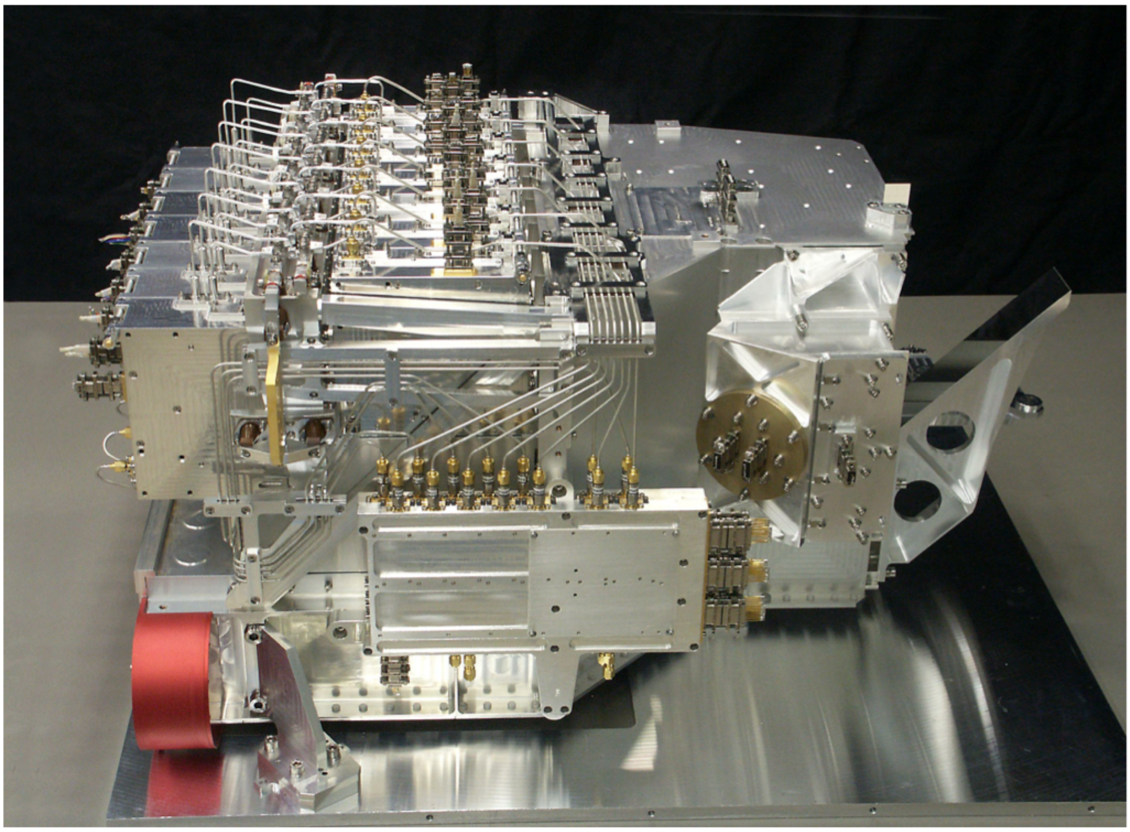
QUICK-START GUIDE TO HERSCHEL-HIFI



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HERSCHEL-HSC-DOC-2129, version 1.2, January 16, 2018

Contents

1 Instrument description

HIFI (the Heterodyne Instrument for the Far-Infrared) was the high-resolution spectrometer flown on-board the Herschel Space Observatory (de Graauw et al., 2010). It offered continuous frequency coverage in the ranges 480–1272 GHz and 1430–1906 GHz (625–240 and 208–157 μm, respectively), by means of 7 dual-polarisation (H and V) mixer bands which could be used one pair at a time. Each of the 7 bands was further split into two subbands (nicknamed “a” and “b”) referring to the respective Local Oscillator (LO) chains covering adjacent frequency ranges (Tab. 1).

HIFI was a Double Sideband (DSB) heterodyne detector, which means that two portions of the electromagnetic spectrum were simultaneously sampled onto the respective spectrometer bandwidths. Those two spectral ranges are called the Upper Sideband (USB) and the Lower Sideband (LSB), see Fig. 1 for more details.

Two types of spectrometers were offered on HIFI: a Wide-Band Spectrometer (WBS) allowing to sample the data on simultaneous bandwidths of 4 GHz (for bands 1 to 5) or 2.4 GHz (for bands 6 and 7) with a constant spectral resolution of 1.1 MHz (0.17 to 0.7 km/s depending on the observed frequency), and a High-Resolution Spectrometer (HRS) with a spectral resolution adaptable between 0.125 and 1 MHz and four different modes (*High-resolution*, *Nominal resolution*, *Low resolution* and *Wideband resolution*, respectively), and a simultaneous bandwidth between 230 MHz and 2 GHz.

HIFI was a single pixel instrument with diffraction-limited spatial resolution. This implied Half-Power Beam Widths (HPBWs) in the range 11–44 arcsec. Further details about the instrument design and components can be found in Chapter 2 of the HIFI handbook.

Band	Tuning frequency range (GHz)	Mixer type	Instantaneous bandwidth (GHz)	Typical HPBW at band centre
1a	487.5–553.5	SIS	4.0	$40''.4$
1b	562.5–628.5	SIS	4.0	$35''.3$
2a	634.0–718.0	SIS	4.0	$31''.1$
2b	722.0–794.0	SIS	4.0	$27''.7$
3a	807.0–852.0	SIS	4.0	$25''.3$
3b	866.0–953.0	SIS	4.0	$23''.1$
4a	957.0–1,053.0	SIS	4.0	$20''.9$
4b	1,054.5–1,114.0	SIS	4.0	$19''.4$
5a	1,116.2–1,236.0	SIS	4.0	$17''.9$
5b	1,235.0–1,272.0	SIS	4.0	$16''.8$
6a	1,430.0–1,558.0	HEB	2.4	$14''.1$
6b	1,578.0–1,698.0	HEB	2.4	$12''.8$
7a	1,701.0–1,794.0	HEB	2.4	$12''.0$
7b	1,793.0–1,902.0	HEB	2.4	$11''.4$

Table 1: Frequency tuning ranges of HIFI subbands.

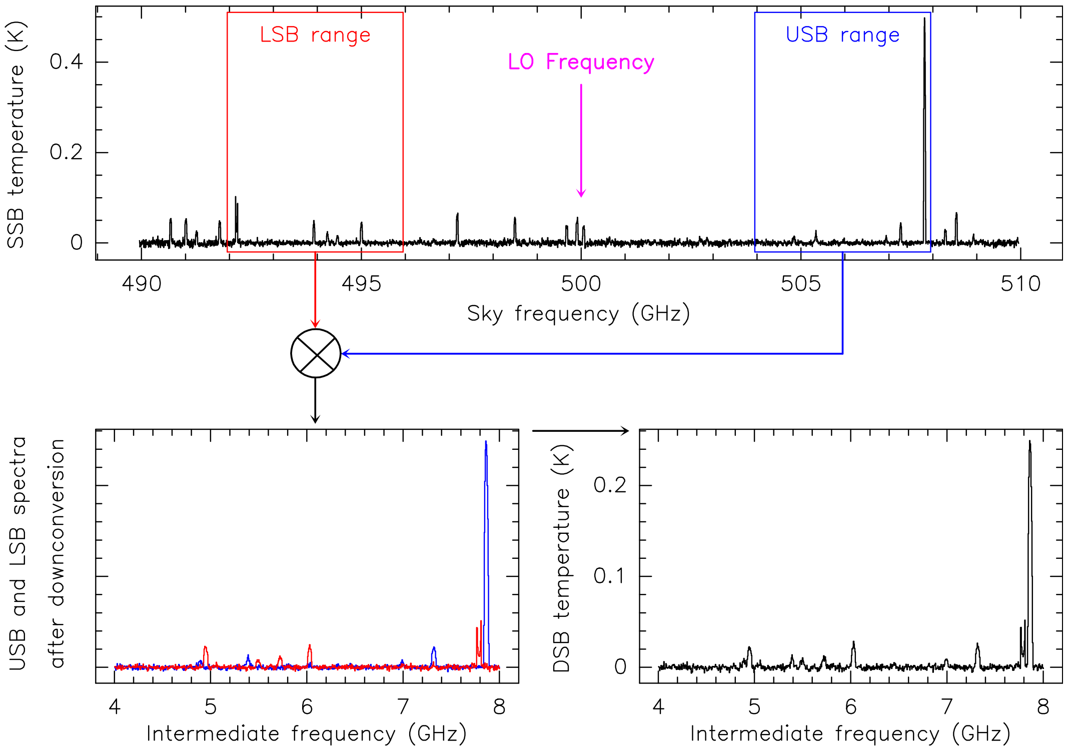

Figure 1: Illustration of the heterodyne mixing on an HIFI spectrum taken in band 1a on IRC+10216. The upper panel shows the spectrum on a sky frequency scale, together with the respective LSB and USB frequency ranges implied by tuning frequency tuning of 500 GHz, and a separation (also called Intermediate Frequency, or IF) of 6 GHz. The lower left panel shows how the respective sideband spectra (LSB in red, USB in blue) get combined in the Double Sideband spectrum by the heterodyne down-conversion. Note how the LSB spectrum gets flipped around its frequency scale. The final DSB spectrum, shown in the lower right panel, is the sum of the respective USB and LSB spectra.

2 The HIFI Observing modes

For HIFI, three Astronomical Observing Templates (AOTs) were offered to the community for mission planning:

- **Single Point**, for observing science targets at one position on the sky;
- **Mapping**, for covering extended regions;
- **Spectral Scanning**, for surveying a single position on the sky over a continuous range of frequencies within one of HIFI's 14 LO subbands.

Each AOT could be used with different modes of operation, or Observing Modes, developed from principles found at many single-dish submillimeter telescopes on the ground for providing the widest practical range of reference measurements suited to the calibration accuracy and Signal-to-Noise Ratio (S/N) goals in a variety of astronomical settings (see Fig 2).

Further details about the HIFI observing modes characteristics can be found in Chapter 3 of the HIFI handbook.

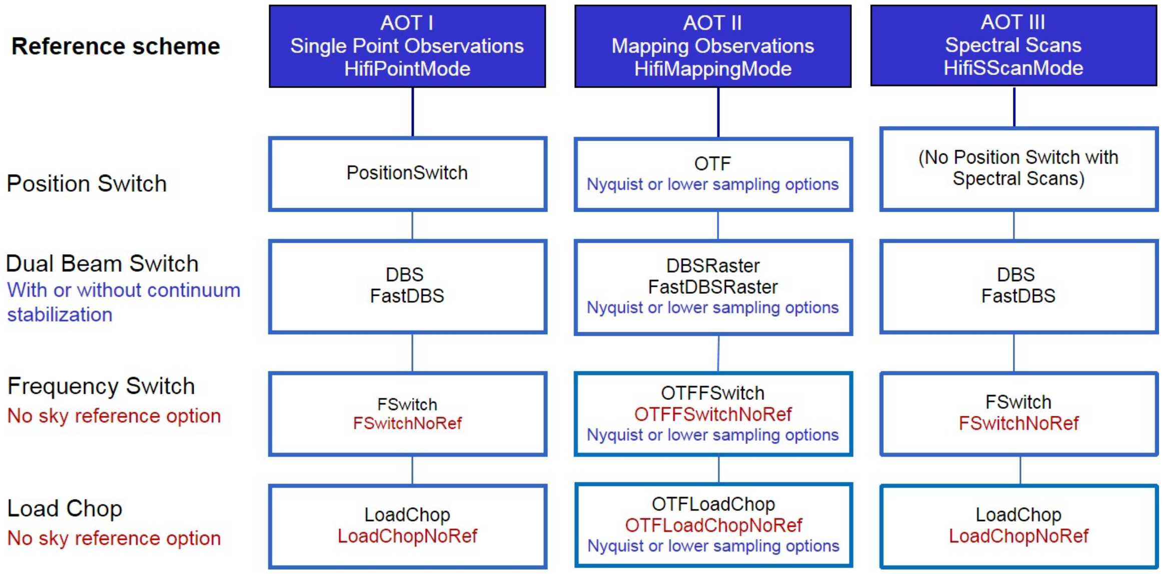

Figure 2: Overview of available AOT Observing Modes for HIFI.

3 The HIFI Pipeline and Data Products Overview

3.1 Products of the standard pipeline processing

The latest HIFI data products generated by the standard pipelines are available in the Herschel Science Archive with version 14.1.0[1]. All HIFI data come as a directory-tree structure organised by processing level. The HIFI Science data are found in the Level 0, 1, 2, and 2.5 contexts and are the result of each stage of the pipeline:

- **Level 0:** The Level 0 Context contains products not yet calibrated either in frequency or flux. It is the first data stage following that of raw telemetry and is essentially the generation of the data-frames forming the observation building blocks (calibration, science) and merged to the relevant Housekeeping. Products at this stage come as detector counts (intensity scale) against frequency channel number (”wave” scale)
- **Level 0.5:** This stage of the pipeline focusses on removing the spectrometer instrumental effects – essentially this is where the frequency calibration is performed. There are separate pipelines for the WBS and HRS spectrometers. This context is actually absent from the Observation Context as soon as the Level 1 products are successfully generated. It can, however, be re-generated if needed.
- **Level 1:** Level 1 data are frequency and intensity calibrated, and are also corrected for the velocity of the spacecraft. The application of observing mode specific calibrations, i.e., the subtraction of reference and OFF positions, and the bandpass calibration using the internal hot and cold loads, is done at that stage. Data processed to Level 1 are in the Intermediate Frequency (IF) scale (in MHz) and on the T'_A temperature scale (in K), i.e. they does not yet take into account losses due to the rearward beam.

[1]A dozen of observations needed reprocessing with HIPE 14.2 in order to correct for an isolated error

- **Level 2:** Level 2 data are converted to the antenna temperature scale T_A^* (in K) and to sky frequency (GHz). Due to the DSB frequency degeneracy, products are generated both on a USB and on an LSB frequency scale. Spectra are averaged together, per each spectrometer, for each LO setting, and each spatial position in the observation. This results in a single spectrum (for each spectrometer) for point observation mode, individual frequency tuning for spectral scans, and individual spectra per position and frequency tuning for maps. These data products may be at a publishable quality level, although corrections for baseline issues are likely required.
- **Level 2.5:** The Level 2.5 pipeline combines the Level 2 products into final products and depend on the observing mode:

  Point mode spectra are stitched, folded (in the case of Frequency Switching), and converted to a `SimpleSpectrum` format. HRS data are stitched only in the case that subbands overlap in frequency.

  Mapping mode Level 2.5 Timeline Products contain spectra that are stitched and folded (in the case of Frequency Switching). Together with those, regridded spectral cubes constructed from the stitched and folded (if applicable) spectra are present. Stitching of HRS data is done as for *Point mode* observations. In the case of spectral mapping observations carried out with a non-zero rotation angle, cubes generated from the Level 2.5 spectra and with the rotation angle applied are also made available

  Spectral Scan Level 2.5 contains a deconvolved single sideband spectrum per polarisation.

Please refer to Section 6.1 of the HIFI handbook and to the HIFI Data Reduction Guide for further details.

3.2 Other HIFI Products in the HSA

3.2.1 User-Provided Data Products

User Provided Data Products (UPDPs) are sets of products delivered by observing time holders. In the vast majority those will correspond to data collected in the framework of Guaranteed Time programmes. Since some of those products have been delivered already quite some time ago, they may actually be of inferior quality to the most recent pipeline products from the HSA. As such, the main added value of those products most likely lies in ancillary products such as catalogues, models, or combinations of data products not contemplated by the standard pipeline. The list of available products is given in Herschel UPDP page. We recommend to carefully read the release notes associated to each of those deliveries.

3.2.2 Highly-Processed Data Products

Highly Processed Data Products (HPDPs) are sets of products generated by expert scientists from the Herschel Science Centre, the NASA Herschel Science Center, and the Instrument Control Centres. In the case of HIFI, emphasis is given on those datasets where particular post-processing is deemed necessary in order to produce science-ready data, although some added-value products are also provided (see Section 5). The HPDPs contemplated by HIFI are summarised in Table 2.

HPDPs can be fetched via a dedicated query panel in the HSA, and are also available at the Herschel HPDP page.

HPDP name	Description	Release note
Spectral Scans	Baseline-subtracted deconvolved data	Teyssier et al. (2017)
Spectral Maps	Baseline-subtracted cubes, optimally regridded. These products also offer integrated intensity maps around the strongest line of interest in a given observation	Morris et al. (2016)
OFF positions	Post-processed versions of the pipeline-generated OFF position spectra. In particular, spectra are stitched. For spectral scans, deconvolved data are provided, and for DSB raster maps, OFF positions cubes are prepared	Teyssier et al. (2016c)
Uncertainty tables	Extracted uncertainty tables from the Calibration Context of the HIFI pipeline output	Teyssier (2016a)
Line lists	Line identification catalogues for each observation	Benamati et al. (2017)

Table 2: List of contemplated HIFI HPDPs

3.2.3 Ancillary Data Products

Ancillary Data Products (ADPs) are products not necessarily associated with an observation. Although a large fraction of them cover information of little interest to the archive user, we can highlight the following items of relevance for science exploitation:

- the HIFI beams (Mueller et al., 2014)
- the Mars models used by HIFI as primary calibrator, in particular to derive its beam coupling efficiencies (see Section 4)
- the database of HIFI gas cell measurements collected during the Instrument Level Tests. These are laboratory measurements that were taken with HIFI pre-launch. In particular a full methanol survey was performed during this period. Details about this dataset can be found in Higgins (2011) and Olberg et al. (2017)

ADPs can fetched via a dedicated query panel in the HSA, and are also available at the Herschel ADP page. See also Section 6.2 of the HIFI handbook for further details.

4 The HIFI Calibration

4.1 Calibration scheme

Like most radio-telescopes using heterodyne detection, the HIFI data are calibrated against a set of internal black bodies (called *hot* and *cold loads*), and a blank sky position (also called *OFF*, or *Reference* position). While the internal load measurement allows someone to calibrate out the instrument bandpass (i.e. the instrument spectral response function), the *OFF* position measurement allows to cancel out to first order the instrument response drift (Ossenkopf, 2003).

Mixer	Frequency GHz	η_{mb}	η_A	HPBW arcsec	K-to-Jy Jy/K
1H	480	0.62	0.65	43.1	482
1V	480	0.62	0.63	43.5	497
2H	640	0.64	0.64	32.9	489
2V	640	0.66	0.66	32.8	474
3H	800	0.62	0.63	26.3	497
3V	800	0.63	0.66	25.8	474
4H	960	0.63	0.64	21.9	489
4V	960	0.64	0.65	21.7	482
5H	1120	0.59	0.54	19.6	580
5V	1120	0.59	0.55	19.4	569
6H	1410	0.58	0.59	14.9	531
6V	1410	0.58	0.60	14.7	522
7H	1910	0.57	0.56	11.1	559
7V	1910	0.60	0.59	11.1	531

Table 3: Adopted values for η_{mb} (main beam efficiency), η_A (aperture efficiency), HPBW, and point-source sensitivity S/T_A^* (i.e. Kelvin to Jansky conversion factor) for one spot frequency per mixer and polarisation (Mueller et al., 2014)

This calibration scheme brings the HIFI data into an antenna temperature scale measured in Kelvin, and called T_A^*. This scale is, however, HIFI-centric and does not take into the optical coupling between the HIFI detectors and the sky through the *Herschel* telescope. This coupling loss is most commonly accounted for through the conversion of the T_A^*-calibrated data in a so-called *main beam antenna temperature* scale ($T_{\rm mb}$), or in flux density (Jansky). Detailed recipes on how to perform those conversion are given in Section 5.8.5 of the HIFI handbook. Tab. 3 summarises the corresponding coupling efficiencies measured against Mars, which is the prime calibration source for HIFI. The Mars model used to derived those is the one developed by R. Moreno (`(http://www.lesia.obspm.fr/perso/emmanuel-lellouch/mars/`). Models used specifically for the HIFI calibration can be found in the Herschel calibrator model page

4.2 Calibration Accuracy

The HIFI flux calibration accuracy is summarised in Tab. 4. Although HIFI was designed for spectroscopy, it also proved an accurate continuum detector down to flux levels as low as a few tens of Jansky (Müller et al., 2014). The absolute flux calibration uncertainties quoted in Tab. 4 are 1-σ random errors applying to the data calibrated in the T_A^*, i.e. the data coming out of the instrument pipelines and provided by the Herschel Science Archive. A systematic uncertainty of $\sim 5\%$ coming from the Mars model has to be added to those numbers.

The relative calibration uncertainty is a repeatability figure of the flux calibration measured over multi-epoch observations of secondary calibrators (essentially point sources). These numbers are not affected by the uncertainty applying to the prime calibrator model.

For the comparison of lines belonging to the same simultaneous bandwidth of a given measurement, the in-band accuracy is assumed to be $\sim 5\%$ in band 1, and below 2% in any other band.

	Band						
	1	**2**	**3**	**4**	**5**	**6**	**7**
Absolute line and continuum flux accuracy (%)							
Total uncertainty on the T_A^* scale	1.6–4	1.3–3	1.5–3	2–3	3–4	5–5.5	6
Beam efficiency	1.1	1.4	1.3	1.3	1	1.2	1.3
Aperture efficiency	1.1	1.4	1.3	1.3	1.1	1.2	1.3
Planetary model	5	5	5	5	5	5	5
Flux calibration repeatability (%)							
Line flux repeatability	NM	3–4	5–8	NM	6–9	9–12	11–12
Continuum flux repeatability	2	3–3.6	2.5–5	6	6.5	8	10

Table 4: Ranges of absolute and relative intensity flux calibration uncertainty per band. For flux calibration, a breakdown is made between uncertainties uncertainties applying to the T_A^*–calibrated data and those applying to data converted further to other scales via the coupling efficiencies. All uncertainties are given as a 1-σ root mean square error in percentage, with the exception of the planetary model which should be considered a peak-to-peak uncertainty. NM indicates that the uncertainties were not measured.

Special caution must be taken when dealing with absorption lines against a continuum. The calibration scheme of HIFI can indeed not accurately calibrate both line and continuum intensities at the same time. In practice, this implies that the line-over-continuum ratio is not necessarily correct for products obtained from either single point mode and spectral mapping observations (note: it **will** be correct for Spectral Scan deconvolved products).

Finally, the numbers presented in this section apply to a perfectly pointed observation, i.e. a source perfectly centred on the commanded telescope aperture. In practice, the pointing will always suffer from a combination of random and systematic errors that will lead to certain flux loss.

The frequency calibration accuracy is well within the instrument specification and of order 100 kHz and 20 kHz for the WBS and HRS (in High-Resolution mode), respectively.

Further details about the HIFI calibration uncertainty budget can be found in Section 5.8 of the HIFI handbook, and in Teyssier et al. (2018)

5 Science-readiness of the HIFI products and residual artefacts

In most cases, the HIFI Level 2 and Level 2.5 products offer a scientific quality that is sufficient to directly perform further data analysis (e.g. line or continuum intensity extraction). The one step that will always be necessary in any of the HIFI product, though, consists in passing from the HIFI-centric antenna temperature intensity scale to a scientifically-meaningul scale. This is explained in Sections 5.8.4 and 5.8.5 of the HIFI handbook, both for line and continuum science exploitation.

Whenever residual artefacts remain, they are mostly in the form of baseline distortion of various nature. Figure 3 illustrates the most representative cases of baseline distortion to be still expected in a fraction of the HIFI products. On top of that, spurious signals can also be present in the final data, showing up mostly as more or less narrow spectral glitches. Figure 4 shows a selection of the typical

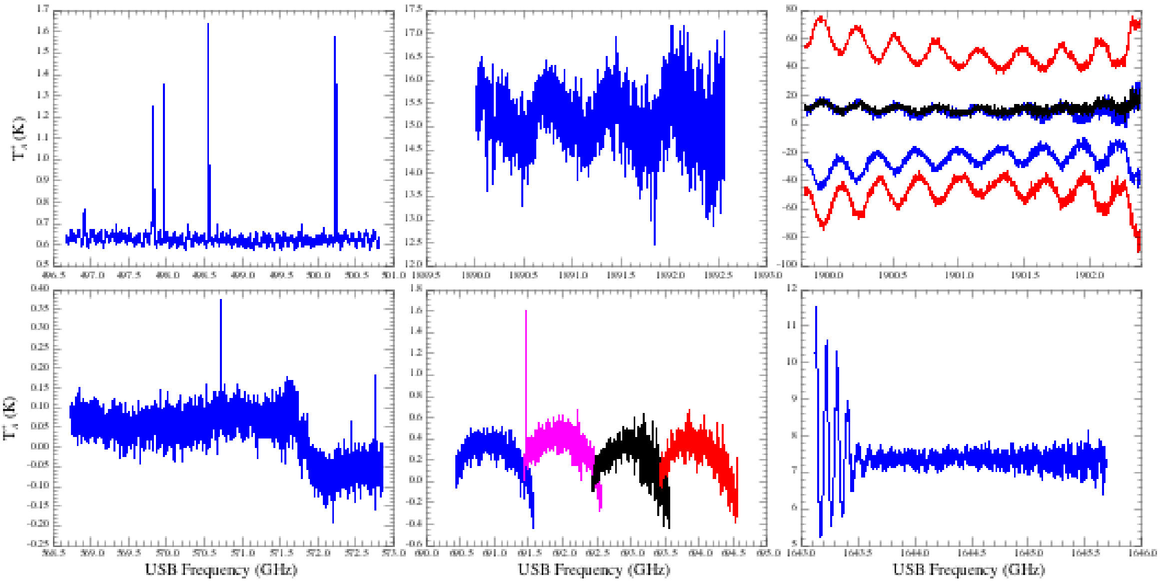

Figure 3: Overview of representative baseline distortion artefacts in the final HIFI products. Top row: various types of optical (left and middle) and electrical standing waves (right - bands 6 and 7 only). Bottom row: example of platforming (left - applies to WBS data only), parabolic residual baselines (middle - essentially for position switching observations), and residual oscillation typical of certain tunings in bands 6a.

spurs one might find in the data. For more details about those respective artefacts, please refer to Section 5.3 of the HIFI handbook.

We estimate that about 20% of the pipeline products could still be affected by such baseline distortion. As most of those cases can be easily dealt with using standard baseline correction tools, although those products are not strictly speaking *science-ready*, they can be considered at least *science-friendly*. Mitigation recipes against those effects are provided in the various sections of the HIFI Data Reduction Guide.

Because those residual artefacts are actually taken care of some of the HIFI HPDPs (Section 3.2.2), the best product to use depends basically on the availability or not of the latter. This will be particularly true for Spectral Scans and Spectral Maps taken in bands 6 and 7, which will account for about half of the residual unruly baselines in the pipeline products. Finally, the HIFI products will usually come with two different spectral resolutions (WBS and HRS data) – we leave it to the user's decision as to which of those data are the most suitable to their science (apart from isolated exceptions, the data quality will be the same in both spectrometers). The following provides a summary of the products that should be used depending on the observing mode.

5.1 Pointed Mode Observation

No dedicated artefact correction has been performed for this mode in the form of HPDPs, and we estimate that about 20% of all the pipeline products taken in this mode could still be affected by residual baseline distortion. One can distinguish the following use cases:

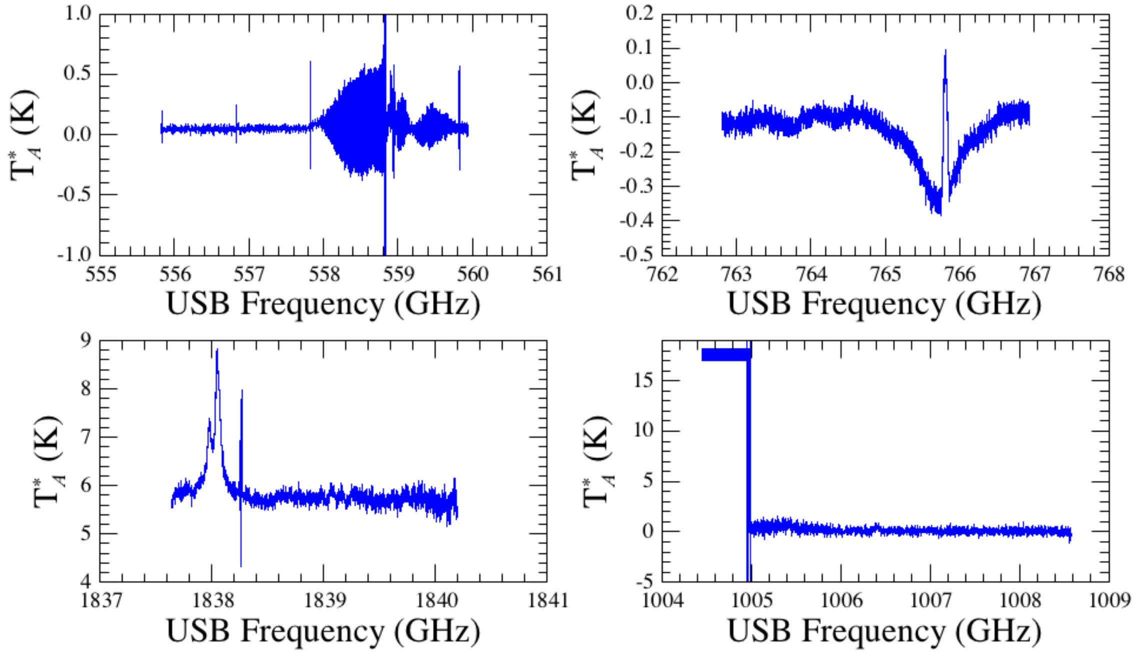

Figure 4: Example of strong narrow and broad spurious signals. Upper left: spur present in band 1a for data taken up to OD496. Upper right: example of broad spur present in band 2b. Lower left: spur present in band 7b for data taken up to OD-779. Lower right: example of saturation due to very strong spurious signals.

- Unless the data are affected by noticeable platforming or parabolic residual baseline distortion (Figure 3), the Level 2.5 stitched products should be used. Otherwise, Level 2 products are best in order to correct for those residual artefacts on a spectrometer subband basis.
- For users wishing to inspect individual Level 2 products prior to their averaging, the SPG products are not fit, instead the corresponding User Provided Data Products should be used (Section 3.2.1).

5.2 Spectral Mapping Observation

While the first use case above can also apply to HIFI spectral mapping data, HPDPs have been generated for a subset of those products, offering a higher quality level than the standard generation products. We recommend the following:

- whenever an HPDP exist for a given Spectral Map observation, this product should be primarily used. It will offer both a baseline-cleaned version of the cubes, with cube grid cell sizes optimised for signal-to-noise ratio, and integrated intensity maps centred on cherry-picked species of interest belonging to the observation. HPDPs for Spectral Maps are provided for about 1/3 of all maps obtained by HIFI, with particular emphasis on observations taken in bands 6 and 7.
- if HPDPs do not exist, the Level 2.5 spectral cubes should be used.

- irrespective of the above, in case users would like or need to re-build the spectral cubes with either improved baseline quality, or simply different re-gridding dimension, Level 2 products should be used as input for those manipulations.

5.3 Spectral Scan Observation

About 2/3 of the $\sim$ 500 Spectral Scans collected over the mission have been corrected for residual baseline distortion, and provided as such as an HPDP. When they are available, we recommend to use those as primary products for exploiting products from this observing mode. Even so, the HPDPs offer different sub-products depending on the science to be performed:

- if the users are only interested in the line information, the HPDP will provide a baseline-subtracted spectrum for each polarisation. Note that line seen in absorption in such data will not be exploitable, unless the continuum information referred to in the next bullet is used.
- in case the continuum information (alone or together with the line) is of interest, the HPDP will also contain the respective isolated continuum and the total spectrum – for this latter, the data quality is usually very similar to that of the SPG (meaning that residual baseline distortion will likely be present), and users will need to estimate a monotonous model for the continuum based on the provided inputs
- finally, in case users would like or need to re-build the deconvolved spectra with either revisited baseline correction, or potentially a different deconvolution algorithm, Level 2 products should be used as input for those manipulations.

6 Link to HELL pages for more in-depth information

The HIFI instrument and calibration page

The Herschel Explanatory Legacy Library for HIFI

The HIFI handbook.

The HIFI Product Explained document

The HIFI Data Reduction Guide

Herschel User-Provided Data Products

Herschel Highly-Processed Data Products

Herschel Ancillary Data Products

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