LWS Grating Wavelength Calibration
Final Report

Cécile Gry & Elisabetta Tommasi

June 8, 1998

Draft 1.1

1. Introduction

The aim of this document is to describe how the wavelength calibration of the LWS grating is performed, to list the files and procedures which are relevant to wavelength calibration, and to assess the achieved accuracy.

2. Basic principles, calibration strategy and existing tools

The LWS diffraction grating is ruled with 7.9 lines per millimetre at a blaze angle of 30° and it is used in the second order for the wavelength range 43-95μm and in first order for the wavelength range 95-200μm. It is mounted in a scanning mechanism which rotates through $\pm 7°$, allowing to cover the extended range of wavelengths of each detector. The nominal spectral resolution elements are 0.29μm in the short-wavelength range and 0.60μm in the long-wavelength range.

The wavelength at each spectral point is determined according to the grating equation by the angle of the grating and the detector angle, which is a constant. Once the ten detector angles are known, the wavelength calibration thus consists in finding the relationship between the engineering units giving the grating position (LVDT, linear variable differential transformer) and the actual grating angle. This is done observing weekly a number of known targets chosen as wavelength standards, and analysing them with CALIBAN chain 1 (ref [1]) :

- the weekly observations are measured with the GWLC procedure to obtain the line centroid (and error) of the lines in terms of LVDT positions, as well as its width and peak height.
- the resulting line center in lvdt, width and peak height are written to the GRLP file, along with the expected wavelength of the line (given by the user - it takes into account the heliocentric velocity of the source)
- the relationship between lvdt and angle is calculated by the GCAL procedure which fits a third-order polynomial to the GRLP data, and writes the polynomial coefficients in the GRCL file.

The relationship is in principle independent of the detector so that all measurements of all lines are used together.

There are actually several GRLP files, with data from various time periods, to allow checking of time dependency. The measurements are also listed in an ascii file (ALL.OUT) giving the object name, the TDT number, the detector name, the lvdt of the center of the

line μm	det	LVDT mean(σ)	# obs	sources
[OIII]51.815	SW1	1327(3)	171	NGC6543 NGC6826 G298.228 IRAS15408 NGC7027
[OIII]51.815	SW2	2783(3)	196	NGC6543 NGC6826 G298.228 IRAS15408 NGC7027 NGC6302
[NIII]57.330	SW2	1993(2)	161	NGC6543 NGC6826 G298.228 IRAS15408 NGC6302
[NIII]57.330	SW3	3376(5)	152	G298.228 IRAS15408 NGC6302
[OI]63.184	SW2	1124(3)	88	G298.228 IRAS15408 NGC7027 NGC6302 NGC7023 IRAS23133
[OI]63.184	SW3	2584(3)	97	G298.228 IRAS15408 NGC7027 NGC6302 NGC7023 IRAS23133
[OIII]88.356	SW5	1579(3)	185	NGC6543 NGC6826 G298.228 IRAS15408 NGC7027 NGC6302
[OIII]88.356	LW1	3142(4)	189	NGC6543 NGC6826 G298.228 IRAS15408 NGC7027, NGC6302
[NII]121.889	LW2	2176(2)	7	NGC6302
[OI]145.525	LW3	1878(4)	76	G298.228 IRAS15408 NGC7027 NGC7023 IRAS23133
[OI]145.525	LW4	3250(5)	80	G298.228 IRAS15408 NGC7027 NGC6302 NGC7023 IRAS23133
[CII]157.741	LW3	945(4)	90	G298.228 IRAS15408 NGC7027 NGC6302 NGC7023 IRAS23133
[CII]157.741	LW4	2374(3)	91	G298.228 IRAS15408 NGC7027 NGC6302 NGC7023 IRAS23133

Table 1: *Lines from astronomical sources used for grating wavelength calibration.*

line, the error on the center lvdt, the width of the line in lvdt units, the gcpn of the line center when measured, the error on the gcpn, the expected wavelength of the line (taking into account the heliocentric velocity of the source), and the peak height of the line.

This ascii file can be used to check a set of calibration coefficients by converting the lvdt values in wavelengths with the coefficients and compare the results with the expected wavelengths. This can be done with the procedure CONV_PLOT_RES.PRO, which also creates an IDL structure RESIDUALS.XDR containing the differences between derived and expected wavelengths (residuals) and allows to plot those and check them statistically.

3. Calibration sources and types of observations

The wavelength standards are mainly planetary nebulae and HII regions. They have been chosen so as to provide the largest possible sample of lines and so that several of them are visible from ISO as much as possible during the mission (see Table 1 and Figure 1). The lines used must be strong enough to give good signal-to-noise and must be unresolved by the grating.

The observations are performed weekly with end-to-end grating scans and provide measurements of seven different emission lines, spread between $51\mu m$ and $158\mu m$, and appearing on two detectors each.

Note that there are no measurement for SW4 and LW5, as no strong line was found in

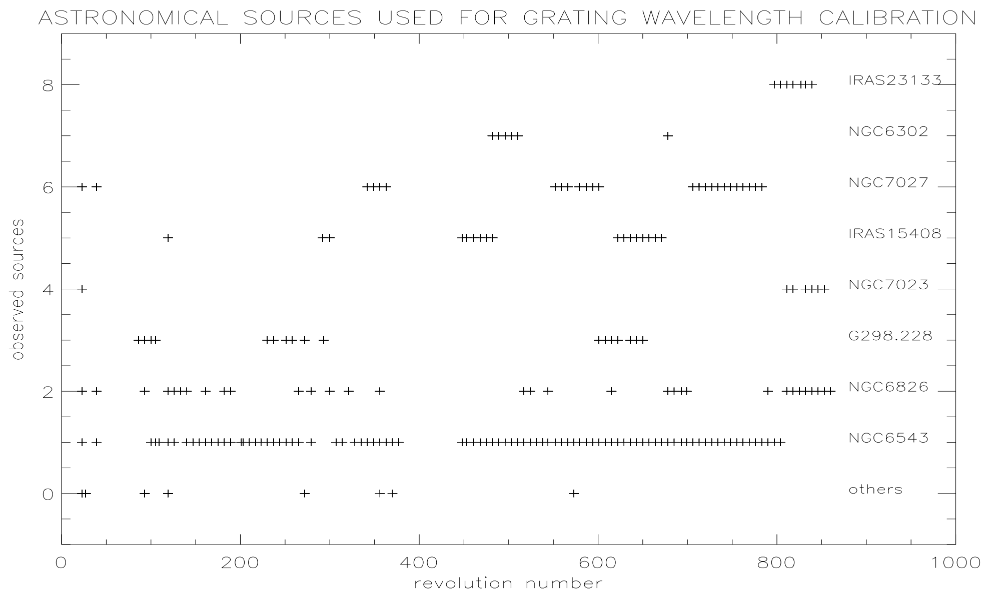

Figure 1: *Main LWS grating wavelength standards observed during the mission. The gap between revolutions 378 and 442 (also evident in fig. 2) corresponds to the period when LWS was not used because of a problem with the FP interchange wheel.*

their wavelength range.

The observation types are really homogeneous from revolution 342 onwards, with AOT L01, with 3 forward and 3 backward scans, and an oversampling of 8. Before that, the AOT observations could have only 5 scans, or not an equal number of forward and backward scans, and during PV phase the observations were performed with COIFs, generally with a higher number of scans and a higher oversampling. Some of them were short scans over a limited number of lines. However it has been check that these differences do not affect the wavelength determination.

4. Wavelength calibration in pipeline version 7.0

4.1 Detector angles

The plot of the residuals (normalised differences between the wavelengths derived from the LVDT with the polynomial relationship and the expected wavelengths) has shown systematic offsets for some detectors. This suggested that some of the detector angles had changed after launch. Therefore their values have been slightly adjusted to minimize the offsets for all detectors. The new angles used from pipeline version 6.0 on are listed below together with the corresponding shifts relative to the first angles used (determined on the ground). The angle shift for detectors SW4 and LW2 were adapted from the neighbouring detectors.

	SW1	SW2	SW3	SW4	SW5	LW1	LW2	LW3	LW4	LW5
angle	67.80	58.74	49.71	40.73	31.72	63.26	54.29	45.27	36.275	27.32
shift	-.1	-.01	0.0	0.0	+.02	+.02	+.01	+.01	+.04	+.04

4.2 Time dependence

The stability of the system is checked by monitoring the measured LVDT at the line centers in the weekly observations. It is found to be remarkably stable for measurements performed close to the rest (central) position of the grating (LVDT $\sim$ 2100). But elsewhere, a little jump has happened in revolution 346. The jump is bigger the farther away the grating from its rest position, and the jump has opposite signs for opposite angles (see Figure 2). In the worst case, the jump is less than half of a resolution element. This jump implies that the relationship between grating angle and LVDT reading has changed on revolution 346 for an unknown reason and it was decided to derive a time-dependent wavelength calibration, which for the version 7.0 considers two distinct periods, i.e. pre- and post-revolution 346. After the jump, only a very slow drift is observed in the LVDT measurements.

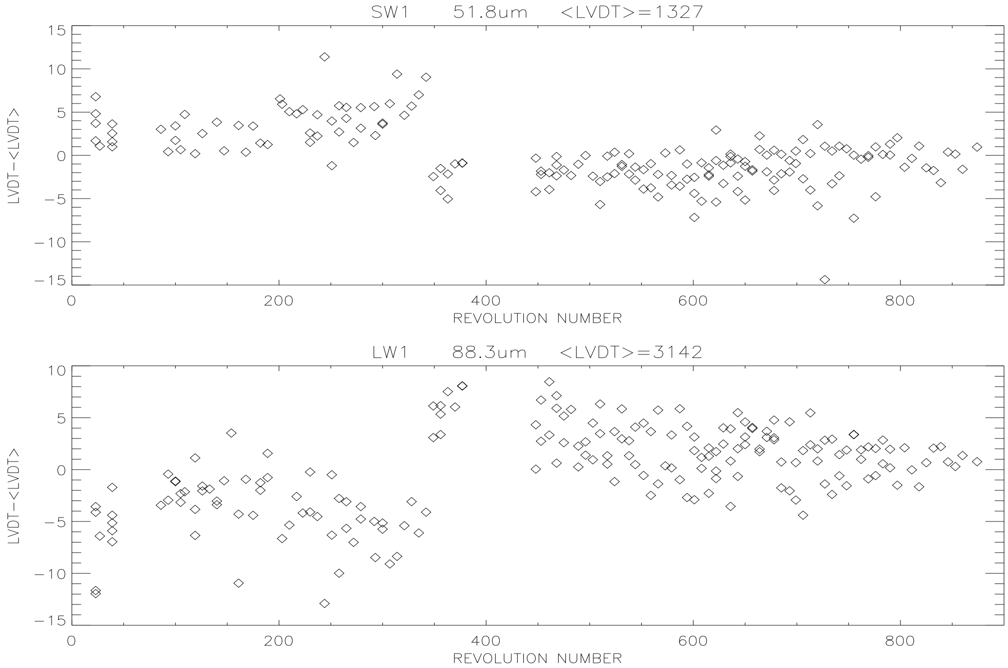

Figure 2: *Deviation of the measured line center (in engineering units LVDT) from the average value as a function of time, for two lines recorded at opposite grating directions relative to the rest position. 40 LVDT units correspond to 1 resolution element of the grating.*

In the current version of the off-line pipeline (V7) only one calibration file is used to transform the LVDT values of the LWS grating observations into wavelengths. It is the LCGW file, which contains the coefficients of the relationships for the two identified time periods.

To allow checking for time-dependence of the calibration the GRLP file has been split in several time periods. For each of them a GRCL file exists, listing the coefficients found for this period. Only two time periods are being considered for version 7 : the first one from PV-phase up to revolution 342, the second one from revolution 349 up to revolution 875, when LWS was turned off.

Here below the values of the coefficients used by pipeline v7 are reported (those for the second period had actually been derived using only data up to revolution 538, but it has been checked that they do not change significantly when all revolutions were used) :

revs	0th-order	1st-order	2nd-order	3rd-order
1-345	69.624422	-5.16459527e-03	5.02618935e-07	-8.20047303e-11
346-875	69.554848	-5.13190430e-03	5.02794834e-07	-8.18631699e-11

5. Assessment of the achieved accuracy

5.1 Check of the residuals.

As mentioned in section 2, besides the GRLP file, the Caliban's GWLC procedure produces an ASCII file easier to handle (.OUT file) in which all the information regarding the line measurements are recorded. All the .OUT files have been merged in a big file ALL.OUT which is used to test the calibration on the calibration measurements themselves. The CONV_PLOT_RES.PRO procedure mentioned in section 2 has been run with the two sets of coefficients on this file and the residuals are plotted in Figure 3. The residuals are the wavelength differences divided by the resolution element so that all detectors can be compared together. They are plotted versus LVDT with different symbol for each detector. Statistics on the residuals are presented below :

	SW1	SW2	SW3	SW5	LW1	LW2	LW3	LW4	all
mean	0.012	0.024	0.007	0.058	0.093	0.15	-0.008	0.022	0.029
sigma	0.056	0.056	0.072	0.039	0.073	0.040	0.069	0.070	0.069

They show that the mean and the dispersion values of the residuals are always well within a quarter of a resolution element.

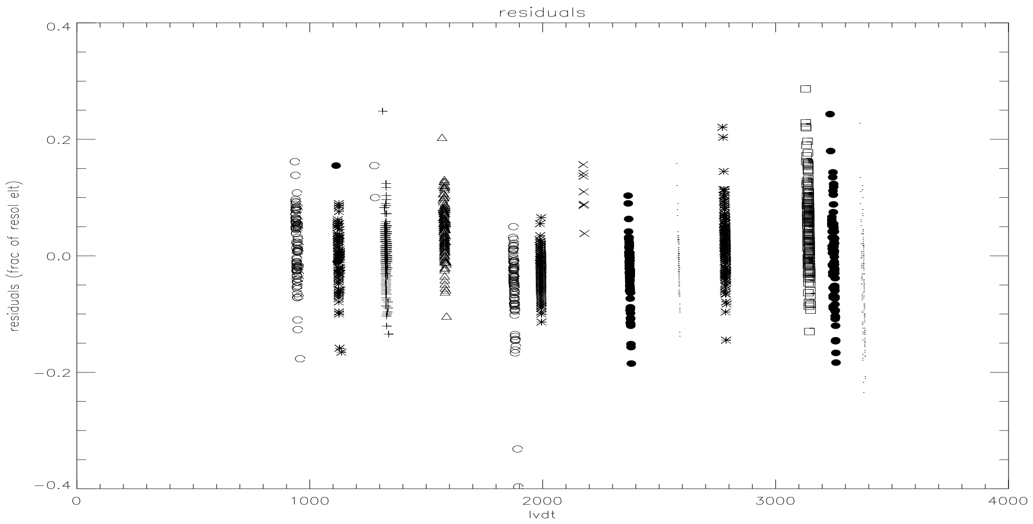

Figure 3: *Residuals calculated for all calibration observations (up to revolution 875) using the pipeline V7 coefficients. The crosses near lvdt=2200 correspond to the 122 μ line with LW2 ; their displacement towards positive values might indicate that the LW2 angle value has to be increased slightly.*

5.2 Wavelength measurements in the fully calibrated spectra (AAR products) : Wavelength precision and width of the resolution element

Emission lines have been measured on the AAR products of more than 65 observations. The results of this study are included in more details in the report on the scientific validation of the pipeline version 7.0. In summary, the precision in the wavelength determination is better than 25% of a resolution element. Only one case has been encountered where higher errors on the wavelength -although less than 1/3rd of a resolution element- have been found for an observation performed just before the jump in revolution 346, when the noise on the lvdt reading was the highest.

The mean of the resolution element width is .27 μm for SW detectors and .58 μm for LW detectors, with a dispersion of respectively .02 and .03, somewhat smaller, although not significantly, than the nominal values of .29 and .60 μm.

6. Mixed-mode observations

A second independent calibration method was planned before launch. It consists in using observations in which the Fabry-Perot is scanned with the grating at a fixed position and pointing at a strong continuum source. This observation produces a scan of the grating spectral element at each FP order position. It thus mimics a series of emission lines with the grating profile. Assuming that the wavelength position of the FP orders is well known, this observation provide a good number of (pseudo)-lines with predicted wavelength and measured lvdt and allows to derive one relationship between grating position and wavelength per detector. We can thus in principle check if it is justified to use a unique relationship for all detectors.

Two mixed-mode observations were performed in revolution 158 with FPS and revolutions 317 and 341 with FPL, both pointing at Jupiter. The position of the FP orders have been measured in grating lvdt units and a wavelength calibration relationship has been derived for each detector. This procedure has lead to significantly different coefficient sets for different detectors, which is difficult to explain physically, as the only moving part during a wavelength scan is the grating.
The mixed-mode measurements are thus still under investigation and are not used for wavelength calibration for the time being.

References

[1] CFDP - Calibration File Derivation Procedures, LWS/IDT/N/0019.3

Appendix

List of relevant files for grating wavelength calibration :

- GRLP : MC-fits format file, created by the GWLC procedure in CALIBAN. It contains the results of the individual line measurements on the LSPD or LCPD files of the weekly grating wavelength calibration observations. It lists target name, coordinates, detector, lvdt, error on lvdt, line width in lvdt, expected wavelength and line peak height. It is used as input by the GCAL procedure to derive the calibration coefficients. GRLP has been split in several files called GRLPnnn-mmm for the time period comprised between revolution nnn and revolution mmm

- GRCL : MC-fits format file, created by GCAL in CALIBAN, which lists the coefficients resulting from the polynomial fit in the GRLP data. As for GRLP, several time periods have been considered, resulting in various GRLPnnn-mmm files.

- LCGW : MC-fits format file, which contain the coefficients for the two time periods in the time-dependent calibration, is used by the pipeline to convert lvdt in wavelength.
- ALL.OUT : ASCII file listing basically the same information as the GRLP file, with the significant advantage of listing also the TDT number (hence the revolution number). It lists : target name, TDT number, detector number, lvdt, error on lvdt, line width in lvdt, gcpn when measured, error on gcpn when measured, expected wavelength, line peak height. This file is used to check the calibration relationship with the procedure CONV_PLOT_RES.PRO.
- LCPD34188888 : MC-fits file containing the merged FPL mixed-mode observations in LCPD format.
- GPAR_FPL_ALL.DAT : ascii file listing the results of the FPL mixed-mode observations measurements including for each detector (col1) and each grating lvdt position (col2), the wavelength derived from the FP calibration (col3) and its error (col4), the wavelength derived from the grating calibration (col5), the fwhm (col6) and the FP order (col7).
- COEF_MM.TXT : ascii file listing for each detector the grating wavelength calibration coefficients derived from the GPAR_FPL_ALL.DAT file.
- results of the auto-analysis products measurements for pipeline 7 validation, listed in four IDL structures : NGC7027_V7.XDR, S106_V7.XDR, NGC6543_V7.XDR (contains only 1/4 revolutions), NGC6543_57_V7.XDR (contains the 57 μ line data for all revolutions).

List of relevant IDL procedures :

- GWLC, GCAL, ... are part of CALIBAN chain 1, and are described in the CFDP document (ref[1]).
- CONV_PLOT_RES.PRO : reads data from ALL.OUT, converts lvdt into wavelength, calculates the residuals, plots them versus TDT number with a symbol per detector (i.e. fig. 3 of the present report) and prints their mean and sigma values. It also creates an IDL structure, RESIDUALS.XDR, which allows further operations on the results.
- CONV_PLOT_RES_MM.PRO : basically same as CONV_PLOT_RES.PRO but for the mixed-mode, reading data from GPAR_FPL_ALL.DAT
- READGRLP.PRO : reads the mc-fits file GRLP.DAT and writes the content in an ascii file GRLPASCII.LIS and to an IDL structure (GRLPSTRUC.XDR).
- READ_OUT_XDR.PRO : reads the ascii .OUT file which is given as argument and creates the IDL structure OUT.XDR with the content.
- REF.PRO : reads the IDL structure OUT.XDR previously created by READ_OUT_XDR.PRO from the .OUT file ; prints statistics (mean, sigma and number of observations) on the measured LVDTs ; creates the "famous" plot monitoring the lvdt values over revolution number for two lines (FAMOUS.PS, fig.2 of this report) ; creates two variables : diff is the difference lvdt-[mean of lvdt for the line] and normdif is this difference normalized by the lvdt dispersion for the line.

- SOURCE_REV.PRO : reads the IDL structure OUT.XDR previously created by READ_OUT_XDR.PRO from the .OUT file and plots the use of calibration standards over the revolutions (i.e. fig.1 of this report).
- LVDT_TO_WAVE.PRO : transforms an lvdt given for a given detector into wavelength with a set of coefficients and detector angles (input : detector and lvdt)