DOCUMENT

HIFI pre-launch laboratory gascell data: Release notes

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1 Introduction

Prior to the launch of Herschel, an extensive test campaign was performed as part of the HIFI Instrument Level Tests (ILT), in order to characterize the HIFI mixer sideband gain ratio, a key component of the flux calibration of this instrument, via laboratory gascell measurements of various gases ([1], [2]).
In particular, the HIFI gas cell was designed to present a saturated column of ^{12}CO, ^{13}CO, OCS and H_2O gas to the instrument detectors. By measuring these gases at various LO frequencies a sparsely sampled picture of the sideband ratio was generated ([3]). In addition, a full spectral scan of methanol (CH_3OH) was conducted over the seven HIFI mixer bands. It is this dataset that is now being made available to the public.
This release note describes the method applied to generate those products following a data structure identical to the in-orbit science products made available in the HSA, and presents the various products delivered in the gascell data archive. In particular, data quality caveats are reminded in order to optimise the data exploitation.

2 Description of the Ancillary Data Product

The gascell data products emulate the data structure used in standard science products acquired over the Herschel mission for HIFI, and therefore can be used and treated a similar manner. This implies in particular that standard data processing and reduction tools from the Herschel Interactive Processing Environment (HIPE[1]) can be directly used on those data. For references to the observational procedure used in the laboratory to collect the data, please see [2] and references therein. We provide in the following detailed about the processing pipeline applied to generate intermediate and top-level products provided in the gascell data archive.

2.1 Method for the product generation

The collected datasets were processed in HIPE to produce full HIFI observation contexts, albeit with non-flight observation ids, following following the procedure listed thereafter. Top-level products are also delivered in a stand-alone fashion, as will be explained in Section 3.

1. Create an empty observing context with appropriate meta data about creator, instrument etc.
2. Generate a level 0.5 product in the observing context by retrieving data from local pool of the original gas cell data.
3. Check for saturation.
4. Average spectra at level 0.5 per phase, i.e. cold/hot load, unfilled/filled gas cell.
5. Run spur finding algorithm on level 0.5 data and add resulting spur table to `Quality` product of the observing context.

[1] `https://www.cosmos.esa.int/web/herschel/hipe-download`

6. Calibrate data: $C = (h_f - c_f)/(h_e - c_e)$, where h and c stand for hot and cold, and subscripts f and e for filled and empty, respectively.
7. Insert the calibrated dataset at level 1 of the observing context.
8. For HEB data, perform an ESW (electrical standing wave) correction.
9. Generate meta data for mean continuum and noise level from pre-calculated tables. If these deviate from band specific, expected values, generate a quality comments and add these to a `Quality` product of the observing context.
10. Generate frequency scales for upper and lower sideband, i.e. USB and LSB, do a frequency conversion of the level 1 data to these scales and generate products WBS-H-USB ... WBS-V-LSB at level 2. Note, that sideband gains are kept fixed at exactly 0.5, i.e. perfect balance between upper and lower sideband is assumed.
11. Rescale spectra at level 2 such that perfectly calibrated data will have a level of 1.0 for no absorption and 0.0 for fully absorbed spectral lines. This was achieved by subtracting half the tabulated mean continuum level from step 9 above.

The original datasets from the ILT campaign contain both WBS and HRS data. However, here only WBS datasets were processed, there are no HRS data present in the resulting observing contexts.

2.2 Layout of the observation context

The layout of the observing contexts generated following the procedure described in Section 2.1 is described in the following tree diagram. Note, that `History` entries, which appear at various levels, have been omitted.

```
obs
 |__ auxiliary (empty)
 |__ calibration (empty)
 |__ level0 (empty)
 |__ level0_5
 |    |__ WBS-H
 |    |    |__ summary
 |    |    |__ 1 ...  There will typically be several datasets at level 0.5,
 |    |    |    |     in level 1 and 2 these will be averaged into one.
 |    |    |    |__ dataset
 |    |    |__ ...
 |    |         |__ dataset
 |    |__ WBS-V
 |__ level1
 |    |__ WBS-H
 |         |__ summary
 |         |__ 1 ...  only one dataset at level 1.
 |              |__ dataset
 |__ level2
 |    |__ WBS-H-LSB
 |    |    |__ summary
 |    |    |__ 1 ...  only one dataset at level 2.
 |    |         |__ dataset
 |    |__ WBS-H-USB
 |    |__ WBS-V-LSB
 |    |__ WBS-V-USB
 |__ logObsContext
 |    |__ LOG
 |__ quality
      |__ comments
      |__ SpurTable
           |__ spur
```

Each of the two accousto-optical backends (WBS-H and WBS-V) is represented by one dataset, which is of type WbsSpectrumDataset. At level 2 there are representations of each of these on a LSB and USB frequency scale (WBS-H-LSB, WBS-H-USB, WBS-V-LSB, WBS-V-USB). Table 1 lists the meta data available in a gas cell observation context at top and htp level. Tables 2 and 3 then list the meta data and columns present in each dataset.

2.3 Data caveats and artefacts

The gascell data have been collected at a phase of the Herschel history where several instrument characteristics had yet to be understood. As such, there are residual artefacts in the data that could not be dealt with in that early phase. This includes in particular:

- spectral spurious features: there can be narrow spikes present in the data, that should not be misinterpreted for real spectral features
- spectral impurity issues (esp. in bands 1a, 5a, 5b, 7a and 7b): prior to launch, HIFI was still suffering from spectral impurity in some bands. This manifested as either ghost lines present at unexpected frequencies, and/or intensities of some lines being under-estimated. This was mostly true in bands 5a and 5b. Note that this got repaired once the instrument started operation in orbit.
- the normalised continuum level should be at exactly 1 if the bandpass calibration algorithm described in Section 2.1 would work perfectly. In case of instability, this level might differ from 1, leading to less accurate absorption line levels.
- residual standing waves can still be present in the spectral baselines
- the diplexer settings for bands 3, 4, 6 and 7 were not optimal during the gascell campaign. As such intensities in those band can be wrong by typically a couple of percent.
- there is no sideband ratio correction applied to the data, owing essentially to the fact that those very data were the ones used to derive this calibration parameter. This implies that the line intensities with respect to the continuum might be erroneous up to 10% in bands 1 to 5.

Further details about those general caveats can be found in the HIFI handbook.

Figure 1 shows statistics on the quality of spectra per LO band and backend. For each of the spectral subbands, five statistical properties (min, max, mean, median, rms) were checked against reasonable expectation values[2]. For each criterion passed one point was awarded, so that good quality spectra will reach 20 and 15 points maximum for the SIS and HEB bands (due to fewer subbands), respectively.

[2]Basically we expect all calibrated intensities at level 1 to fall in the intervall 0.5–1.0 with some tolerance.

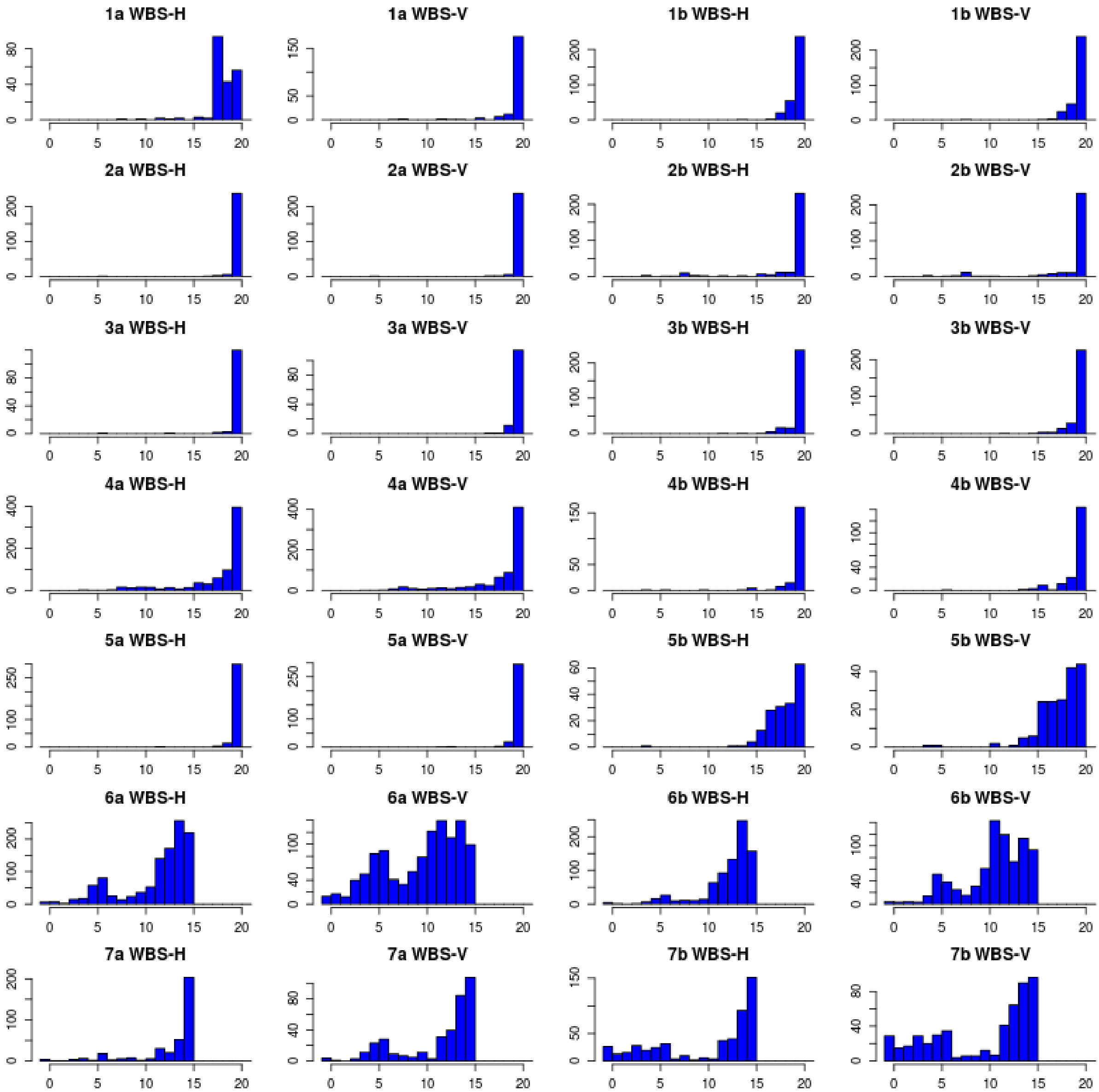

Figure 1: Statistics on quality of spectra per LO band and backend.

3 Content of the Ancillary Data Products

3.1 Deliverable format and structure

The gascell products can be found at the following link:
http://archives.esac.esa.int/hsa/legacy/ADP/HIFI/HIFI_gascell/

They will come in three main forms:

- Individual FITS files containing the stitched level 2 spectra, and hosted in the sub-directory `Individual_spectra_data`. Those are served in tar ball archives per mixer band, with names `HIFI_gascell_<band>.tar.gz`. Within each tar ball, each observation comes as a collection of FITS files named `<obsid>_HIFI_gascell_<backend>_<lof>GHz.fits.gz` with `<backend>` one of `WBS-H-USB`, `WBS-H-LSB`, `WBS-V-USB`, `WBS-V-LSB`. Each file comes with a postcard with name `<obsid>_HIFI_gascell_postcard_<lof>GHz.png`. Fig. 2 illustrates such a postcard.
- On top of that we also provide deconvolved spectra for the methanol spectra covering the whole operational range of HIFI, hosted in the sub-directory `Deconvolved_methanol_data`. The files are named:
  - `HIFI_gascell_methanol_deconvolved_band1-5.fits.gz`
  - `HIFI_gascell_methanol_deconvolved_band6-7.fits.gz`
  - They come with with postcards `HIFI_gascell_methanol_deconvolved_<band>.png` (see Fig. 3 for an illustration)
  - They are bundled together into `HIFI_gascell_methanol_deconvolved_ALL.tar.gz` and illustrated in movies as MP4 files
- Full data pools per mixer band, containing all processing levels described in section 2.2, and hosted in directory `HIPE_pools`. The pool naming convention is `gascell_<band>.tgz`. Those pools are mostly of interest to users willing to explore lower process levels within HIPE but these are not the default products to use for direct science exploitation.

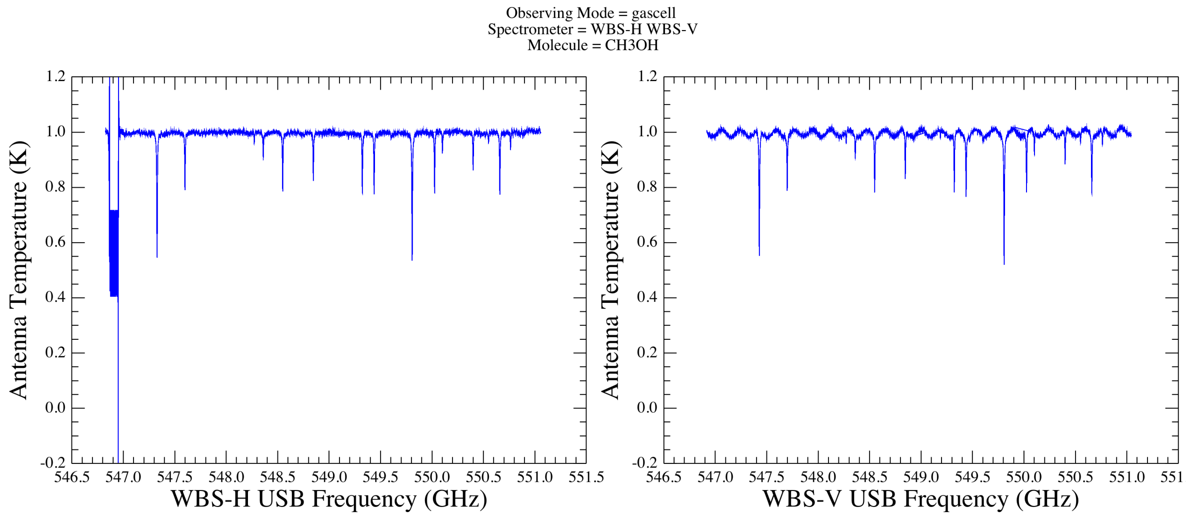

Figure 2: Illustration of a postcard for one of the gascell products in band 1. Note the presence of saturation and residual standing waves

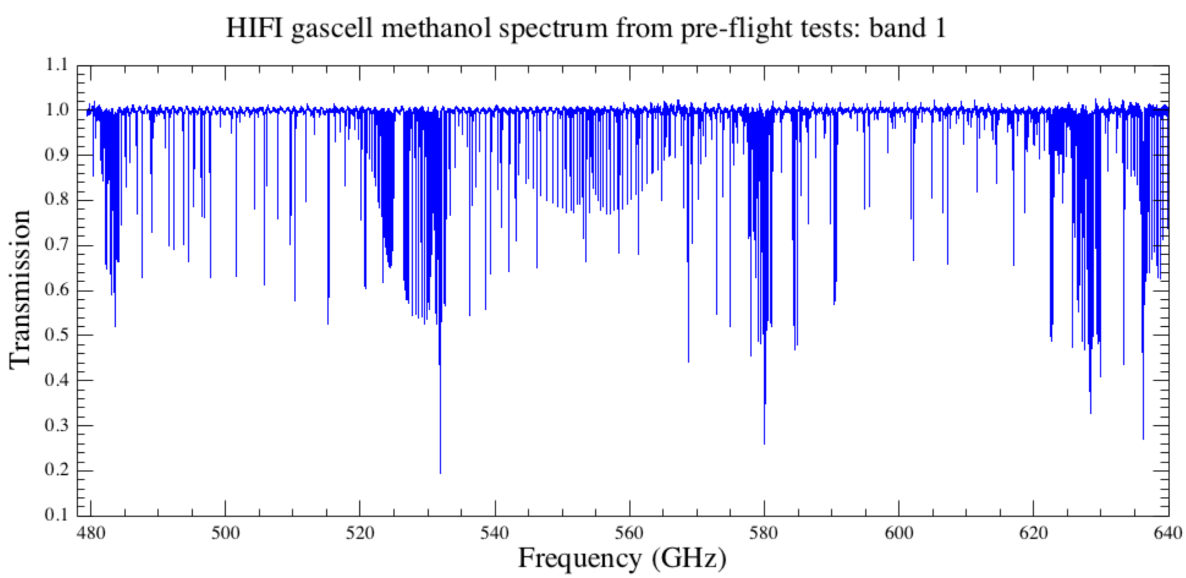

Figure 3: Illustration of a postcard for one of the methanol deconvolved spectra.

References

[1] Higgins, R., 2011, *Advanced optical calibration of the Herschel HIFI heterodyne spectrometer*, PhD National University of Ireland Maynooth.

[2] Higgins, R., Teyssier, D., Borys, C., Braine, J., Comito, C., Delforge, B., Helmich, F., Olberg, M., Ossenkopf, V., Pearson, J. and Shipman, R., 2014, *The effect of sideband ratio on line intensity for Herschel/HIFI*, Experimental Astronomy, 37, 433–452.

[3] Kester, D., Higgins, R. and Teyssier, D., 2017, *Derivation of sideband ratio for Herschel/HIFI*, A&A, 599, A115

[4] Teyssier, D., 2008, *HIFI FM Gas-cell measurements*, SRON-G Technical Report SRON-G/HIFI/TR/2008-002.

4 Appendix: products meta-data

name	value	description	where
type	OBS	product type identification	both
creator	gas cell pipeline	generator of this product	both
creationDate	2014-01-31T13:18:55	creation date of this product	both
description	HIFI gas cell data ...	name of this product	both
instrument	HIFI	instrument attached to this product	both
modelName	GAS CELL	model name attached to this product	both
startDate	2007-06-18T18:04:47	start date of this product	both
endDate	2007-06-18T18:05:02	end date of this product	both
formatVersion	1.0	version of product format	both
obsState	LEVEL2_PROCESSED		both
obsid	268511817	observation identifier	both
odNumber	-1	operational day number	obs
molecule	CH3OH	methanol	obs
aot	n/a	AOT identifier	obs
calVersion	n/a	HIFI calibration version	obs
object	gas-cell	target name	both
obsMode	DBS gas-cell	observing mode	both
Band	1a	active band	both
level	20	pipeline level	htp
apid	1030	apid	htp
fileName	hhifiwbsh...	filename for exporting purposes	htp
sideband	lsb	(only at level 2)	htp
continuum	1.0	observed continuum level	htp
noiseRms	0.0249	observed noise level (rms)	htp

Table 1: Example of meta data in the gas cell observing context and its HIFI timeline products. These data are present at observation context ("obs") or Hifi Timeline Product ("htp") levels, or both. The observation identifiers used during the gas cell campaign are from 0x10000000 (decimal 268435456) and upwards.

Table 2: Meta data of a dataset at level 1 and 2. Fixed values have been indicated in parantheses after the description.

name	*unit*	*description*	
type	–	product type identification	(HifiSpectrumDataset)
creator	–	generator of this product	(HifiPipeline)
creationDate	–	creation date of this product	
description	–	name of this product	
instrument	–	instrument name	(HIFI)
modelName	–	model name	(FM-ILT)
startDate	–	start date of this product	
endDate	–	end date of this product	
formatVersion	–	version of the product format	
apid	–	apid	(1030 or 1031)
obsid	–	observation id	
backend	–	spectrometer	
channels	–	number of channels	
hsdBuildFailure	–		
wavename	–	actual name of the wavecolumn	(frequency)
wavedescription	–	description of wavecolumn	(Double Sideband IF)
waveunit	–	units of the wavecolumn	(MHz)
OBS-revision	–	on board software revision	(3)
OBS-version	–	on board software version	(4)
OBS-patch	–	on board software patch level	(3)
Band	–	active band	
author	–	author of this product	(olberg)
origin	–	site that created the product	(HIFI-ICC)
telescope	–	name of telescope	(Herschel Space Telescope)
odNumber	–	operational day number	(-1)
raNominal	deg	requested RA	(0.0)
decNominal	deg	requested Dec	(0.0)
raDeSys	–	coordinate reference frame	(Equatorial)
posAngle	deg	position angle	(0.0)
equinox	–	equinox of coordinate system	(2000.0)
version	–	version of the product	(0.1)
level	–	pipeline level	(00)
Pipeline applied	–	pipeline modules applied	(122)
isMasked	–	Bad Pixels have been flagged	(true)
resolution	MHz	mean resolution combs spectra	
hassubbands	–	whether it has subbands	
subbandlength_n	–	length of subband ($n = 1 \ldots 4$)	
subbandstart_n	–	starting channel of subband ($n = 1 \ldots 4$)	

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loFrequency	GHz	local oscillator frequency	
polarization	–	description of polarization	
sideband	–	description of sideband	(dsb)
AOT	–	observation template	(gas-cell)
obsMode	–	observing mode	(DBS gas-cell)
sds_type	–	building block type	(science)
room_temperature_avg	K	average of the room temperature	
room_temperature_std	K	standard deviation	
gascell_pressure	mbar	pressure in the gas cell	
gainMethod	–	method used to parametrize the sideband gains	(default)
lsbGain	–	sideband gain level applied in LSB spectrum	(0.5)
lsbGain_0	–	sideband gain polynomial coefficient 0 applied	(0.5)

name	*unit*	*description*
badLo	–	set of raised LO flags (for each subband).
Band_ATT	dB	WBS individual sub-band attenuator setting
bbnumber	–	building block number
bbtype	–	building block type
bitshift	–	bit shift
buffer	–	integration buffer
Chopper	–	actual chopper positions
cmd_chopper	–	commanded chopper positions
flag_n	–	bitwise flag ($n = 1 \ldots 4$)
flux_n	–	flux ($n = 1 \ldots 4$)
{lsb,usb}frequency_n	MHz	frequency scale ($n = 1 \ldots 4$), without {lsb,usb} prefix at level 1
frequency_monitor	–	LSU frequency monitor
frmon_valid	–	valid flag for frequnecy monitor
hot_cold	K	hot and cold temperatures of the calibrator
IN_ATT	dB	WBS global attenuator setting
integrations	–	number of integrations
integrationTime	s	integration time
LOF_code	–	encoded info on local oscillator frequency
LoFrequency	GHz	local oscillator frequency
MJC_Hor	A	calibrated mixer junction current, horizontal polarization
MJC_Ver	A	calibrated mixer junction current, vertical polarization
nrbytes	–	number of bytes
obsTime	–	observation time
packetTime	–	packetization time
rowflag	–	dataframe flag
scancount	–	integrated scan count
weight_n	–	channel weights ($n = 1 \ldots 4$)

Table 3: List of columns in the datasets at level 1 and 2.