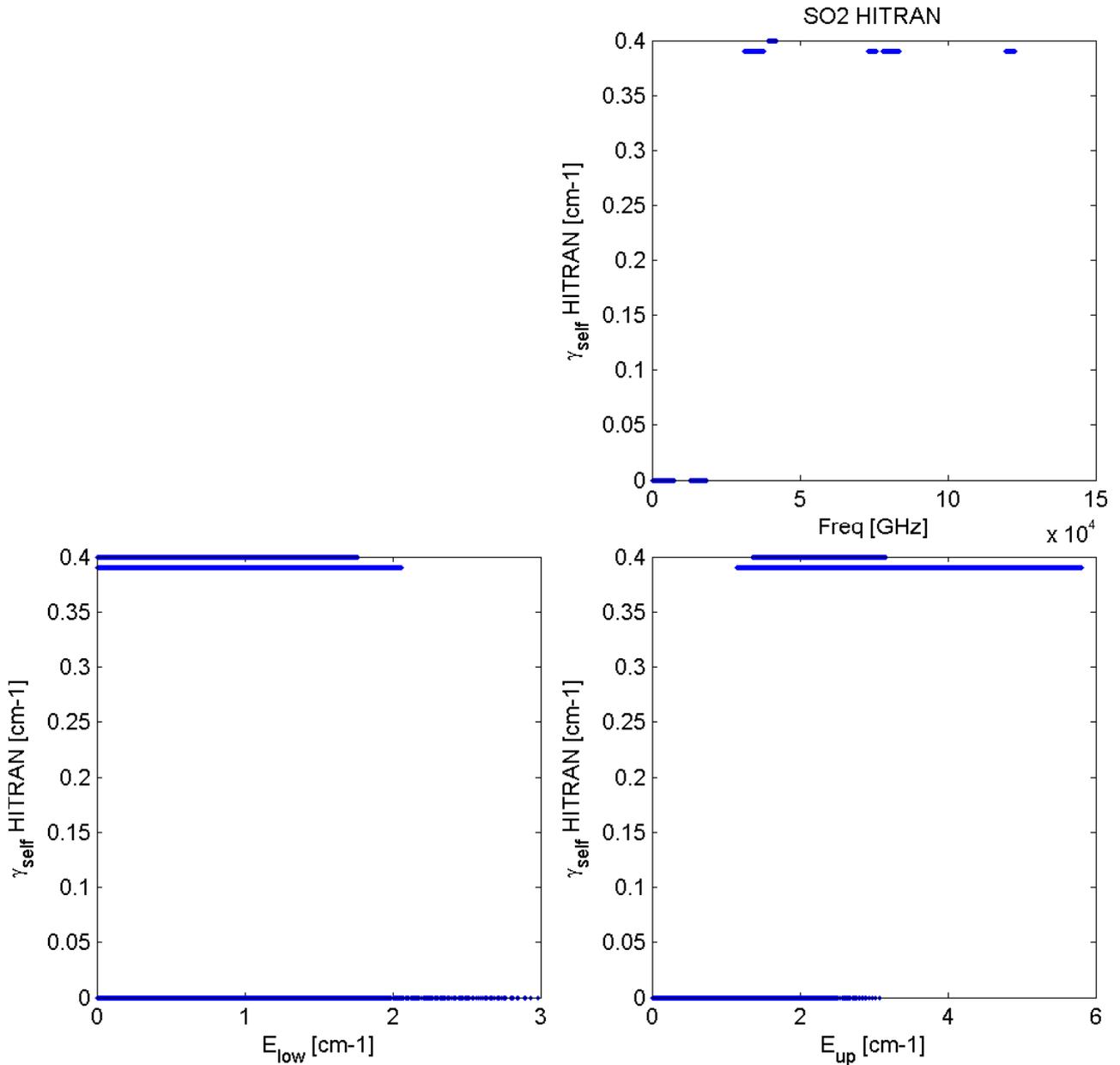
	HIFI FM Gas-cell measurements	Hifi no.: SRON-G/HIFI/TR/2008-002 Inst.no.: n Issue: Draft 1.0 Date: :16-04-08 Category: 2.
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CH3OH HITRAN

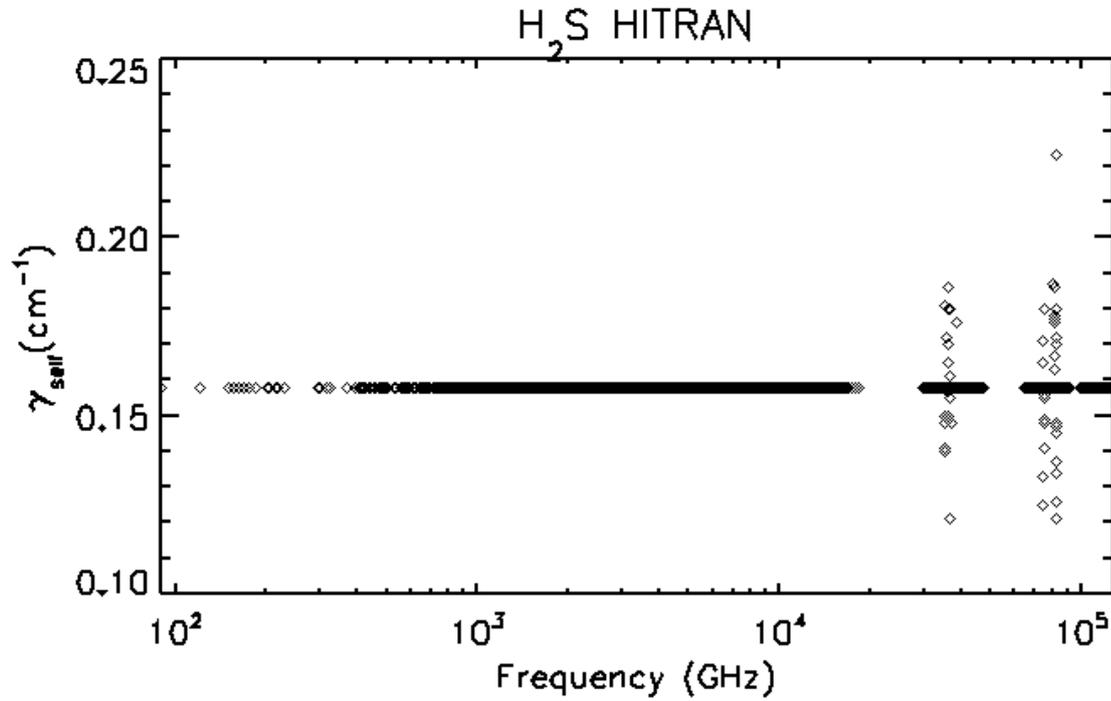


CH₃OH molecule in the HITRAN database

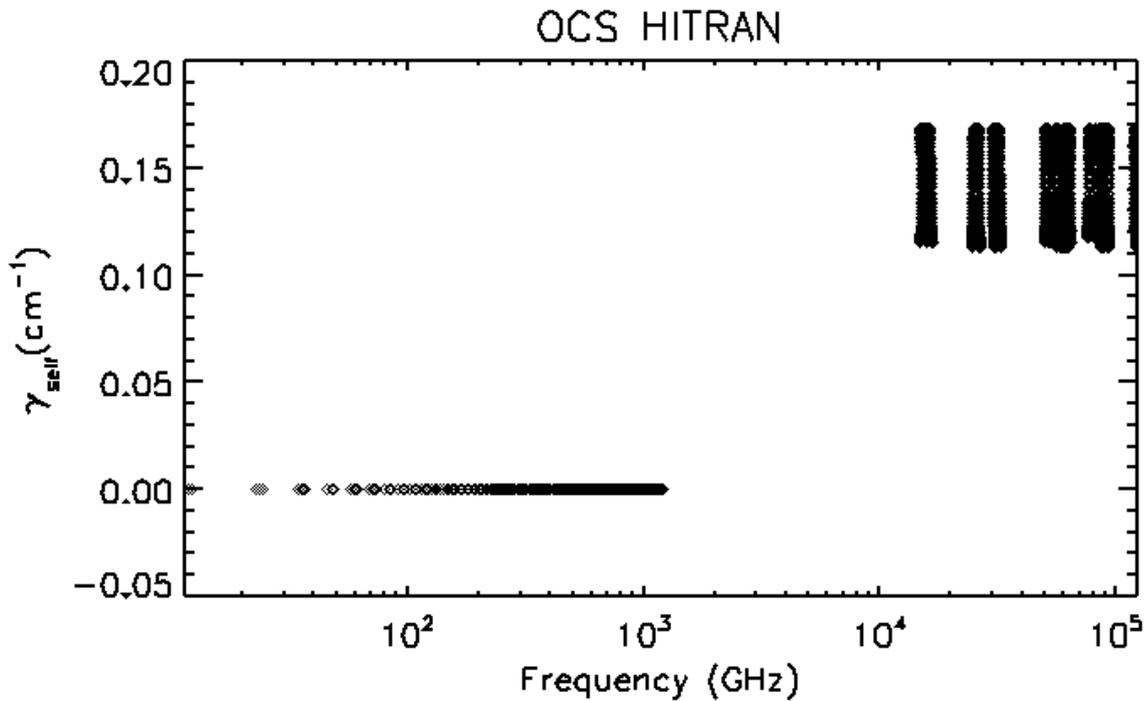
	HIFI FM Gas-cell measurements	Hifi no.: SRON-G/HIFI/TR/2008-002 Inst.no.: n Issue: Draft 1.0 Date: :16-04-08 Category: 2.
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SO₂ molecule in the HITRAN database. Note that $\gamma_{\text{self}}=0.0$ in the HIFI frequency range, so it needs to be measured by a dedicated experiment



H_2S molecule in the HITRAN database.



OCS molecule in the HITRAN database. Note that $\gamma_{\text{self}}=0.0$ in the HIFI frequency range, so it needs to be measured by a dedicated experiment.

HIFI

**HIFI FM Gas-cell
measurements**

Hifi no.: ICC/2008-124 .

Inst.no.: n

Issue: Draft 1.0

Date: :07-04-08

Category: 2 .