SWS AOT-1 High Resolution Processing: Documentation

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Abstract

We present a complete set of 315 high resolution processed AOT-1 speed 3 and 4 spectra. The high resolution is achieved by splitting the integration ramp in several sub-slopes per reset interval. In addition we present a complete set of 439 AOT-1 speed 1 and 484 speed 2 spectra at normal resolution, but processed through an updated pipeline and defringed. All observations are provided in two versions, normal and defringed. In addition, Browse Products were generated from the defringed spectra via a systematic process which also removed bad points detected by an additional format check. Quality reports and so-called up/down-plots are delivered to assess the reliability of specific spectral features and individual observations as a whole. A searchable catalog containing all observations with their average flux and noise per AOT-band is provided as well.

1 INTRODUCTION

1.1 SWS AOT-1

The SWS AOT-1 spectra cover the entire SWS spectral range (2.38 to 45 micron). This broad coverage could be achieved in a limited time using instrumental smoothing by moving the grating scanner over several scanner steps within one integration reset interval. There exist four different speeds for the AOT-1 spectra which are defined by their size and the number of scanner steps. Table 1 describes these speeds in terms of duration, reset interval, dwell time (time during which the grating does not move), scanner step size, number of updown scans and the degradation of the normal AOT-1 wrt. full grating resolution. More information on the AOT-1 observing mode can be found in the ISO handbook, volume V: SWS - The Short Wavelength Spectrometer.

1.2 PIPELINE PRODUCTS

The current AOT-1 products available in the ISO Data Archive (IDA) have been processed with the automatic data-analysis pipeline, i.e. Off-Line Processing (OLP) version 10.1. Each observation has three sets of data products; the ERD (Edited Raw Data), the SPD (Standard Processed Data) and the AAR (AutoAnalysis Results). In addition for some observations there exist the Survey Products, Icons and Postcards, and various Highly Processed Data Products (HPDP).

Speed	Duration [sec]	Reset [sec]	Dwell [readout]	Scanner [step size]	Resolution degradation
1	1200	1	3	4	3.2∼5.4
2	1900	2	3	2	3.5∼6
3	3600	2	3	1	2∼3
4	6500	2	6	1	1.3∼1.5

Table 1: Definition of the AOT-1 observing speeds by reset length, dwell time and the scanner step size. In the last column the degradation of the normal AOT-1 wrt. the full grating resolution is given. The degradation varies with detector band and with wavelength.

2 AOT-1 HPDP: SPEED 3 AND 4

This section describes the automatic processing which produces the high resolution AOT-1 speeds 3 and 4 products. All observations are reprocessed to the AAR using OSIA 4.0 the specific sequence of routines is listed in Appendix A. The calibration files remain the same as for OLP10.1 with the exception of CAL25 3A 060 which is an updated version of the band 3A relative spectral response function.

2.1 ERD to SPD

The pipeline uses the standard ISP_DSPD routine with the addition of the newly introduced keyword SUBSLOPE. This keyword defines the number of subslopes into which each second of the integration ramp is split. For speeds 3 and 4 the value is set to SUBSLOPE=1. This results into two sub-slopes per reset. The implementation of the sub-slope in the pipeline is described in Lahuis & Kester (2003). During the data reduction we encountered some problems in sub-routines used in the high resolution processing. These problems are briefly explained below. The routines in OSIA 4.0 are updated with the fix (see manual OSIA 4.0).

2.1.1 PULSESHAPE CORRECTION

In many observations there were some detectors that showed an improper splitting of the continuum after high resolution processing. Upon further investigation this problem was traced to an improper pulse shape application. The problem only appears when performing high resolution processing and is not deemed a significant problem for the existing OLP10.1 data products.

2.1.2 SUBSLOPE CORRECTION

In the high resolution sub-slope mode, the fitting of multiple slopes to the integration ramp could produce holes in the continuum around strong unresolved lines. This problem was traced back to the fact that the sub-slopes were not completely following the change in the integration ramp. The problem was resolved by processing with more sub-slopes and then combining slope fragments to make up the desired sub-slope. For the data processed here, each integration ramp was effectively divided into two slopes.

2.2 SPD to AAR

Several routines used for processing an SPD have been adapted in order to include the sub-slope configuration (see Appendix A). The user does not notice this, and processing an SPD to AAR uses the standard OSIA procedures in the following order. ANTIMEM reduces the memory effects. The dark current is subtracted for each band with the DARK routine. This routine uses DYNADARK for band 2 to correct for memory effects in this band. FLUXCON is used for the absolute flux calibration. The high resolution pipeline uses RESP INTER instead of the old RESPCAL to correct for the RSRF. The new correction will shift and smooth or enhance the RSRF before applying it to the data. This reduces the amplitude of the fringe residuals, and has been shown to give better results when applying FRINGES on the AAR. In addition an update of the RSRF for band 3A is used. RESP INTER uses by default RESPCAL for band 1,2 and 4 because these bands are not so sensitive to fringes. The velocity correction is done with VELCOR. After these steps, the AAR is produced with EXTRACT AAR.

2.3 DEFRINGING

AOT-band 3 has the most fringing. The RSRF (CAL25s) should remove the fringes from the spectrum. However the calibration was created from a fully extended source in the laboratory before launch and will not fully match the fringes seen in flight. RESP INTER is a routine to help correct the differences seen in flight. RESP INTER removes the RSRF only for bands 3A, 3C, 3D, and 3E by shifting and scaling the calibrated RSRF. This results in better defined fringe residuals.

In addition, the RSRF for band 3A is updated to correct some standard fringe patterns seen within the band. This update to the calibration is available in OSIA 4.0.

The defringing is done using the routine FRINGES with the keyword CYSTEP set to 10. Setting the CYSTEP keyword to a lower value will not significantly affect the found fringe components, but will increase the processing time by a large amount.

We use an updated version of FRINGES which includes the keyword QUALITY. The routine then returns a float array containing quality information of the observation, i.e. average flux, mean flux, standard deviation, and number of points used for statistics. The statistics are calculated for the standard and the defringed data and are per detector per AOT-band.

An example of the necessity for defringing is given in Figure 2. This figure also shows the noise increase of the higher resolution data.

2.3.1 GENERAL NOISE INCREASE

The sub-slope implemented in the high resolution pipeline results in a higher spectral sampling. A drawback is that the integration ramp is split in half (for speeds 3 and 4 at SUBSLOPE=1) and therefore the integration time per data point is half the integration time per point at normal resolution. This results in an increase of the statistical noise by a factor of 1.4 (noise$\approx 1/\sqrt{t}$). Upgrades in the high resolution processing tend to improve the noise. Figure 1 shows as an example the noise increase distribution of the high resolution data wrt. the normal resolution data for band 3A. On average the noise increases by a small amount.

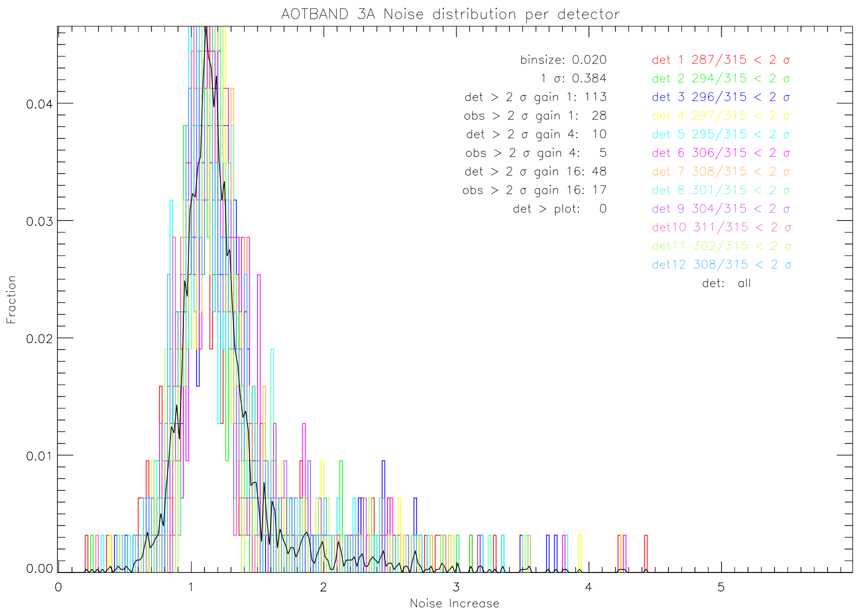

Figure 1: Noise increase distribution in band 3A. The x-axis is the ratio HPDP noise over old pipeline noise. The y-axis is the normalized fraction. The different colors represent detectors 25 to 36 of band 3A. The black line is the overall distribution.

2.3.2 LOW FLUX OBSERVATIONS

Figure 1 shows that there are observations which show a significant noise increase wrt. the low resolution data. This is visible in all bands. In general this noise increase is introduced in the sub-slope calculation for observations with low flux (i.e. around 0).

2.3.3 SHUTTER CLOSED

During the observations of TDTs 12200516 and 13501827 the shutter of the instrument was closed. These have been omitted from this product.

3 AOT-1 HPDP: SPEEDS 1 and 2

The processing of the AOT-1 speed 1 and 2 is done with the same routines as used for the high resolution processing. The only difference is that the ISP_DSPD runs in default (which is SUBSLOPE=0). This means the processing differs from the old pipeline by the pulse-shape correction, RESP INTER for band 3 and an updated RSRF for band 3A. In addition there is again a defringed version, and the statistical information for each observation is in the catalog.

3.1 DEFRINGING of SPEEDS 1 and 2

For the processing of Speeds 1 and 2, we had to be a little careful with stability of the routines. RESP INTER requires rather good signal or high sampling throughout band 3 to operate properly. Since this was not uniformly the case for all speeds 1 and 2, we used the standard RSRF correction routine of RESPCAL.

Also, for the noise determination, we obtained more stable results by turning the routine ANTIMEM off (again only for Speeds 1 and 2). ANTIMEM simply masks the first dark current samples in a dark current measurement. This has the biggest effect in band 3 which masked the first 3 points (reducing the number of dark current samples greatly). By turning ANTIMEM off, we retain more dark current points but also possible include unknown states of the dark current shutter (i.e. shutter could still be closing during the first sample).

3.1.1 FAILED DEFRINGING

For observations 37801819 and 71101311 the defringing failed for AOT band 3E. These are AOT1 speed 2 observations and FRINGES was unable to collect enough usable data points for each detector to calculate a proper continuum level. The other bands successfully completed FRINGES.

3.2 QUALITY INFORMATION

We attempt to assess the quality of our processing based on the noise measured within each AOT band for each detector. This is possible with the FRINGES routine. Spectral fragments such as an AOT band, can have significant spectral structure in terms of slopes and/or features. It is necessary to remove broad features when removing fringes in the spectral fragment. This also provides an opportunity to measure the noise on the spectrum. Without spectral features, the noise can be directly calculated as the standard deviation of the difference of the data and the smoothed continuum.

We calculated the noise on the original data as well as the newly processed AAR data. Noise calculated in this manner is likely an over estimation since it will have a strong contribution from the noise at the AOT band edges, where the sensitivity is low relative to the center of the band. Furthermore, since individual detectors may be offset from each other, the noise is more properly calculated for each detector individually.

However, in the flux-noise catalog, we list per AOT band an average flux (average over the continuum) and the combined RMS of all twelve detectors in the band. The average calculated in this way only gives a rough indication of the flux level but still useful to be able to select observations based on brightness in a particular AOT band (or combination thereof).

NOTE: We must emphasize that the noise and flux values listed in the catalog are measures of two different things and cannot be combined. In other words, the catalog is NOT suitable as low resolution broad band data.

4 CATALOG

We present a catalog of spectral noise and average band flux. The catalog lists 1237 AOT1s by TDT number, the ISO name the spectral noise and average continuum flux per AOT band. There is also a set of flags telling if the defringing was successful, whether the data are processed in high resolution mode, and a coded noise increase and the AOT band with the highest noise increase.

5 BROWSE PRODUCTS

All browse products are based on the defringed HPDP spectra and were generated with an improved version of the Browse Product Generator Software. In addition to the standard browse products – postcards, icons and survey FITS files – quality reports and so-called up/down-plots in PDF format are available to assess the reliability of specific spectral features and individual observations as a whole.

5.1 POSTCARDS AND SURVEY FITS FILES

The processing of the defringed HPDP spectra largely follows the prescription for manual reduction, i.e. sigma-clipping, flatfielding and rebinning. Though glitch recognition is performed, no attempt is made to automatically remove them beyond simple sigma-clipping. The basic processing steps for the survey FITS generation are briefly summarised in the following. Postcard graphics are based on the survey products and provided in a format similar to that available for pipeline data in the archive.

5.1.1 NOISY DETECTOR FLAGGING

Especially some of the BIBIB detectors in band 3 occasionally show increased noise, rendering the data of single detectors sometimes completely useless. In order to improve the performance of the sigma clipping and flatfielding steps, data of apparently unreliable detectors is removed in the first processing step.

Figure 2 shows an example of an affected spectrum, where one of the detectors suffers from a totally erratic behaviour. As with manual processing, the best option to automatically handle such data is to completely exclude the data of the noisy detector from further processing.

Recognition of these detectors is based on a sigma-clipping "test-run". The OSIA routine `sigclip` is applied once with a 2.5σ threshold. The percentage of clipped points with respect to the input data is then counted separately for each detector. Any detector where 50% of more of the data points were catched by `sigclip` is assumed to be affected by abnormal noise and excluded from further processing. Note, however, that not the sigma-clipped spectrum, but the unchanged data of the detectors found to be reliable is passed to the next pipeline stage.

5.1.2 FLATFIELDING

Flatielding of the detectors' signals is performed with OSIA's `sws_flatfield` routine. The flatfielding reference is generated by median combining the sigma-

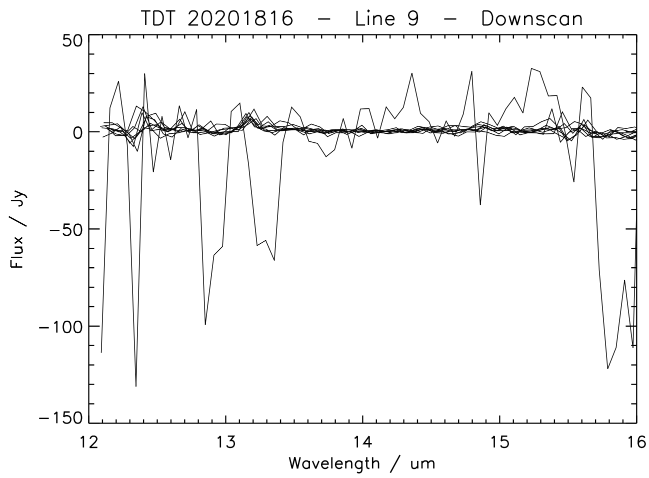

Figure 2: Example of a noisy/unreliable detector. While the signals of most detectors are well aligned, one detector (no. 36 in this case) shows an erratic behaviour, resembling of a series of large glitches or jumps.

clipped data (4σ threshold) to suppress the impact of glitches on the flatfielding result. Only the downscan data is used to minimise the influence of memory effects. The individual detector signals are flatfielded either by adding offsets or by multiplication with a gain factor. The decision which method is actually applied is based on the median flux in each line. At flux values below 100 Jy the offset method is chosen, above this threshold the gain method. Internally, `sws_flatfield` uses a second order polynomial fit to each detector's signal and the reference to determine the correct offset or gain correction.

5.1.3 SIGMA CLIPPING

The final sigma clipping is *not* based on an OSIA procedure, but uses an own algorithm, better adapted to the undersampled speed 1 and 2 data. While sigma clipping in OSIA and ISAP tends to zap away data points belonging to narrow emission lines in these observations, the new procedure avoids this at the cost of slower processing speed.

First, the width of the bins used to compute the local noise and flux is dynamically chosen for each individual line. The resolution of each line is estimated by dividing the median wavelength difference between two data points of a given detector by the median wavelength of the line. In the case of speed 1 and 2 data, the sigma clipping bin width is equal to one such resolution element, and doubled for speed 3 and 4 data. This guarantees that at least one data point of each detector contributes to the statistics in the bin. The typical resolutions for all AOT bands at the different speeds are listed in Table 2. Second, the new sigma clipping routine does not use a series of non-overlapping bins, but centres one bin over each individual data point. While this increases processing time, it is the only working solution to avoid clipping of narrow spectral features in speed 1 and 2 data.

The most extreme point in each bin is excluded from statistics calculation, and median and standard deviation of the remaining points are determined. One round of sigma clipping is performed with a threshold of 2.5σ.

Band	Resolution for speed:		
	1 & 2	3	4
1A	265	1070	2130
1B	220	870	1730
1D	275	1090	2180
1E	180	720	1430
2A	260	1040	2070
2B	155	620	1240
2C	265	1060	2110
3A	230	910	1830
3C	300	1190	2380
3D	185	740	1480
3E	230	920	1820
4	310	1230	2380

Table 2: Single-detector resolution used for the calculation of sigma clipping bin width and rebinning resolution.

5.1.4 AVERAGING & REBINNING

The averaging and rebinning of the detectors and scan directions in each line is performed with OSIA's `sws_rebin`. The end product is five times oversampled with respect to the original resolution, as determined above. Data points are weighted by their standard deviation, and Gaussian smoothing with the instrumental profile is used to suppress high-frequent noise. The standard flux-conserving algorithm of `sws_rebin` is used.
The final survey FITS product is obtained by strict zapping of all off-band data.

5.2 QUALITY REPORT AND UP/DOWN-PLOTS

Each set of browse products includes a quality report in text format and a 12-page PDF file, the so-called up/down plot. Both files help to assess the reliability of an observation and to recognise specific problems with the data.
The text report is divided into the following sections:

5.2.1 INPUT DATA FORMAT CHECK

Prior to any processing, the input data undergoes a simple format check. Data points with offending entries, e.g. invalid detector numbers or wavelength values, are found and reported. At the time being it is not clear where such points originate from.

Data points with a flux value of exactly 0.0 Jy, apparently not corresponding to a real measurement, are reported as well.

5.2.2 AAR REPAIR REPORT

In order to allow smooth processing of the data, all data points marked by the format check are removed from the input data. The actions of this symptomatic repair procedure are summarised in this section of the quality report.

All repaired input files are available as part of the HPDP sets in the archive. While some of the original files cannot be read with standard tools like OSIA and ISAP due to format errors, the corrected versions have been checked for compatibility.

5.2.3 DETECTOR RELIABILITY REPORT

The detectors which were found to show excessive noise and had to be removed from the data are listed in this section together with the affected line numbers.

5.2.4 OUT-OF-LIMITS REPORT

This report summarises the number of points where the integration ramps reached at some point the saturation level (partially out of limit, PoL) or where the signal was completely above the flux limit for reliable measurements (totally out of limit, ToL). Both conditions can be the result of particle hits (glitches), but in some data sets the source flux simply reached the limits. While up to two percent of PoL data in bands 1-3 are normal, higher rates may indicate increased space weather. In band 4, up to 5 percent can be frequently observed under normal conditions.

The presence of ToL-data is generally associated with high glitch rates or very bright source fluxes and should always be a reason to carefully check the raw data.

5.2.5 PHOTOMETRIC GAIN REPORT

For bands 2-4, the photometric gain of each detector block was determined for each observation using the internal calibration sources. The results are available in the FITS headers of the pipeline products. Any deviation of the gain factor from the mean value for the whole mission is flagged in this section of the quality report. Possible reasons are increased space weather, which caused debiasing of the detectors, and problems during the internal calibration.

Please note that observations during the performance verification phase may be flagged in this section due to different settings of the detector bias voltages.

5.2.6 PIPELINE GLITCH FREQUENCY REPORT

The frequency of glitches, that were already flagged by the pipeline, was calculated from the input data and compared to mean values for the whole mission. Significant deviations are reported in this section and are generally indicators for increased space weather.

Observations in the performance verification phase may be flagged due to different susceptibilities of the detectors to particle hits, caused by non-standard bias voltages.

5.2.7 BLOCK GLITCH DETECTION REPORT

The browse product generator tries to identify block glitches, i.e. sudden flux changes in all or most detectors of a band at the same time, caused by particle hits. This is done by checking for significant correlated signal changes in the flux-vs.-time domain. For each identified event, the instrumental time key (ITK), scan direction, and mean wavelength are given. The significance of the detection is encoded in three values:

- **CORREL:** is a measure for the correlated flux change of all detectors at the time of the glitch. The higher this value, the more detectors are affected by the glitch, and the higher is the peak value.
- **SIGNI:** is a measure of the goodness-of-fit when a glitch model is applied to the glitch candidate. The higher this value, the more probable is an impact of the glitch on the final product
- **CORRATIO:** is the ratio of the correlated flux in the two scan directions. The higher this value, the smaller is the probability that this is a real spectral feature and not a glitch that occurs only in one of the scan directions.

Further, the start and end wavelength of the affected data portion are given in the column `WAVES`, and a combined 'glitch penalty' value, computed from the three significance indicators above is printed in the column `PENALTY`. If the glitch does not only affect a single data point per detector, but has an exponentially decaying tail, this is flagged in the last column. A rough estimate of the width of the affected wavelength range is given. Possible detector block jumps, i.e. sudden flux changes lasting for a very long time, are marked in this column as well.

5.2.8 DETECTOR GLITCH DETECTION REPORT

This is similar as the block glitch report, but considers events where only one detector displays a sudden flux change. A glitch penalty value indicates the significance of the detected event. As for block glitches, the length of a possible glitch tail is given.

5.3 UP/DOWN PLOTS

There exist two plots for each line of the observation with slightly different content. In both plots, red data points refer to downscan data (scan direction -1, increasing wavelength) and blue points to upscan data (scan direction +1, decreasing wavelength). The upper plot on each page contains the sigma-clipped spectrum before averaging and rebinning of the data. Visual inspection can reveal obvious up/down differences and help to assess whether a spectral feature in the survey product is real or not.

The second plot shows the difference between an assumed mean spectrum and the up/down data, normalised by the typical noise of the observation. The noise is determined locally, i.e. in a small bin centred over each data point. Significant differences between the signal in the opposite scan directions pop up as vertical gaps between the up/down data. This representation allows the visual identification of up/down differences even in data with high dynamic range, e.g. emission line spectra of planetary nebulae.

Figure 3 shows an example survey product spectrum, in this case band 1A data. The emission feature at 2.55 μm could in principle be a shifted H_2 transition line. The up/down plot in Figure 4 reveals that it is in fact an artefact, caused by a positive glitch in the upscan data.

5.4 REMARKS ON GLITCH DETECTION AND REPORT

The glitch detection information in the quality report cannot replace a careful visual inspection of the raw data if optimal data reduction is needed. However, they can help in a first assessment of the data quality and to check whether a spectral feature in the survey product may have been caused by a glitch. While most of the block glitches reported for AOT speed 1 and 2 observations can be easily found in the up/down plots as well, some may only be identified by looking into the unclipped raw data, e.g. with ISAP.

This is especially true in the case of AOT speed 3 and 4 observations, where only the strongest glitches - with CORREL values well above 100 - will leave a signature in the final product. Still, they are present in the data and should be considered if the data is to be further reduced and analysed. The same holds for detector glitches, which are effectively suppressed by the browse product generator's clipping algorithm.

The glitch reports are best used together with the up/down plots. Visual inspection of the flux differences between the two scan directions and comparison with the list of glitch candidates allows to distinguish between a real spectral feature and a glitch artefact in most cases.

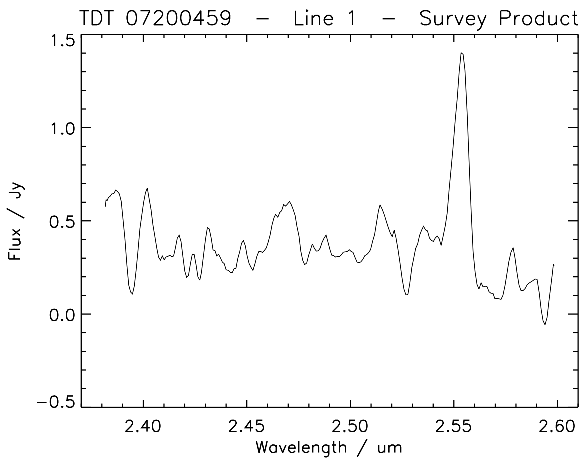

Figure 3: Survey product spectrum with a possible spectral feature or glitch at 2.55 μm.

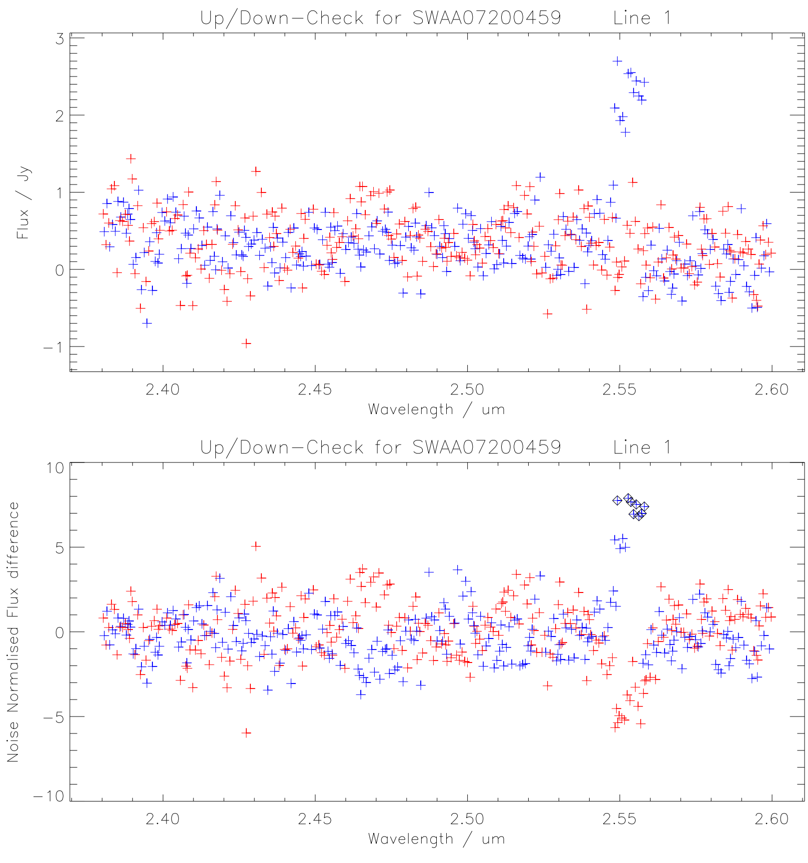

Figure 4: Same spectrum in U/D representation. The feature at 2.55 μm turns out to be caused by a positive glitch in the upscan data (blue points).

6 END PRODUCT

6.1 FILENAME CONVENTION

The high resolution HPDP speed 3 and 4 are available in two versions. The following file convention is used.
swhaC*tdt*.fits : high resolution processed AAR (speed 3/4)
swhfC*tdt*.fits : high resolution processed defringed AAR (speed 3/4)

The HPDP speed 1 and 2 are also available in two versions. A similar convention is used but only indicates that the non-defringed product has been processed with the OSIA 4.0 pipeline as described in this document.
swhaC*tdt*.fits : reprocessed AAR (speed 1/2)
swhfC*tdt*.fits : reprocessed and defringed AAR (speed 1/2)

An original version of this HPDP contained only files named:
swha*tdt*.fits swhf*tdt*.fits

These have been replaced by the swhaC and swhfC files respectively, after having passed through the additional format check which also removed bad points. Please see Section 5.2.2 for more details.

In addition, the following files are provided:

ssph*tdt*.fits :	Survey FITS files, compatible with ISAP.
spch*tdt*.fits :	Postcard graphics, generated from the survey products.
sqrh*tdt*.txt :	Quality report in ASCII text format.
udch*tdt*.pdf :	Up/Down plots as 12-page PDF document.

Appendices

A Scripts

The routines given here can be used to reproduce the AOT-1s. They are implemented and fully upgraded in OSIA v4.0. The manual explains the changes made.

High resolution processing speed 3 and 4:	**ISP_DSPD,SUBSLOPE=1** **ANTIMEM** **DARK** **FLUXCON** **RESP_INTER** **VELCOR** **EXTRACT_AAR** **FRINGES,CYSTEP=10,QUALITY=quality**
Speed 1 and 2 processing:	**ISP_DSPD** **ANTIMEM** **DARK** **FLUXCON** **RESPCAL** **VELCOR** **EXTRACT_AAR** **FRINGES,CYSTEP=10,QUALITY=quality**

B FRINGES

To examine the fringes that have been removed from a specific defringed observation, follow the procedures described here in OSIA 4.0.

Read the standard and defringed AAR
aar=READ_FAAR(swha*tdt*.fits)
aarf=READ_FAAR(swhf*tdt*.fits)

Extract fringe patterns
aarfringes=aar
aarfringes.data.flux=aar.data.flux/aarf.data.flux

Plot fringes for a specific band
plotaar,aarfringes,band='*aot_band*'

C FAILED OBSERVATIONS

There was a small set of observations which failed the DSPD processing. These were 13501827,12200516,12501616,12601620,40201614,14801733,70301713, 87700502, 87702501. These are all indicated in the IDA as having some major failure. There are also 6 which we list as failing FRINGES in one AOTBAND: 37801819, 71101311, 25601404, ,63103501, 07200272, 30101147. Some of these observations failed FRINGES because there was no data for a given aperture while others failed because the noise increase was too high (greater than a factor of 5).

The Observers SWS Interactive Analysis (OSIA) software package is distributed by the SWS consortium and is available at: `http://iso.esac.esa.int/ ==> ISO Data Analysis Software ==> OSIA`

References

Lahuis, F., & Kester D. 2002, *SWS AOT-1 High Resolution Processing*, February 2003 (see ISO documentation under `http://iso.esac.esa.int/`)

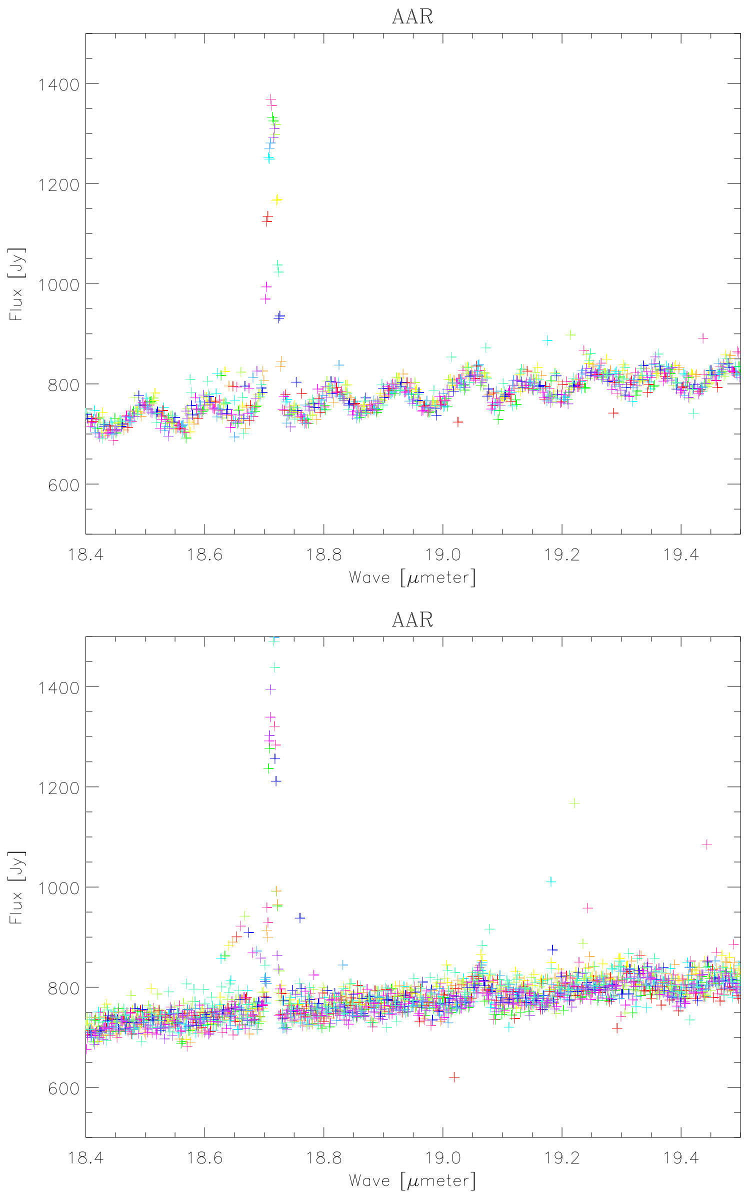

Figure 2: These figures show the utility of FRINGES. The top figure is the OLP10.1 AAR for a spectral fragment in AOTBAND 3C. The SIII forbidden line is quite evident. What is not so clear is the HI 8-7 line at 19.06 μm. This line is clearly seen in the high resolution and defringed product.