PRISMAS Data Release Note

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Contents

1 Introduction 3

1.1 PRISMAS goals . . . 3

1.2 HIFI observing strategy . . . 3

1.3 PRISMAS legacy . . . 4

2 Delivered product description 4

2.1 Reduced HIFI data . . . 4

2.1.1 Reduced data in HIPE format . . . 4

2.1.2 Data reduction summary files . . . 5

2.1.3 Reduced data in FITS format . . . 5

2.2 Quick-look plots . . . 6

2.3 Scripts . . . 6

2.4 Latest update: January 2016 . . . 6

3 Caveats and warnings 7

4 An example 7

4.1 Starting point . . . 7

4.2 Storing the (repipelined by the HSA) level2 dataset . . . 8

4.3 Compiling the necessary routines . . . 8

4.4 Reducing the level2 product . . . 9

4.4.1 Section 1 . . . 9

4.4.2 Section 2, block 1 . . . 11

4.4.3 Section 2, block 2 . . . 11

4.4.4 Section 2, block 3 . . . 11

4.4.5 Section 2, block 4 . . . 12

4.4.6 Section 2, block 5 . . . 12

4.4.7 Section 2, block 6 . . . 12

4.4.8 Section 2, block 7 . . . 12

4.4.9 Section 2, block 8 . . . 12

4.4.10 Section 2, block 9 . . . 12

4.4.11 Section 2, block 10 . . . 12

4.5 Saving and exporting . . . 13

5 Acknowledgements 13

A Sideband corrections in the continuum-divided spectra 14

1 Introduction

PRISMAS (PRobing InterStellar Molecules with Absorption line Studies) is a comprehensive spectroscopic study of key molecular line carriers, probing interstellar hydrides and carbon chains with the Herschel Space Telescope. The reference HIPE version, for both the pipeline and the data reduction scripts were initially developed, is HIPE 11.0. However part of the data was reduced with HIPE 12, and the routines were modified accordingly (see section 2.4). Since the modifications were minor and for clarity reasons, we do not discuss them in the present document.

1.1 PRISMAS goals

Our investigation is based on high-resolution HIFI spectroscopy of some 25 molecules (hydrides containing the elements H, D, C, N, O, F and Cl, see the proposal for a complete list) and full spectral scans with PACS. We take advantage of the strong dust emission from massive star-forming regions to detect multiple absorption components from foreground clouds of diverse properties that are known to intersect the selected sight-lines, along with emission and absorption intrinsic to the background sources. Our investigation is progressing on the comprehension of several topics concerning the interstellar medium (ISM), like the role of high-temperature chemical reactions in the formation of interstellar molecules, and the question of how such reactions might be driven; the role of grain surface reactions in interstellar chemistry; the growth of carbon molecules, bridging the gap between molecules and aggregates.

The updated list of the observed sources is reported in Table 1. Note that not all the target species have been observed in all the sources. Choices have been made depending on sensitivity, specific characteristics of each source, superposition with other projects, and time availability. In particular, only a few lines have been observed towards Sgr A* (+20km/s), W3–IRS5, and Circinus.

Name	R.A. (J2000) ($^{h:m:s}$)	Dec. (J2000) ($^{\circ:\prime\prime:\prime}$)	distance (kpc)
Sgr A* (+50km/s)	17:45:51.7	-28:59:08.7	8.6
G005.88-0.39 (W28A)	18:00:30.4	-24:04:00.0	3.8
G10.62-0.39 (W31C)	18:10:28.7	-19:55:50 .0	4.8
W33A	18:14:39.4	-17:52:00 .0	4.0
G34.3+0.1	18:53:18.7	+01:14:58.0	3.8
W49N	19:10:13.2	+09:06:12.0	11.4
W51	19:23:43.9	+14:30:30.5	7.0
DR21(OH)	20:39:00.7	+42:22:46.7	1.0
Sgr A* (+20km/s)	17:45:37.4	-29:05:40.0	8.6
W3 - IRS5	02:25:40.6	+62:05:51.0	1.8

Table 1: List of PRISMAS sources.

1.2 HIFI observing strategy

Except for a few Load-Chop and On-The-Fly observations of CI, CII and NII, all the HIFI PRISMAS data have been taken in double beam switching mode with a throw of 3'. Since we do not perform a systematic frequency scan, but aim at specific transitions, we are not able to deconvolve the spectra to separate the upper from the lower sideband. Nevertheless, for each transition, we use three or more different local oscillator tunings, with a separation of about 15 km/s (identified by 'A', 'B' or 'C' in the AOR names), allowing to address whether a line comes from one sideband or the other. We have also taken a few spectra using the continuum-stabilization observing option, in order to have a more reliable estimate of the continuum emission (AORs labeled with the suffix 'cont').

1.3 PRISMAS legacy

The large database of high quality spectroscopic observations acquired by PRISMAS is a precious source of information, concerning both the foreground gas and the background sources, for which we serendipitously detect a large amount of emission lines. It thus constitutes an important Herschel legacy to astrochemistry and ISM science. In order to facilitate the exploitation of this database, we provide, as described in this guide, the calibrated reduced data, corrected for instrumental effects, together with quick-look plots, spotting the main transitions, and various scripts useful to reproduce or to independently perform the data reduction.

2 Delivered product description

For each executed HIFI observation[1], the following products were generated:

- 6 files with reduced data in CLASS-readable FITS format;
- 24 files with reduced data in generic FITS format;
- four quick-look plots.

We also provide the user with all the HIPE/CLASS scripts used for the data reduction.

2.1 Reduced HIFI data

2.1.1 Reduced data in HIPE format

For each executed HIFI AOR, at the end of the data reduction, a folder is produced and stored in the Reduced_HIPE11 folder with the following naming convention:

obsid_telescope-phase_target-source_HIFI-band_target-line-approx-freq_A_target-species_HIPE11_red[2].

The products available from the latest version of the Herchel Science Archive (HSA) to date are now repipelined by default. The script Repipeline_PRISMAS.py downloads and locally stores them. After compiling the Routines_PRISMAS.py script, the data reduction procedure Reduction_PRISMAS.py can be run, generating products that are finally stored and exported in various FITS formats using the SaveExport_PRISMAS.py scripts. Eventually, in addition to the level2 products, our reduction process creates the following, so-called 'level3' products:

- level3_fringes_stitched, where the subbands in the level2 spectra have been stitched and the standing waves removed by applying the *fitHifiFringe* HIPE task;

[1] Only part of the products described in what follows is provided for the few Load-Chop and On-The-Fly observations.

[2] Telescope-phase, when present, refers to one of the 'Science Demonstration' (SDP), 'Priority Science 1' (PSP1) or 'Priority Science 2' (PSP2) phases of the HIFI observing campaign; and A, B or C, when applicable, refer to the three tunings obtained using slightly different Local Oscillator frequency (see Section 1). When present, the suffix '_cont' indicate that the observation has been performed with continuum stabilization (see Section 1) for a more reliable estimate of the continuum emission. The folders lacking the '_red' suffix have been repipelined but not yet reduced.

- level3_WBS_base_sub, where a baseline has been fitted and subtracted (using the *fitBaseline* HIFI task) to the WBS spectra obtained in the previous step. This product is intended for emission line studies, while absorption line studies should use the product level3_WBS_base_div ;
- level3_HRS_base_sub, where the WBS polynomial found in the previous step is applied to the HRS spectra. The use of such polynomial comes from the considerations that i) there is often very little free frequency range in the HRS spectra for fitting the baseline, and ii) the HRS and WBS baselines overlap always perfectly;
- level3_WBS_base_div, where the WBS spectra are normalized to the continuum value. This level, intended for absorption line studies, aims at providing the correct line–to–continuum ratio. It is built with the same polynomials previously determined and taking into account the sideband gains as described in Appendix (equations 1 and 2);
- level3_HRS_base_div, where the WBS baseline polynomials have been used, as in the previous step, to normalize the HRS spectra to the continuum values.

A few observations may lack some of these levels because of problems either in the data or encontered in the reduction procedure. Please, refer to the reduction summary files for a possible explanation.

2.1.2 Data reduction summary files

When running our scripts, the text files stored in the folder Reduction_summaries (with the naming convention described in Section 2.1.1) contain a record of the main input/output parameters for each step of the HIPE data reduction, together with comments, written by the people performing the reduction, signalling possible data artefacts or problems in the procedure. These files keep note, for instance, of the periods and amplitude of the dominant standing waves, of the polynomial parameters of the subtracted baseline, and of the value of the sideband ratio. Moreover, with the information stored here and the scripts provided, the user can reproduce the final products and, in case of need, perform a new reduction with different parameters.

A small number of the observations present significant artefacts, so, be careful when using the reduced data products. In order to check for possible problems, please, read carefully the comments, when present, in the summary file relative to the products you are interested in.

2.1.3 Reduced data in FITS format

A total of 30 FITS file is provided for each observation. 6 of them are in CLASS-compatible FITS format (their name finishes with'_Class.fits'), corresponding to the levels described in the previous question: level2, level3_fringes_stitched, level3_WBS_base_sub, level3_HRS_base_sub, level3_WBS_base_div, level3_HRS_base_div. 24 of them are in the HIPE FITS format (their name finishes with'_HIPE.fits'): 8 for the level3_fringes_stitched level (4 HRS-, 4 WBS-related, each of them comprised of both USB and LSB for the H and V polarisations), 4 for the level3_WBS_base_sub level (USB and LSB for the H and V polarisations), 4 for the level3_HRS_base_sub level (USB and LSB for the H and V polarisations), 4 for the level3_WBS_base_div level (USB and LSB for the H and V polarisations), and 4 for the level3_HRS_base_div level (USB and LSB for the H and V polarisations). The file naming convention is the same as in Section 2.1.1, with the additional suffixes referring to the corresponding levels. For instructions about how to read the fits files in CLASS, please refer to the *hiClass* task documentation in HIPE.

2.2 Quick-look plots

Four quick-look plots accompany each AOR. They have been generated running a CLASS routine over the level2 data (more specifically the level2 CLASS-compatible FITS format mentioned in the previous section), as they are the best suited to a quick-look of both absorption and emission data. The CLASS routine has been designed by T. A. Bell, and later modified by M. De Luca, who adapted its use to the release of the PRISMAS dataset. It produces one .eps file for each sub-band and takes into account ONLY the WBS-V data, resulting in three/four quicklook plots. We have then converted these .eps files to .jpeg format and made the thus generated files available in the PRISMAS database. The quick-look plots allow the user to immediately identify the main lines present in the considered sub-band, also indicating the band (signal or image) to which they belong: C I, C^+, CO, ^{13}CO, $C^{18}O$, $C^{17}O$, CH_3OH, SO, ^{34}SO, H_2CO, HCO^+, $H^{13}CO^+$, $HC^{18}O^+$, HCN, $H^{13}CN$, $HC^{15}N$, HNC, $HN^{13}C$, $H^{15}NC$, CCH, SiO, ^{29}SiO, ^{30}SiO, H_2S, H_2CS, OH, H_2O, HDO, $H_2{}^{18}O$, H_3O^+, NH_3, $^{15}NH_3$, NH_2D, CH, ^{13}CH, CH^+, $^{13}CH^+$, CS, ^{13}CS, $C^{34}S$, CN, ^{13}CN, $C^{15}N$, based on both JPL and CDMS spectroscopic data.

2.3 Scripts

Together with the reduced data and the plots, we provide all the HIPE/CLASS scripts used for the data reduction, that can be used for checking the details of the reduction procedure or for performing a new reduction using different input parameters. All the scripts are extensively commented, with evocative names chosen for routines and variables. It should thus be easy to follow and modify the procedure for all users, including those not familiar with HIPE and Jython.

The file Repipeline_PRISMAS.py is used to locally store the repipelined observations, whose names must be provided in an input file. To run this script yourself, please, read the instructions at the beginning, create the appropriate input file as described in the instructions, and adapt it to your working session. The main data reduction script is called Reduction_PRISMAS.py . It asks for an input file that has to be written by the user as described in the script itself. This script makes use of the routines defined in the file: Routines_PRISMAS.py , that should be executed entirely once, before performing the reduction. Finally, the script Save_Export.py allows the user, after adaptation to his working session as explained in the file, to save the reduced Observation Context in the local store and to save fits files readable by CLASS.

Any advice about possible improvements or report of mistakes will be very welcome. To this purpose, please use the email addresses reported in the front page of this guide. Please, keep in mind that the scripts have been developed and optimized to work with HIPE version 11.0 and, in general, we are not planning to check for compatibility with further HIPE versions.

2.4 Latest update: January 2016

The processing of all *Herschel*/HIFI AORs was a bit longer expected. Part of the reduction was conducted using HIPE version 11 (namely the following sources: W3-IRS5, DR21(OH), W28A, W31C, and W33A), and part using HIPE version 12 (G34.3+0.1, Sgr A^* - +20 and +50 km s^{-1}, W49N, and W51). The procedure that are described in the present document relate to the routines that were designed to work with version 11 of HIPE. These routines were updated to be compatible with version 12 of HIPE. The routines that we used to produce quick-look plots were also updated to be compatible with the latest version of the GILDAS/CLASS software, 'nov15b'. The principles and objectives of all updated routines remained unchanged, however, and the modifications were very minor. We provide all of the routines in both cases.

3 Caveats and warnings

Please, read carefully the data reduction summary file relative to the observation of interest before using the reduced products for pubblication, in order to check whether such observation is affected by baseline, standing wave or other serious artefacts.

Some observations, especially those taken in bands 6 and 7, present irregular baseline patterns that do not allow a meaningful global fit. There are also cases in which, although the global baseline is reasonably well fitted, individual transitions present local fluctuations in the baseline that cannot be properly taken into account with the general data reduction procedure and that deserve a more careful subtraction.

The presented data reduction does not concern the few observations taken in Load-Chop mode and the On-The-Fly modes, for which an ad-hoc data reduction will be addressed in the near future. The present data reduction does not include the treatment of observations that were designed to measure the continuum level in various *Herschel* bands, whose name contains the 'cont' character string (example: 'PSP2_PRISMAS_W28A_hifi5a_1113GHz_cont').

We would be grateful if you could acknowledge the work of the people who have performed the data reduction, in case you use the reduced data directly for publication.

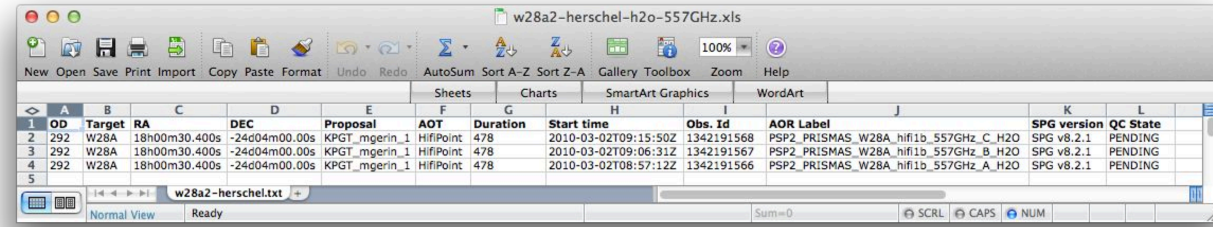
4 An example

Assume one wants to reduce the observation of the o-H_2O line at 556.936 GHz for the W28 A2 (a.k.a. G5.89–0.39) source, starting from the raw data available in the HSA with HIPE, and getting to a version that one will be able to work in a publication context in any reduction software, like CLASS. This document shows all the necessary steps to this aim.

4.1 Starting point

The Herschel Observing Log. An *Herschel Observing Log* search provides the information given in the Table shown in Figure 1. The .xls table thus retrieved indicates the observation date (OD), target name, right ascension and declination, the proposal for which the observation was done, its astronomical observation template (AOT), duration and start time, as well as its observation identity (Obsid), the label of the corresponding astronomical observation request (AOR), the standard product generation (SPG) version and quality control (QC) state. The only necessary information for the treatment described here are the Obsid and AOR label. Such information can also be retrieved from the *Herschel Science Archive* (HSA).

The o-H_2O line at 556.936 GHz in W28 A2. In our present case in point, the Table shows that three observations were done corresponding to the observation of the o-H_2O line at 556.936 GHz in



OD	Target	RA	DEC	Proposal	AOT	Duration	Start time	Obs. Id	AOR Label	SPG version	QC State
292	W28A	18h00m30.400s	-24d04m00.00s	KPGT_mgerin_1	HifiPoint	478	2010-03-02T09:15:50Z	1342191568	PSP2_PRISMAS_W28A_hifi1b_557GHz_C_H2O	SPG v8.2.1	PENDING
292	W28A	18h00m30.400s	-24d04m00.00s	KPGT_mgerin_1	HifiPoint	478	2010-03-02T09:06:31Z	1342191567	PSP2_PRISMAS_W28A_hifi1b_557GHz_B_H2O	SPG v8.2.1	PENDING
292	W28A	18h00m30.400s	-24d04m00.00s	KPGT_mgerin_1	HifiPoint	478	2010-03-02T08:57:12Z	1342191566	PSP2_PRISMAS_W28A_hifi1b_557GHz_A_H2O	SPG v8.2.1	PENDING

Figure 1: The information Table retrieved from the *Herschel Observing Log* for the observations of the o-H_2O line at 556.936 GHz in W28 A2.

W28 A2 in the PRISMAS KPGT. These observations are associated with the following (Obsid, AOR label):

- (1342191566, PSP2_PRISMAS_W28A_hifi1b_557GHz_A_H2O)
- (1342191567, PSP2_PRISMAS_W28A_hifi1b_557GHz_B_H2O)
- (1342191568, PSP2_PRISMAS_W28A_hifi1b_557GHz_C_H2O)

4.2 Storing the (repipelined by the HSA) level2 dataset

The process. The first step of the treatment consists of locally storing the already repipelined level2 product made available by the latest HSA version. This step is done by running the Repipeline_PRISMAS.py routine, for which:

- the input file is list_tobepipelined.txt in the working directory;
- the output file is list_repipelined.txt in the working directory;

The actions. Three modifications must be done:

- updating the list_tobepipelined.txt file;
- specifying the list_tobepipelined.txt file path in the routine;
- specifying the list_repipelined.txt file path in the routine;

The o-H_2O line at 556.936 GHz in W28 A2. The updated list_tobepipelined.txt file is shown in Figure 2. The paths of the input and output files are given within the Repipeline_PRISMAS.py routines at respective lines 54 and 56, as indicated in Figure 3. The run took ∼10 minutes on a standard Desktop computer for the whole three obsids considered here, and generated the list_repipelined.txt file that can be seen in Figure 4.

Important note. This treatment's step has not been tested for the load-chop observing mode, and is not expected to work for the otf-mapping mode.

4.3 Compiling the necessary routines

The process. This step simply consists in defining all the routines effectively used in the reduction, that is the next step in the whole treatment. This is done by running the Routines_PRISMAS.py routine, which takes the time to press the corresponding button on your computer.

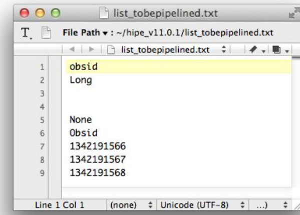


Figure 2: The list_tobepipelined.txt file for the reduction of the o-H_2O line at 556.936 GHz in W28 A2.

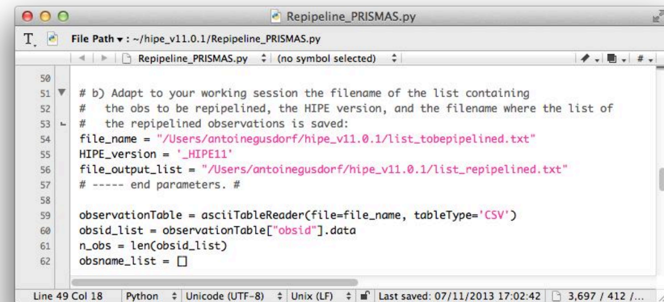


Figure 3: The modified portion of the Repipeline_PRISMAS.py file for the reduction of the o-H_2O line at 556.936 GHz in W28 A2.

4.4 Reducing the level2 product

The process. This step is the core of the treatment, as it generates the user-defined level3 product from the repipelined data (so-called level2 product). The corresponding routine, Reduction_PRISMAS.py , consists of two sections:

- Section 1, in which parameters are specified;
- Section 2, in which the reduction is done in 10 blocks.

The sections must be run block by block, each block's effect being explained below.

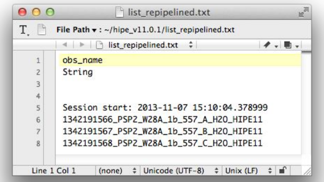
Preliminary action. The Reduction_summaries directory must be created in the working one prior to the running of the Reduction_PRISMAS.py routine. In this example, the working directory is /Users/antoinegusdorf/hipe_v11.0.1/ (see Figure 3 above).

4.4.1 Section 1

The process. The first section of this step consists of specifying parameters for the writing of the outputs generated by the Reduction_PRISMAS.py routine, which are mostly the HIPE variables related to the level3 product, and reduction summaries files (that contain details on the reduction process). For this section:

- the input file is list_tobereduced.txt in the working directory;
- the reduction summaries files are located in the Reduction_summaries directory.

The actions. Three modifications must be done:



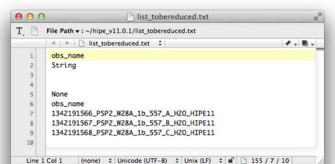
```
obs_name
String


Session start: 2013-11-07 15:10:04.378999
1342191566_PSP2_W28A_1b_557_A_H2O_HIPE11
1342191567_PSP2_W28A_1b_557_B_H2O_HIPE11
1342191568_PSP2_W28A_1b_557_C_H2O_HIPE11
```

Figure 4: The list_repipelined.txt file for the reduction of the o-H_2O line at 556.936 GHz in W28 A2.

- updating the list_tobereduced.txt file;
- specifying the list_tobereduced.txt file path in the routine;
- specifying a character string useful to the creation of the reduction summaries files.

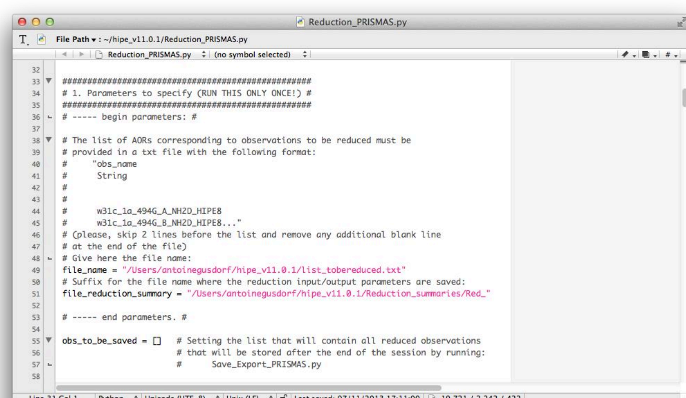
The o-H_2O line at 556.936 GHz in W28 A2. The updated list_tobereduced.txt file is shown in Figure 5. It can easily be created copy-pasting the last lines from the list_repipelined.txt file for instance (see Figure 4). The paths of the input file, and the character string mentioned above are given within the Reduction_PRISMAS.py routines at respective lines 49 and 51, as indicated in Figure 6.



```
obs_name
String


None
obs_name
1342191566_PSP2_W28A_1b_557_A_H2O_HIPE11
1342191567_PSP2_W28A_1b_557_B_H2O_HIPE11
1342191568_PSP2_W28A_1b_557_C_H2O_HIPE11
```

Figure 5: The list_tobereduced.txt file for the reduction of the o-H_2O line at 556.936 GHz in W28 A2.



```
32
33 ################################################
34 # 1. Parameters to specify (RUN THIS ONLY ONCE!) #
35 ################################################
36 # ----- begin parameters: #
37
38 # The list of AORs corresponding to observations to be reduced must be
39 # provided in a txt file with the following format:
40 #     "obs_name
41 #      String
42 #
43 #
44 #      w31c_1a_494G_A_NH2D_HIPE8
45 #      w31c_1a_494G_B_NH2D_HIPE8..."
46 # (please, skip 2 lines before the list and remove any additional blank line
47 # at the end of the file)
48 # Give here the file name:
49 file_name = "/Users/antoinegusdorf/hipe_v11.0.1/list_tobereduced.txt"
50 # Suffix for the file name where the reduction input/output parameters are saved:
51 file_reduction_summary = "/Users/antoinegusdorf/hipe_v11.0.1/Reduction_summaries/Red_"
52
53 # ----- end parameters. #
54
55 obs_to_be_saved = []    # Setting the list that will contain all reduced observations
56                         # that will be stored after the end of the session by running:
57                         #      Save_Export_PRISMAS.py
58
```

Figure 6: The modified portion of the Reduction_PRISMAS.py file for the reduction of the o-H_2O line at 556.936 GHz in W28 A2.

Important note. Only run this treatment once per block of treated observations. For instance, here it is only necessary to run it once for the three obsid 1342191566, 1342191567, and 1342191568. The section 2, though, will be run once per observation.

4.4.2 Section 2, block 1

The process. This part of the treatment defines the observation that is about to be dealt with.

The actions. Nothing to modify here, just interactively select the name of the AOR that is about to be reduced in the next blocks of this routine. The name's list is read from the list_tobereduced.txtfile.

The o-H_2O line at 556.936 GHz in W28 A2. In this case, the choice is to be made between the following names:

- (1342191566, PSP2_W28A_1b_557_A_H2O_HIPE11)
- (1342191566, PSP2_W28A_1b_557_B_H2O_HIPE11)
- (1342191566, PSP2_W28A_1b_557_C_H2O_HIPE11)

4.4.3 Section 2, block 2

The process. The aim of this step is to fit the WBS fringes.

The actions. A list of parameters can be modified in order to properly fit the fringes: the number of fringe components (nfringes), their start, end, and typical period, a usermask and associated flag. However, in the case of WBS fringes-fitting, the combination (usermask, automask) can be set to ([(0,0)],True). The quality of the fitting result is checked a posteriori, as the routine shows the fringes components that will be removed, the associated spectrum (before and after treatment), baseline and mask. A list of controlling quantities is also provided to verify that the treatment parameters are correct.

The o-H_2O line at 556.936 GHz in W28 A2. We use the (usermask, automask)=([(0,0)],True) setup, and check that the applied treatment is correct with the a posteriori displayed values for e.g., the amplitude of the removed sine waves in units of baseline fraction.

4.4.4 Section 2, block 3

The process. The aim of this step is to fit the HRS fringes.

The actions. Similar to what is done for the WBS, a list of parameters can be modified in order to properly fit the fringes: the number of fringe components (nfringes), their start, end, and typical period, a usermask and associated flag. The doglue option is also available to signal the possible lack of connection of subbands. In the case of the HRS fringes fitting, it is recommended that the number of used fringes be set to 1, and that a usermask be defined with multiple intervals corresponding to the mask that must be used for both the LSB and USB. The quality of the fitting result is again checked a posteriori, as the routine shows the fringes components that will be removed, the associated spectrum (before and after treatment), baseline and mask. A list of controlling quantities is also provided to verify that the treatment parameters are correct.

The o-H_2O line at 556.936 GHz in W28 A2. We define the usermask by inspecting the level2 obs variable data (resp. HRS-V-USB and HRS-V-LSB, for instance). The final used mask for the 1342191566, PSP2_W28A_1b_557_A_H2O_HIPE11 observation is [(556,77,557.01), (569.83,570.05)] We check that the applied treatment is correct with the a posteriori displayed values for e.g., the amplitude of the removed sine waves in units of baseline fraction.

4.4.5 Section 2, block 4

The process. The block 4 of section 2 stitches the subbands and creates the corresponding variables.

The actions. No other action than running the block is required here.

4.4.6 Section 2, block 5

The process. The block 5 of section 2 subtracts the WBS baseline and creates the corresponding variables.

The actions. No other action than running the block is required here. The used masks, and the subtracted polynomials are controlled throughout the process in an interactive mode. They can be however modified if necessary.

4.4.7 Section 2, block 6

The process. The block 6 of section 2 subtracts the WBS baseline from HRS and creates the corresponding variables.

The actions. No other action than running the block is required here.

4.4.8 Section 2, block 7

The process. The block 7 of section 2 divides the WBS by the baseline and creates the corresponding variables.

The actions. No other action than running the block is required here.

4.4.9 Section 2, block 8

The process. The block 8 of section 2 divides the HRS by the WBS baseline and creates the corresponding variables.

The actions. No other action than running the block is required here.

4.4.10 Section 2, block 9

The process. The block 9 of section 2 restores the original level2 and calibration data.

The actions. No other action than running the block is required here.

4.4.11 Section 2, block 10

The process. The block 10 of section 2 allows to save the desired data.

The actions. No other action than running the block is required here.

4.5 Saving and exporting

Preliminary action. The Reduced_fits directory must be created in the working one prior to the running of the SaveExport_PRISMAS.py routine. In this example, the working directory is /Users/antoinegusdorf/hipe_v11.0.1/(see Figure 7 below).

The process. The SaveExport_PRISMAS.py routine saves and exports the reduced data in .fits format. The checkup file list_reduced.txt is created, and contains the list of reduced data (see Figure 8). The run took ∼10 minutes on a standard Desktop computer (for the total of the three obsids considered here).

The actions. The name of the file with list of reduced data must be given as a parameter (see Figure 7).

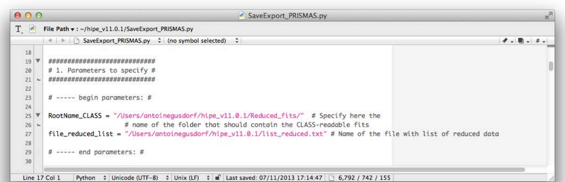


Figure 7: The modified portion of the SaveExport_PRISMAS.py file for the reduction of the o-H_2O line at 556.936 GHz in W28 A2.

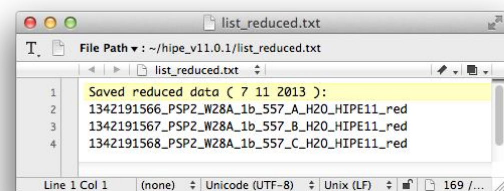


Figure 8: The list_reduced.txt file for the reduction of the o-H_2O line at 556.936 GHz in W28 A2.

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A Sideband corrections in the continuum-divided spectra

Using the following definitions:

- signal (S): the sideband where the line of interest is found, with gain $G_{\rm S}$;
- image (I): the sideband opposite to S, with gain $G_{\rm I}$;
- l: line;
- C: continuum;
- P: polynomial fit to the level2 data,

the line in the level2 signal sideband, corrected for the gain is:

$$T_{\rm level2} = T_{\rm l} + T_{\rm C,S} + (G_{\rm I}/G_{\rm S}) \cdot T_{\rm C,I}.$$

The polynomial fit to the baseline thus gives:

$$P = T_{\rm level2} - T_{\rm l} = T_{\rm C,S} + (G_{\rm I}/G_{\rm S}) \cdot T_{\rm C,I}.$$

Assuming a spectral shape of the continuum source changing slowly with the frequency (through the $T_{\rm C,I} = (1+\epsilon) \cdot T_{\rm C,S}$, relation):

$$P = T_{\rm C,S} \cdot [(1+\epsilon) \cdot (G_{\rm I}/G_{\rm S}) + 1].$$

So, the corrected continuum values are:

$$T_{\rm C,S} = \frac{P}{(1+\epsilon) \cdot (G_{\rm I}/G_{\rm S}) + 1},$$

and

$$T_{\rm I,S} = (1+\epsilon) \cdot \frac{P}{(1+\epsilon) \cdot (G_{\rm I}/G_{\rm S}) + 1}.$$

Defining the sideband ratio: $SBR = G_{\rm USB}/G_{\rm LSB}$, the correctly divided spectra for the upper and the lower sideband, are, respectively:

$$T_{\rm div}^{\rm LSB} = \frac{T_{\rm level2}}{P} \cdot [(1+\epsilon) \cdot {\rm SBR} + 1] - (1+\epsilon) \cdot {\rm SBR} \simeq \frac{T_{\rm level2}}{P} \cdot [{\rm SBR} + 1] - {\rm SBR}; \quad (1)$$

$$T_{\rm div}^{\rm USB} = \frac{T_{\rm level2}}{P} \cdot [(1+\epsilon)/{\rm SBR} + 1] - (1+\epsilon)/{\rm SBR} \simeq \frac{T_{\rm level2}}{P} \cdot [1/{\rm SBR} + 1] - 1/{\rm SBR}. \quad (2)$$