JWST TECHNICAL REPORT

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1.0 Abstract

Analysis has been carried out for the observations of photometric standards in the NIRISS Single Object Slitless Spectroscopy mode, involving re-analysis of the commissioning calibration observation of the standard star BD+60°1753 and new analysis of observations of standards GSPC P177-D, G191-B2B, and 2MASS J17430448+6655015 made in cycle 1. The reductions are affected by three main issues that are difficult to address at a high level of precision: (1) all the spectra are adversely affected by bad pixels in the two-dimensional spectral images, which affect some wavelengths in the extracted spectra; (2) for the fainter standards GSPC P177-D, 2MASS J17430448+6655015, and G 191-B2B the sky background subtraction presents difficulties that are currently under investigation; (3) for 2MASS J17430448+6655015 and G 191-B2B spectral contamination from nearby objects limit the amount of useful data obtained in cycle 1.

There have been changes in the data reduction pipeline since commissioning which affect the results, primarily because there was a revision in the spectral extraction from a simple box extraction along the trace used initially to a more complex extraction that models the overlap between spectral orders 1 and 2 which is used currently. The change in the extraction reduces the order 1 photometric calibration scaling factors determined from the commissioning observations of BD+60°1753 by about 1% over the entire wavelength range, which led to a revision of the SOSS photometric calibration in late 2023. The cycle 1 observation for G 191-B2B and GSPC P177-D produce results consistent with the revised calibration within ±1% for order 1 subject to the background or contamination issues at some wavelengths, and the results for 2MASS J17430448+6655015 show roughly a ±2.5% range of variation from the current calibration values in order 1 subject to the same issues at some wavelengths. The order 2 calibration seems of similar accuracy to the order 1 calibration for wavelengths less than about 0.9 μm but not at longer wavelengths especially where the signal is low, while the order 3 calibration seems to have issues that need to be addressed.

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For the A-type standard stars we observe wavelength shifts in the pipeline extracted spectra that cause a mis-match in the Paschen line wavelengths compared to the stellar models for the stars. These shifts are much larger than the radial velocity corrections for these stars. The cause of these shifts is currently under investigation, but they are currently assumed to be due to issues in the pipeline spectral trace determination.

2.0 Introduction

The NIRISS Single Object Slitless Spectroscopy (SOSS) mode observes individual bright stars, generally for time-series exoplanet science. There is a requirement for 10% or better photometric calibration of the mode in order 1 over the wavelength range. The goal is to do considerably better than this in practice. In the commissioning of the instrument an observation of the A0mA1V type photometric standard star BD+60°1753 was taken in program 1091, and this formed the basis of the initial NIRISS SOSS absolute calibration delivered to the Common Reference Data System (CRDS) in June 2022. At that time the spectral extraction within the JWST data reduction pipeline was using a very simple column extraction over the entire sub-array, which ignored the presence of spectral orders 1, 2, and 3 within the SUBSTRIP256 sub-array wherein most of the calibration observations were taken. This was a result of the pipeline not yet having the "ATOCA" extraction algorithm from the Université de Montreal (Darveau-Bernier et al. 2022) in place at that time. Due to this issue, the initial spectral extractions in the commissioning analysis used a simple box extraction following the spectral traces in orders 1, 2, and 3 individually to obtain a count-rate spectrum as a function of wavelength in each order. Comparison of the count-rate values to the theoretical expectation for the stellar flux density was used to derive a response function from ADU/s units to Jansky for each order. These functions were delivered to CRDS around the end of NIRISS commissioning.

Additional photometric standard star observations in the SOSS mode were obtained in cycle 1 calibration programs 1536, 1537, 1538, and 1539. In the early part of 2023, the ATOCA algorithm was successfully incorporated into the JWST data reduction pipeline. A re-analysis of the commissioning and cycle 1 SOSS photometric observations was undertaken in the summer of 2023 after the cycle 1 observations were completed. Further work was carried out in June 2024, mostly to improve the background subtraction for the fainter sources. This report discusses the results of this analysis and the resulting revision of the SOSS mode photometric calibration.

3.0 Observations and Data Analysis

The cycle 1 calibration observations of concern for this analysis are: program 1536, observation 9, of photometric standard star 2MASS J17430448+6655015 (type A8III), program 1537, observation 2, of photometric standard star G 191-B2B (type DA0.8), and program 1538, observation 12, of photometric standard star GSPC P177-D (type G0V). In addition, the commissioning observation in program 1089, observation 2, of BD+60°1753 was re-reduced with the ATOCA algorithm. Cycle 1 program 1539 involves roughly monthly monitoring of BD+60°1753 in SOSS mode. Those observations were also re-reduced, but the main concern there was to make sure that there is no sign of variability in the star. There was no indication of variability in the star, so the program 1089 observation was used because that observation has much better signal-to-noise (S/N) ratio than the shorter subsequent observations in program 1539 or in the cycle 2 equivalent program 4499.

The standards G 191-B2B, 2MASS J17430448+6655015, and GSPC P177-D are all somewhat fainter than BD+60°1753, with K_s magnitudes of 12.764±0.023, 12.772±0.028, and 11.861±0.024 respectively while the Ks magnitude for BD+60°1753 is 9.645±0.015. The signal-to-noise ratio (S/N) for the BD+60°1753 observation in program 1089 during commissioning is much higher than what was obtained in cycle 1 for the other standards, both because the observation was several times longer and because the star is brighter.

For each observation the spectrum was extracted in the level 3 pipeline using the ATOCA algorithm. The set of individual spectra in each order were then averaged over the sequence of extracted spectra from the observation at each wavelength point with outlier rejection using the `sigma_clipped_stats` routine from `astropy.stats` package to produce a mean spectrum for each order and each object. These spectra were calibrated to Jansky using the photometric calibration which was derived during commissioning but with the correction described in the next paragraph. The subsequent analysis involves comparing the spectra in physical units to the expected spectrum from stellar atmosphere models to see what adjustments, if any, need to be made to the photometric scaling values.

Prior to the start of this work, it was pointed out by Löic Albert of the Université de Montreal that there was an issue in the SOSS photometric calibration file submitted in commissioning, in that it injects noise into the spectra. This was found to be due to an error in making the commissioning photometric calibration file: in the commissioning analysis the ratio of the count rate values with wavelength to the stellar model spectrum at the same wavelengths was calculated, and then a smooth polynomial function of wavelength was fit to the values. The idea was to use the smoothed function to produce the photometric calibration file, but by mistake the original ratio values with noise were used to create the reference file instead. Thus, it was required to make a revision to the CRDS SOSS photometric reference file in any case to correct from the raw ratio values to the polynomial function and thereby reduce the noise in the output pipeline spectra.

3.1 Background Subtraction in the SOSS Photometric Reductions

In the original commissioning analysis of the observations in program 1089 the photometric calibration was derived from the directly extracted spectra with no subtraction of the background signal. The star BD+60°1753 is relatively bright and so the effects of the background on the output spectrum are small enough that these were several times smaller than the measurement uncertainties as determined at the time. However, the other standard stars observed in cycle 1 are fainter than BD+60°1753 and for these stars the background subtraction cannot be neglected.

The JWST data reduction pipeline does not carry out a background subtraction step for the SOSS mode observations. The targets of the SOSS observations are generally bright stars for which the background is comparatively small, and also the exoplanet community generally wish to carry out their own data reduction beyond what the pipeline produces, so it was considered better to leave the background component untouched in the pipeline data products given that there are significant uncertainties in how best to carry out the background subtraction.

In commissioning there were some limited full-frame SOSS mode observations carried out in program 1092, the SOSS wavelength calibration program, with the target offset out of the normal position in the SUBSTRIP256 sub-array to a position in the middle of the detector. These exposures were used to create a background template for the SOSS mode by masking out the source signals and using a low-order polynomial to fit a smooth variation over the detector. Due to the presence of a "step" in the background at about x of 698-700 in the upper part of the images, the fitting was done in two sections with a linear fit used to join the two sections up at the pixels where the step is seen. For the normal background subtraction on science data, the template values were extracted in the SUBSTRIP256 subarray area of the full image (y pixel range 1793 to 2048, and all x pixels). The full-frame template image is shown in Figure 1 below. In the full frame image, the area in the upper right with the largest signal is where the GR700XD grism orders 0, 1, 2, and 3 are all overlapping from different points within the full field of view of the NIRISS pick-off mirror. In the area to the upper left the order zero spectra no longer contribute and the signal is from orders 1, 2, and 3 at different positions within the pick-off mirror field of view. The area at the bottom of the detector receives little signal because the grism shifts light up in the y direction on the detector, and nominally no signal will be directed to the bottom 400 or so rows on the detector. Some faint signals are present in this area, the cause of which is not understood.

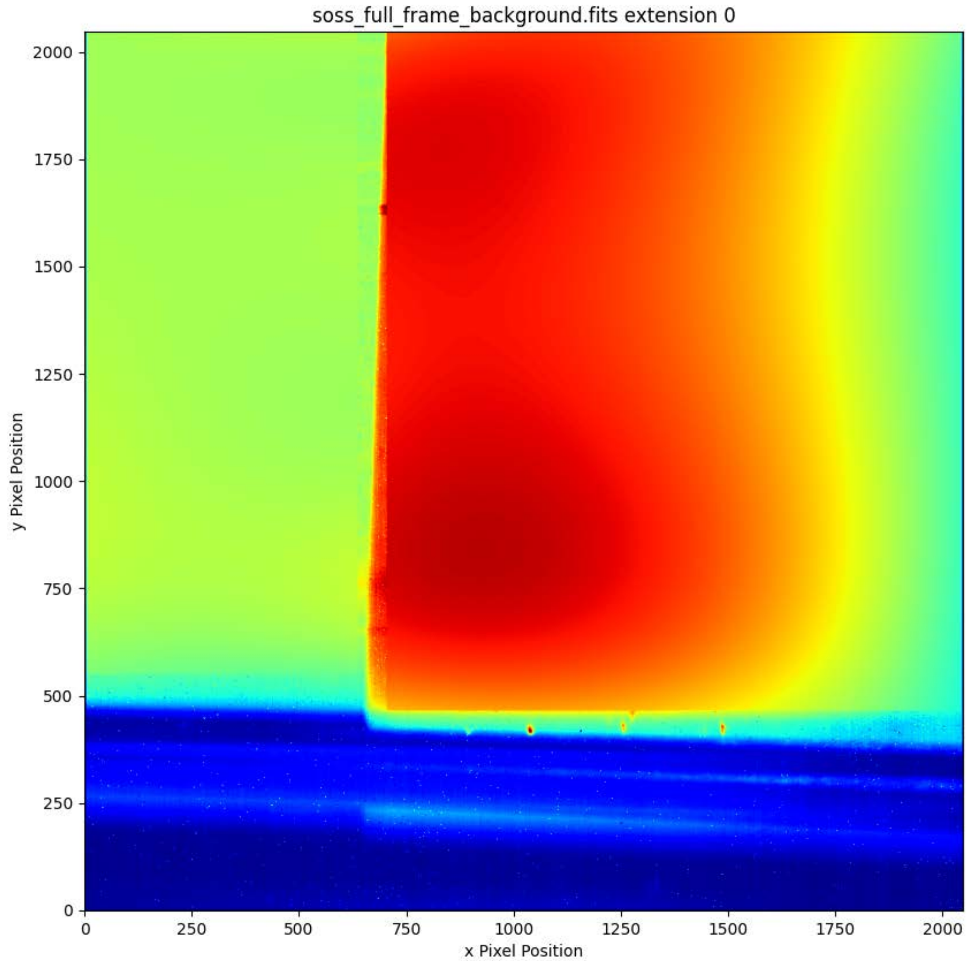

Figure 1: The template SOSS full frame background image derived from observations in commissioning program 1092. The display range is from 0.0 to 3.5 ADU/s.

Each pixel in the background image is receiving photons from multiple orders and many wavelengths. The shape of the background can be approximated by convolving the total point spread function of the GR700XD grism in all orders (which was observed in ground testing by taking several exposures of a lamp "point source" at different positions) with a uniform sky background. Those simulations show that the step in the background is due to having orders 0, 1, 2, and 3 for the region to the right on the detector, while having only orders 1, 2, and 4 for the region to the left on the detector. The initial assumption was that the background shape should be uniform for different lines of sight on the sky, but that the level would change from observation to observation as the zodiacal light component changes in total signal for different ecliptic latitudes. Experience in cycle 1 has shown that there are variations in the background shape from different observations, the causes of which are not understood. Cycle 2 calibration program 4479 and the upcoming cycle 3 program 6658 are specifically intended to provide more background observations for the SOSS mode in order to evaluate the changes that are seen as a function of the ecliptic latitude and longitude. The analysis of these observations has shown that there is a definite change in the shape of the background along the wavelength dimension (pixel x) as well as a change in the relative signal between the left and right parts of the detector where the contributing orders are different. This variation is approximated by a constant offset of both sections of the background, but the reason for this type of variation is not clear. The background subtraction is done using a tool that takes the background template and applies a multiplicative scaling by one parameter plus an additive offset by a second parameter. Currently it is difficult to determine what the best combination of the two parameters is for the background removal. For the fainter sources this becomes a limiting factor in the analysis.

The dominant contribution to the SOSS background is the zodiacal light background, with a possible minor contribution from the telescope background at long wavelengths. As the background signal in Figure 1 is the integrated intensity over a wide range of wavelengths in multiple spectral orders, it is not clear why the template shape changes. At the main SOSS wavelengths, the zodiacal light background is scattered solar radiation. There is also a thermal component at longer wavelengths which becomes significant at wavelengths greater than about 4 μm. The NIRISS detector has response out to about 5.5 μm, but the GR700XD grism response is much reduced at long wavelengths and one would not expect large changes to the total signal due to small changes in the local zodiacal dust temperature, although such changes would affect the thermal part of the zodiacal spectrum. One also does not expect changes in the shape of the scattered solar light component, although this can be caused by changes in the overall size distribution or composition of the local zodiacal dust near the spacecraft. Such changes are not expected to be large over the relatively narrow range of solar distances for JWST in its orbit.

In the new reductions the background subtraction was carried out using a tool created for this purpose, which allows one to scale and shift the background template as described above, and then to subtract it off of a SUBSTRIP256 rate image from the pipeline. The tool allows the user to plot cuts in the x and y directions to see the effect of the background subtraction, and to look at a simple extracted order spectrum before and after the subtraction. Unfortunately, it is not practical to incorporate the pipeline ATOCA extraction into the tool because that process is rather slow. The background subtraction analysis is carried out using the average rate image from the observation, which can then be applied to the individual ramp slope images in the "rateints" file. The general approach is to scale the background template to remove the discontinuity in the background near x=700 in the rate images, and then to look at the residual signal level away from the object spectra and adjust the parameters until the background-subtracted image is close to zero away from the source signal. Once the background subtraction is done, revised level 1 rate and rateints files are written out for use in the level 2 and level 3 stages of the pipeline.

The background subtraction was done for all the cycle 1 standard star observations and for the commissioning observation of BD+60°1753. The background subtraction needs more work in the future, when it is hoped to be able to understand the possible variations in the shape better. For some of the observations, particularly the case of GSPC P177-D, the background subtraction is the limiting factor in the analysis/

3.2 Observations of BD+60°1753

As noted previously the longest available observation of this star is observation 2 of program 1091. This consisted of a time series observation of the star with 3 groups per integration and 876 integrations. The total science time for this observation was 5.3475 hours. This observation is significantly longer than the other individual observations of this star in program 1091or the individual photometric observations in the stability monitoring programs 1539 and 4499. Figure 2 shows the mean rate image from this observation, with an IRAF-style logarithmic scaling to show order 3 and a very faint contaminating source that affects that spectral order.

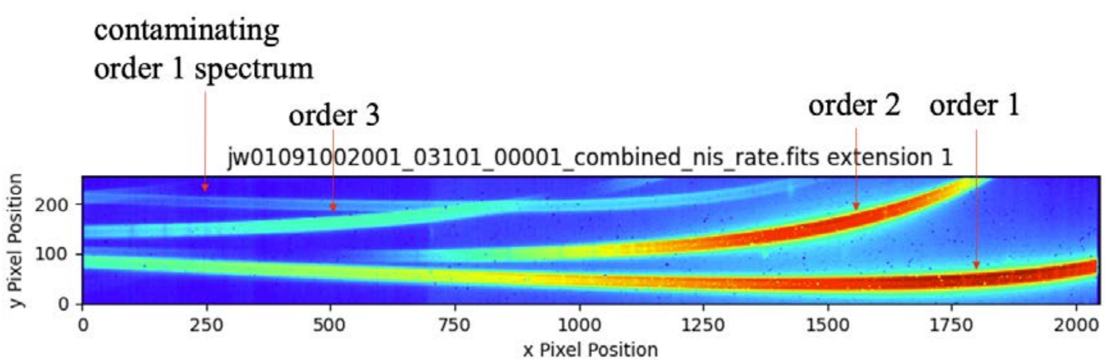

Figure 2: The mean rate image for program 1091 observation 2, the time series observation of the photometric standard star BD+60°1753. Spectral orders 1 to 3 for the standard are marked. As can be seen above, there was some contamination in order 3 from the first order spectrum of a much fainter star in the field.

The contaminating source appears to be the star 2MASS 17244630+6025483 also catalogued as SDSS J172446.31+602548.3, Gaia DR3 1435897078467442432, and WISE J172446.32+602548.2. This is a roughly 16^{th} magnitude K-type main sequence star at a distance of about 43″ from BD+60°1753. Figure 3 shows the configuration of the observation from the Astronomer's Proposal Tools (APT). The background image is from the Sloan Digital Sky Survey. The contaminating object is marked with the arrow.

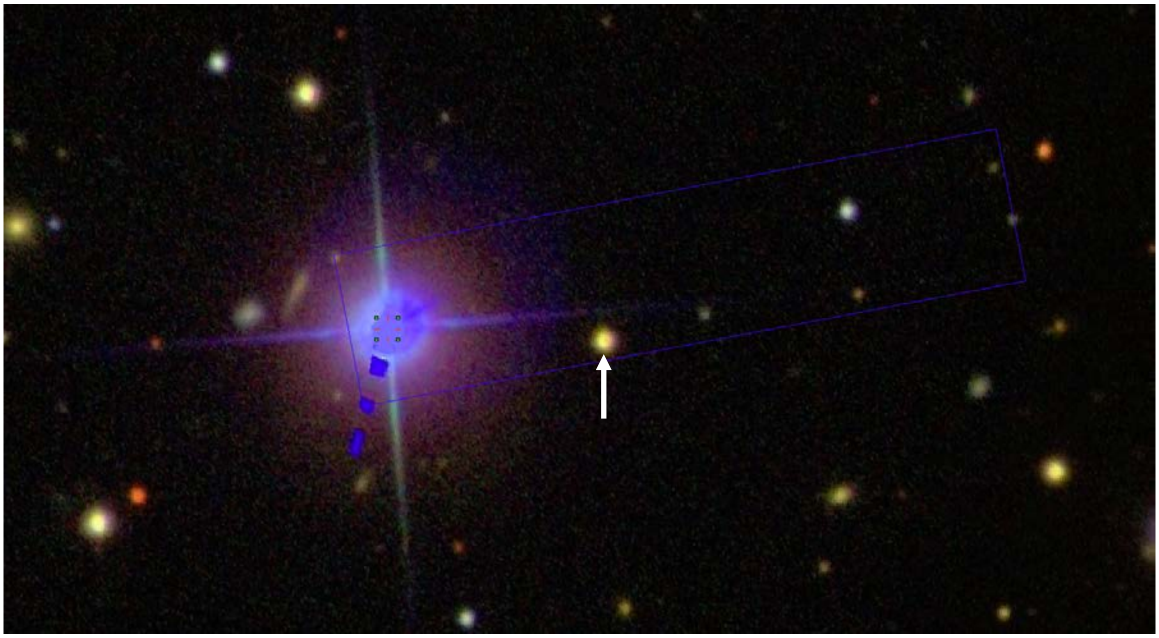

Figure 3: The Sloan Digital Sky Survey image of the field near BD+60°1753 for observation 2 of program 1091, from the Astronomer's Proposal Tools. The blue outline is the SUBSTRIP 256 field of view for the orientation of the observation. The arrow points to the contaminating star that affects the order 3 spectrum of the standard in this observation.

The available Sloan (Gunn et al. 1998, Fukugita et al., 1996, York et al. 2000), 2MASS (Skrutskie et al. 2006), WISE (Wright et al. 2010), and Gaia DR3 (Gaia Collaboration 2016, Gaia Collaboration 2023, Babusiaux et al. 2023) photometry for this star is listed in Table 1, along with the magnitudes for the standard star BD+60°1753 for comparison. At K-band the star is 41.6 times fainter than the standard star. In the Gaia DR3 G_{RP} filter, which is roughly equivalent to the short wavelength end of the SOSS order 1 wavelength range, the brightness ratio is 227.8.

The peak order 1 signal for BD+60°1753 is about 1383 ADU/s, while the peak zodiacal background level is about 4 ADU/s. This is why for the commissioning observations it was not vital to carry out a background subtraction. The background correction is roughly 1% at most for order 1 in this case, and usually it is rather smaller than a 1% relative correction. The uncertainties in the spectral extraction were clearly larger than any background issues. For BD+60°1753 the background subtraction process in the 2024 re-reduction was difficult to carry out with high precision because the signal contrast between the star and the background is large. A scaling value of 0.9544 was used in the background subtraction, which was derived by looking at the signal in the corners of the rate image away from the spectral orders and scaling to make the background value as close to zero as was feasible. It is not clear that this is the best way to determine the proper scaling value.

3.2.1 Revision of the Photometric Reference File to Reduce the Noise in the Spectra

In dealing with the re-reductions of the photometric observations a correction was made to the photometry reference file to correct the noise issue discovered by Löic Albert. This was not noticed in the commissioning observations because of two factors. First, the application of the reference file to the BD+60°1753 spectra did not produce noisy output values because the noise is with respect to the BD+60°1753 stellar model that was used in the determination of the response. Second, the only other star for which the values could be tested was the SOSS wavelength standard in program 1092, the M-type dwarf star TWA 33, and the spectrum of this star shows complex band structure at all wavelengths covered by the GR700XD grism. Hence it was not obvious that the extracted spectrum was noisier than expected.

Table 1: Photometry for the contaminating star in Figure 3 and for the photometric standard star. BD+60°1753 does not have Sloan photometry.

Filter	SDSS J172446.31+602548.3 Magnitude	BD+60°1753 Magnitude
SDSS u	20.34±0.06	
SDSS g	17.610±0.005	
SDSS r	16.384±0.004	
SDSS i	15.920±0.004	
SDSS z	15.668±0.006	
Gaia DR3 G	16.3892±0.0006	9.6839±0.0004
Gaia DR3 G_{BP}	17.1303±0.0058	9.6884±0.0008
Gaia DR3 G_{RP}	15.5521±0.0028	9.6582±0.0008
2MASS J	14.543±0.041	9.612±0.022
2MASS H	13.868±0.042	9.651±0.018
2MASS K_S	13.694±0.048	9.645±0.015
WISE W1	13.727±0.024	9.612±0.023
WISE W2	13.727±0.024	9.639±0.020
WISE W3	>13.217	9.664±0.033
WISE W4	>9.512	>9.068

Once this issue was discovered the SOSS photometric reference file was regenerated using the intended polynomial functions for each order. This new file was then used in all the re-reductions described in this report. Figure 4 shows the magnitude of the corrections for all orders from program 1091. The main thing to note is that there is no overall change in the values as a function of wavelength but the excursions seen are due to the noise patterns from the extracted spectra. (The F277W order 1 spectrum ends at about 2.38 μm because of the short wavelength cut-off of the filter, and the noisy values for shorter wavelengths are due to there being little or no signal.). This change was entirely based on the extraction and fitting carried out in June 2022 and does not involve any reprocessing of the data.

Figure 5 shows the output commissioning spectrum calibrated with the revised reference file. Also shown in the plot is the reference stellar model that was used in the calibration from https://www.stsci.edu/hst/instrumentation/reference-data-for-calibration-and-tools/astronomical-catalogs/calspec (Bohlin, Gordon, and Tremblay 2014). There are some issues in the calibrated spectra. The order 3 spectrum is a little high at all wavelengths; this was assumed to be due to the contamination from the other star. As the JWST data reduction pipeline did not at that time extract or calibrate order 3 in SOSS mode, this discrepancy was not followed up with further analysis. The order 2 spectrum has issues at wavelengths above about 1.0 μm. In this wavelength range the order 2 signal is low, and it goes to a value very close to zero at the grism blaze wavelength of about 1.3 μm. The concern in commissioning was the fidelity of the order 2 spectrum in the wavelengths below 1 μm where there is no order 1 coverage, and as is seen in the Figure the agreement there is good. The intent was to fix these issues later once the ATOCA extraction was operational and other standard star data was available to cross-check the results.

3.2.2 Revisions With the New Extraction

Once the revised photometric calibration file was produced, as it should have been at the end of NIRISS commissioning, then the re-reduction was carried out. The background subtraction carried out using the commissioning background template shape with a scaling of 0.954 and no offset, and then the spectra were extracted with the ATOCA algorithm in pipeline version 1.14.0 and CRDS reference file rmap version 11.17.19. The output order 1 and order 2 spectra were averaged and then compared with the CALSPEC stellar model file bd60d1753_stiswfc_004.fits as the "truth" spectrum. There was relatively little change in the overall spectral level with the new extraction. For wavelengths where there are no bad pixels to affect the ratio and where the S/N ratio is good, the theoretical spectrum and the newly extracted calibrated order 1 and order 2 spectra agree to within about ±1%.

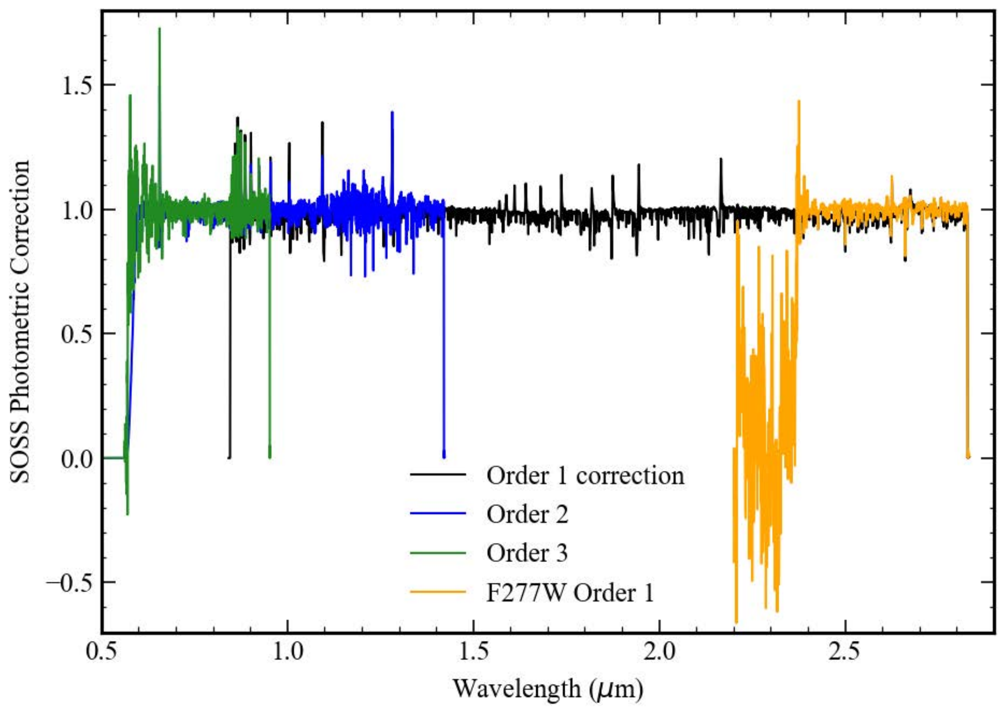

Figure 4: Corrections to the SOSS photometric calibration using the commissioning values from observation of BD+60°1753. The correction is the ratio of the revised values to the values delivered to CRDS in 2022. For F277W the noisy values at wavelengths below 2.35 μm are due to having no actual signal at these wavelengths.

Unfortunately, the comparison is hampered by the effects of bad pixels in the spectral extraction. The cross-dispersion width is 31 pixels for the ATOCA extraction, and there is a significant chance of getting a bad pixel within each wavelength slice. As there is no correction for the effects of these pixels in the extraction, and the original "not-a-number" (NaN) value from the bad pixel is set to zero to avoid getting a large fraction of NaN pixels in the output spectra, what one sees is generally an upper envelope of good values along with many single wavelength "drops" of order 6%, and sometimes much larger drops, in the output spectra.

In commissioning the CALSPEC file bd60d1753_mod_005.fits was used in making the photometric response file. Some part of the relative change in value is due to the change in the comparison spectrum between commissioning and the re-reduction. In Figure 6 below the ratio of the order 1 output signal to the CALSPEC model predicted flux density values is given for the new reduction with a small background subtraction correction. The ratio values show discrepancies in the line core which produce ratio values up to 1.12 in the Paschen series line cores below 1 μm wavelength. Examination of the lines show that the pipeline extraction has a small wavelength shift with respect to the model. Scaling the model wavelengths by a factor of 1.0013 produces much better line matching, although in the line cores there are still peaks up to 1.03 due to differences in the detailed line profile shape between the SOSS spectrum and the CALSPEC model. The measured radial velocity for the star is −27.13±0.79 km/s, which is far smaller than this wavelength shift. The wavelength shift appears to be due an issue in the ATOCA spectral extraction. One also sees the very numerous "drop-outs" due to bad pixels that affect the spectral extraction. The upper envelope of points seems to be within the range 0.98 to 1.0 for most of the order 1 wavelength range. This, a value of 0.99 seems representative of the average ratio value away from the line cores where there are no effects of the bad pixels. However, this is difficult to estimate at high accuracy because of the many excursions outside this range.

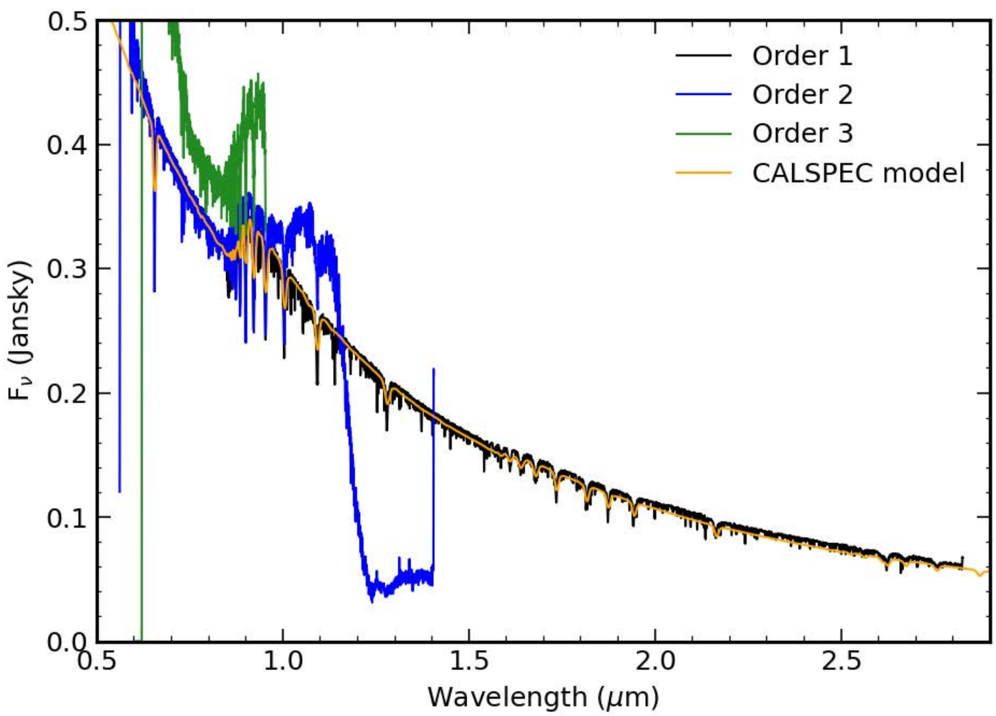

Figure 5: The revised extracted spectra of BD+60°1753 from the original reduction and extraction done in NIRISS commissioning in June 2022, applying the smoothed response functions rather than the "noisy" versions. The wavelength regions where order 2 shows large discrepancies with the model spectra are where the signal level is very low in Figure 2 above. The discrepancy in order 3 is partially due to the low signal level and partially due to the order contamination. The model spectrum is from the CALSPEC database https://www.stsci.edu/hst/instrumentation/reference-data-for-calibration-and-tools/astronomical-catalogs/calspec .

For order 3 the results are improved by the revised fit, but again the low S/N limits the accuracy of the output spectral calibration. In the brighter parts of order 3 where there is no contamination the ratio values are within about 0.98 to 1.02, but in the region around 0.62 μm where the response is very low the ratio goes down to 0.85. Once again as in order 2 this is due to the limitations of fitting a polynomial to the noisy data across the wavelengths with very low response. Cycle 2 GO program 3279 is specifically concerned with calibration of order 3, which we expect will improve the photometric calibration of this order, but that will be a future revision.

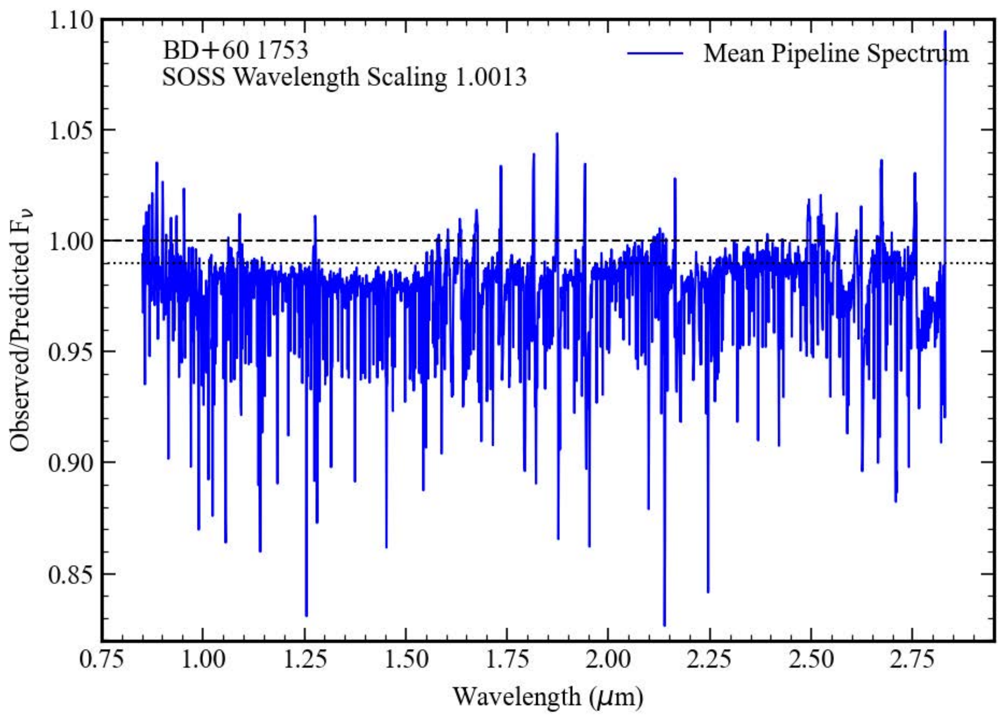

Figure 6: Ratio of the observed flux density to the CALSPEC model flux density for the re-reduction of the commissioning observation of BD+60°1753 in order 1. The dotted line at a ratio value of 0.99 seems to define the level of agreement of the two spectra in wavelengths where the bad pixel "drop-outs" are not an issue.

With the revised extraction for order 2, and using the same code as in commissioning to extract order 3 in the re-reduction, some work was done on improving the overall fits for order 2 and order 3 to try to remove the large discrepancies seen in Figure 5 above. This work was partially successful. There are still issues with the fitting of order 2 in the wavelength range of very low signal near the blaze wavelength, from 1.1 to 1.3 μm in particular. A higher order Legendre polynomial fit was used, but the observed values are very noisy and cover a very large range of response values. The best compromise fit that was obtained is still not entirely satisfactory over the response minimum of order 2, and one sees residual wavy values in the ratio of the order 2 spectrum observed to the CALSPEC model. Although this is not ideal, the low S/N of this wavelength range plus the fact that it is redundant with order 1 means that this limitation of the fitting is not important from the standpoint of the SOSS science in normal observations. It might be an issue if order 1 was saturated and order 2 was the only source of spectral information at these wavelengths.

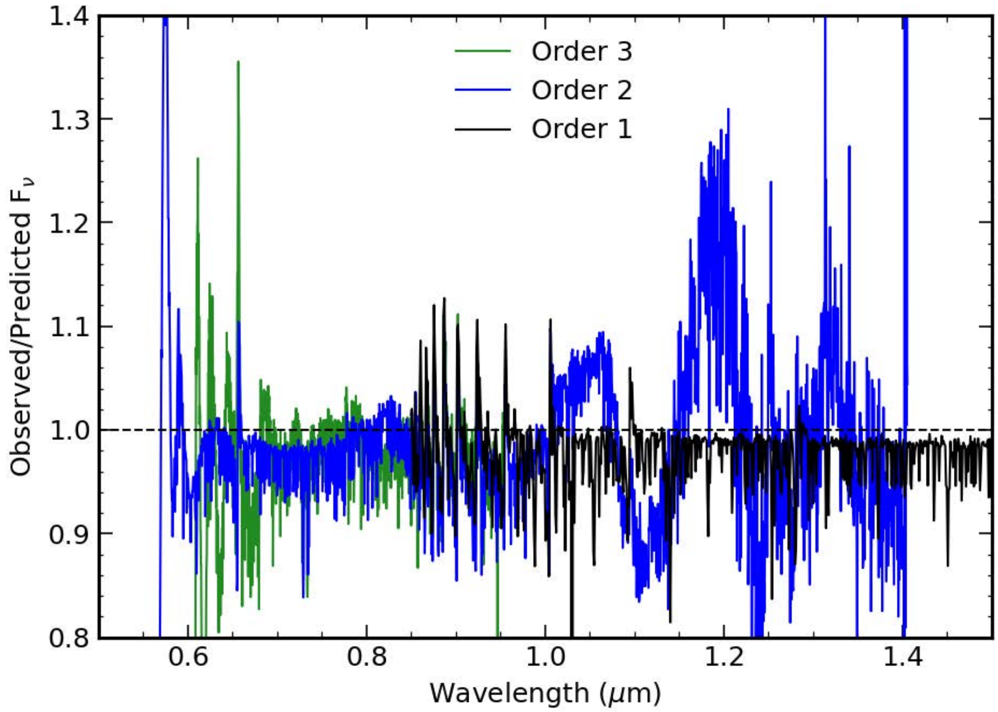

Figure 7: The ratio of the observed to predicted signal for the short wavelength part of the order 1 spectrum plus the order 2 and 3 spectra from the re-reduction. The order 3 spectrum was extracted using the non-pipeline code that was used in commissioning. Some adjustments to the fitting of orders 2 and 3 was carried out to improve the results for the regions of low signal. Nonetheless one still sees the "wave-like" ratio discrepancies from the limits of fitting order 2 through the region of very low signal around 1.0-1.3 μm.

3.3 Observations of G 191-B2B

The white dwarf standard star G 191-B2B, which is one of the three primary HST spectrophotometric standard stars, was observed in observation 2 of program 1537. The output rate image of the observation is shown in Figure 8. In this figure the display is logarithmic between the minimum and maximum values of the rate image, so as to show the zodiacal background component and some contamination from other stars near the white dwarf star. There are two order zero order images in the field of view, one being close to the order 1 spectrum around x = 1520 near the bottom of the subarray, which is the brightest thing in the field of view.

The most serious contamination effect is for the longer wavelength part of both order 2 and order 1, where the first order spectrum of another star is contaminating the data. The brightest part of order 2 is affected by contamination from two faint first order spectra, and the order 3 spectrum is affected by another faint first order trace at this orientation.

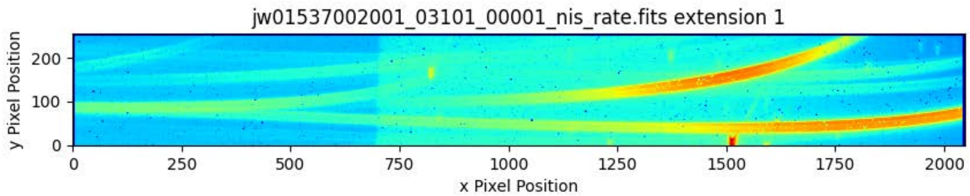

Figure 8: The mean rate image for the observation of standard G 191-B2B in program 1537. The display is using an IRAF-style logarithmic display to show the background component.

Figure 9 shows the SUBSTRIP256 sub-array with the Digital Sky Survey image of the field in the background for the specific orientation of program 1537 observation 2. Although the orientation avoids the brighter stars nearby, the three faint stars that are close to the standard star are unavoidable. These three stars are between 6.5 and 8.8 magnitudes fainter than G 191-B2B in the Gaia DR3 catalogue.

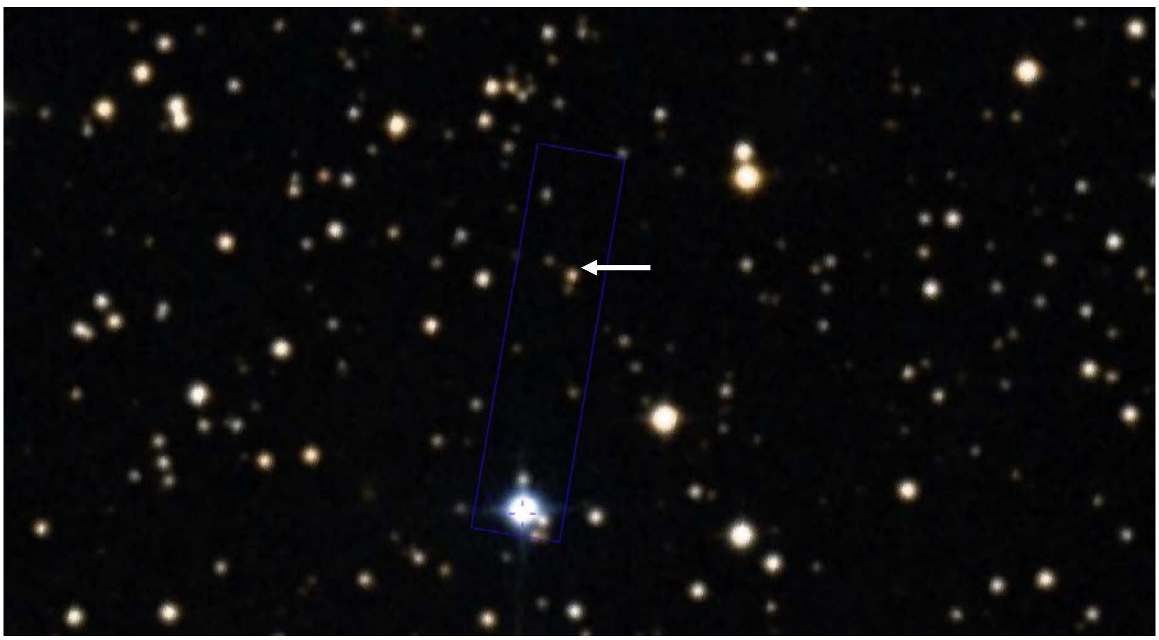

Figure 9: The Digital Sky Survey image of the field of G 191-B2B with the orientation of the SUBTRIP256 subarray for observation 2 of program 1537 overlaid. Although this orientation avoids the bright stars in the vicinity, a number of faint stars are within the subarray area, including the star marked with the arrow that produces the long wavelength order 1 contamination for G191-B2B.

The star marked with the arrow is probably the source of the first-order spectrum that contaminates the order 1 spectrum of G 191-B2B at long wavelengths. That star is Gaia DR3 266080164657064192 or 2MASS J05052871+5251151 or WISE J050528.71+525114.8. This star appears to be a late K-type main sequence star with moderate reddening from the Gaia DR3 observations. Table 2 shows the Gaia/2MASS/WISE photometry for this star compared to the corresponding values for G 191-B2B.

Table 2: Photometry for the marked contaminating star in Figure 9 and for the photometric standard star.

Filter	2MASS J05052871+5251151 Magnitude	G 191-B2B Magnitude
Gaia DR3 G	17.1671 ± 0.0009	11.7184 ± 0.0007
Gaia DR3 G_{BP}	18.2387 ± 0.0130	11.7184 ± 0.0007
Gaia DR3 G_{RP}	16.1552 ± 0.0040	12.0707 ± 0.0006
2MASS J	14.893±0.042	12.543±0.021
2MASS H	14.107±0.044	12.669±0.025
2MASS K_S	13.905±0.049	12.764±0.023
WISE W1	13.726±0.035	12.816±0.024
WISE W2	13.805±0.035	12.957±0.020
WISE W3	>12.139	>12.656
WISE W4	>9.047	>9.061

Observations of G 191-B2B in SOSS mode were strongly desired despite the moderately crowded field and the chance of contamination because this is the only available white dwarf photometric standard that NIRISS can observe in this mode at a reasonable S/N. If it were possible to observe the brightest white dwarf star Sirius B and get much better S/N that would be preferable, but the close proximity of Sirius A makes this impractical.

Another issue beyond the contamination is the zodiacal light background. At this pointing the zodiacal background is about 1.38 times higher than the standard template shown in Figure 1 above (with no offset parameter used), and there are some discrepancies in the shape as well. This makes proper extraction of the spectrum difficult even ignoring the effects of contamination. A second background subtraction with a scaling value of 1.25 and no constant offset was used, and this seems to produce better results in the extracted spectrum. Figure 10 shows the ratio of the extracted spectrum of G 191-B2B to the CALSPEC model (g191b2b_stiswfcnic_004.fits) for the original rate image and for the background-subtracted case with the two scalings, in first order only since order 2 and 3 are subject to contamination. In the original spectrum one sees the background signal effect in the discontinuity in the spectral ratio around 2.15 µm. At longer wavelengths the contamination from 2MASS J05052871+5251151 strongly affects the spectrum. There are also discrete peaks due to contamination from order 0 spectra at several wavelengths, around 1.25, 1.32, 1.70, and 2.0 µm.

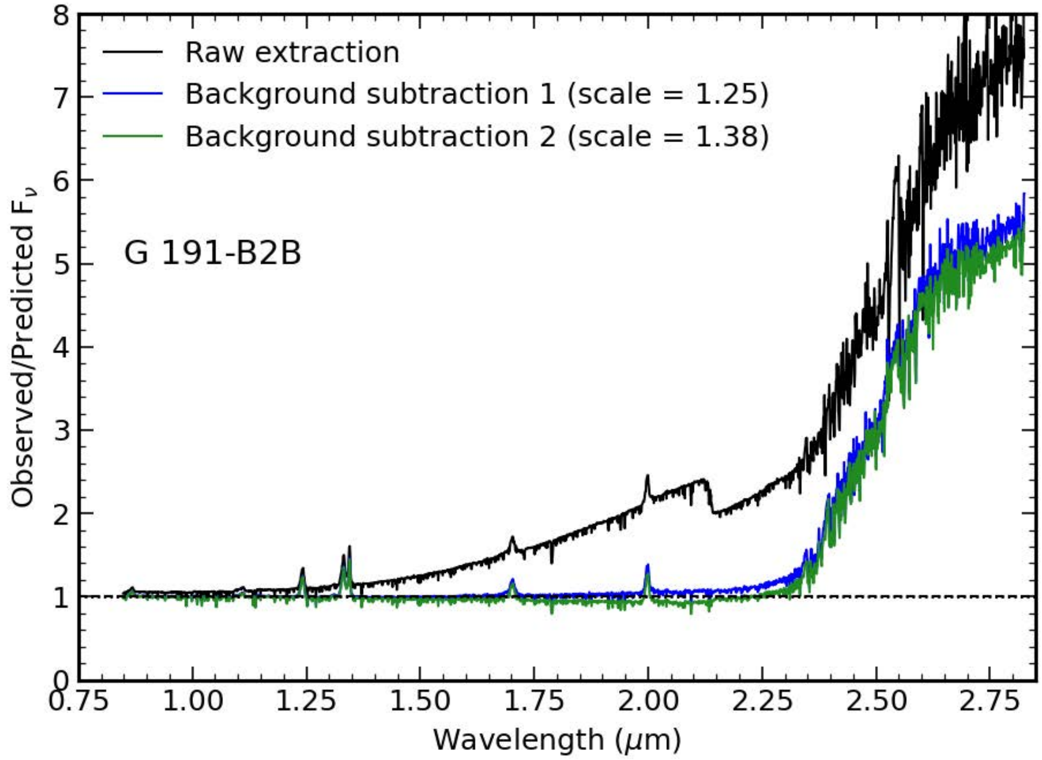

Figure 10: The ratio of the extracted first order SOSS spectrum of G 191-B2B to the CALSPEC model spectrum for the original rate image (black) and for the two background-subtracted rate images (blue and green). At wavelengths longer than 2.25 μm or so there is contamination from the K-type star 2MASS J05052871+5251151. The blue curve, for a background scaling factor of 1.25, appears to produce the best result. In both cases the offset parameter was set to zero and only the pure scaling was used.

Figure 11 and Figure 12 show the order 1 signal ratio compared to the model for the background-subtracted spectrum. As is seen in Figure 11 the spectrum is contaminated at wavelengths longer than about 2.15 μm. At short wavelengths the upper envelope of the ratio values is flat with values close 1.0, but from approximately 1.3 μm onward there is a slope of the ratio values as they decline from about 0.99 to 0.95. It is not clear whether this is a real effect due to a small discrepancy in the CALSPEC model spectrum or whether there is some issue in the spectral extraction or the background subtraction star which has lower S/N than the observations at shorter wavelengths. However, the uncertainties in the background subtraction may also explain this issue, particularly because the background template shape may be subtly wrong for this sky position. The star is at ecliptic latitude +29.8°, while the background observations have been taken near the ecliptic equator to maximize the signal that is measured. We do not know if this affects the background template shape.

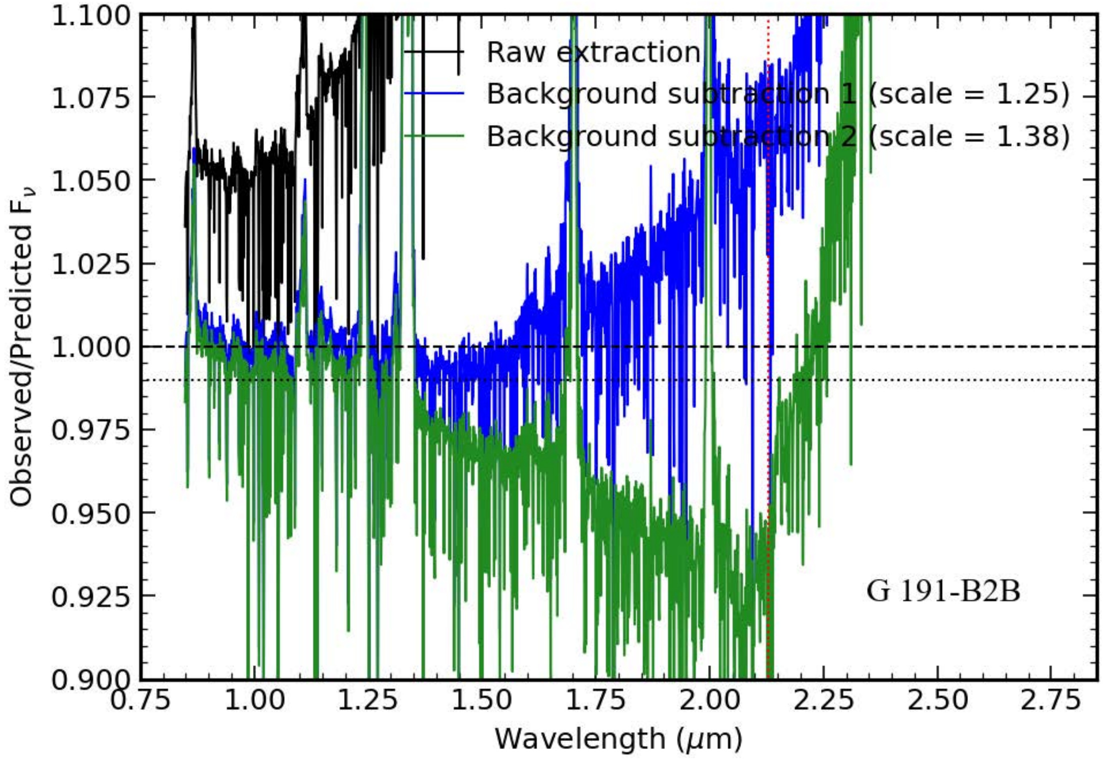

Figure 11: As in Figure 10 but zoomed in to show the background-corrected spectral ratio. The red dotted line marks the wavelength at which contamination from the K-type star starts to have a significant effect.

Given the uncertainties the most trustworthy part of the spectral ratio plot is the shorter wavelength part at wavelengths below about 1.6 μm. That part of the ratio spectrum plot is shown in Figure 12. These values are consistent with the results for BD+60°1753 shown in Figure 6, with the ratio values generally being between 0.99 and 1.01 over this range of wavelengths in the positions where there is no contamination.

In the future with better knowledge of the possible changes in the zodiacal background template shape it may be possible to improve these results and extend the useful wavelength range to 2.13 μm. Note that both order 2 and order 3 have too much contamination to allow useful comparisons with the stellar model to be made, which is why these orders are not shown for this standard star.

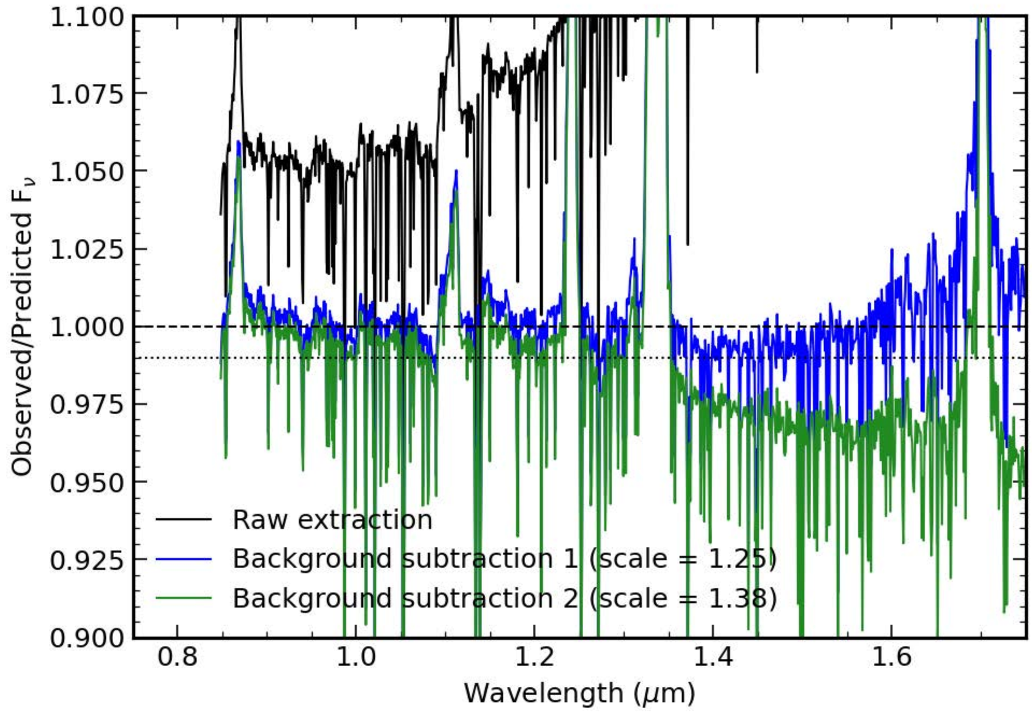

Figure 12: As in Figure 10 and Figure 11, but showing the shorter wavelength part of order 1 where the ratio values do not show a systematic change with wavelength. As is the case for the observation of BD+60°1753 in Figure 6 above, the upper envelope of values for the background-subtracted spectrum with scaling 1.25 (the blue curve) in this wavelength range are between ratio values of 0.99 and 1.01 where there is no contamination or bad pixel drop-outs.

3.4 Observations of GSPC P177-D

This G-type photometric standard was observed in observation 12 of program 1538. The rate image from the observation is shown in Figure 13 below. There is minimal contamination of the image; there are several faint zero order spectra present but these are not very close to the main spectral traces.

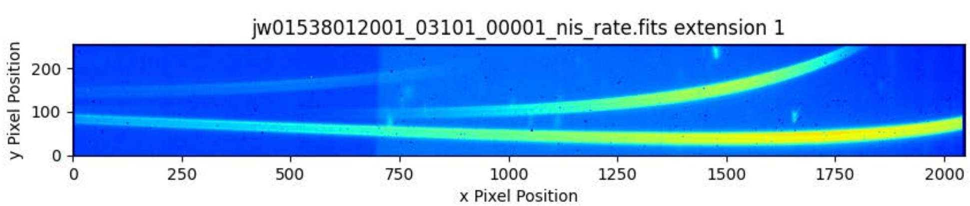

Figure 13: The mean rate image for the observation of standard GSPC P177-D in program 1538. The display is using an IRAF-style logarithmic display to show the background component.

Figure 14 shows the ratio of the extracted order 1 spectrum for GSPC P177-D to the CALSPEC model file p177d_stisnic_010.fits using the raw rate file for the processing. One sees significant effects due to the zodiacal background. There is also some type of excess signal just on the short wavelength side of the background discontinuity.

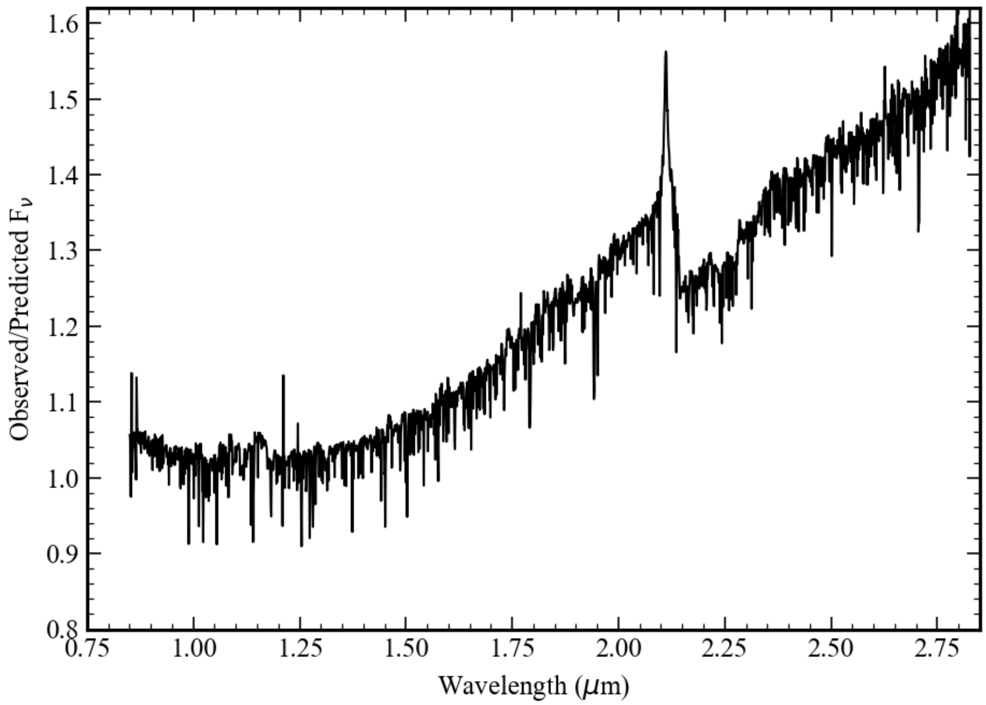

Figure 14: The ratio plot of the pipeline extracted spectrum for GSPC P177-D in order 1 with the CALSPEC model spectrum from p177d_stisnic_010.fits. The effect of the zodiacal background is obvious from the spectral ratio discontinuity at about 2.13 μm.

Attempts were made to remove the zodiacal background with the commissioning template. A few different combinations of the parameters were tried. The best background subtraction appears to be for a scaling of 0.730 and an offset of 0.119 ADU/s. This leaves a residual constant background across the image at a low signal level. If one scales to make the background-subtracted image go to zero away from the spectral orders the result is always an over-subtraction of the background that causes the extracted spectrum to be low by 10% or more across the order 1 wavelength range. Why there needs to be a residual signal over the subarray when the background is properly subtracted off to produce the right signal level is not understood. It may be that there is a scattered light component from the GR700XD grism when a bright star is observed that is not produced in the background observations with only faint sources in the field, and that this is what is left after the background subtraction, but at this point this is speculation. This situation makes the background subtraction difficult to carry out automatically, since it is not clear what signal level to aim for in the subtraction.

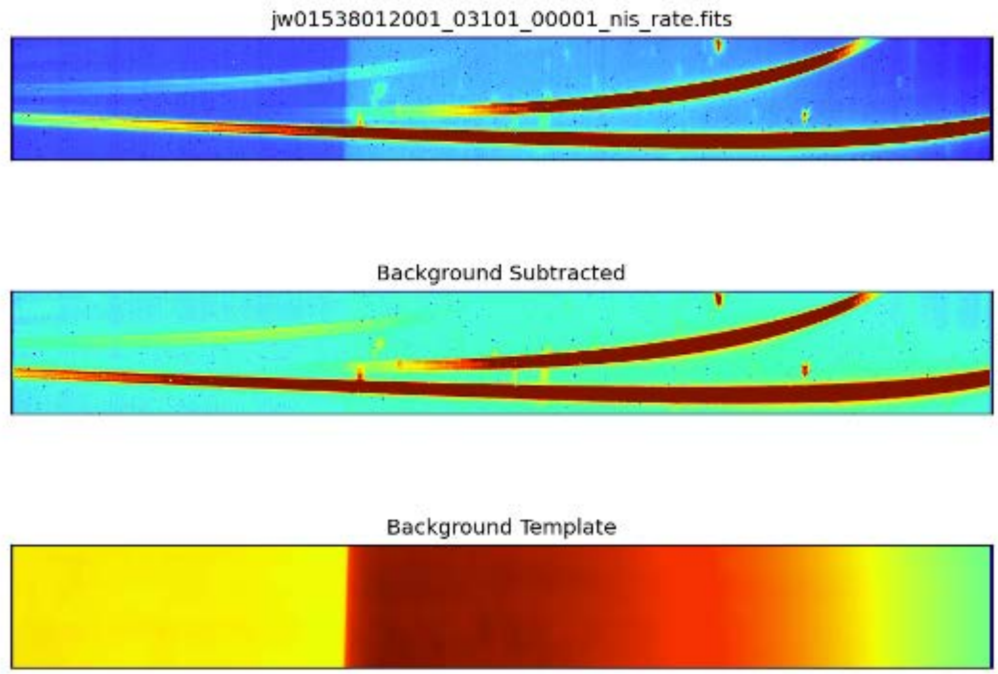

Figure 15: The background subtraction for the observation of GSPC P177-D. The upper panel shows the original rate image. The middle panel shows the best background subtracted rate image that was obtained. The low panel shows the background template used, which is scaled by a factor of 0.73 compared to the original template image, and then offset by 0.119 ADU/s.

Figure 16 shows the ratio plot of the extracted order 1 spectra for no background subtraction and for the best background subtraction that was found. The two-parameter change in the default background template from NIRISS commissioning is able to produce a fairly good match to the predicted spectrum using the photometric calibration from BD+60°1753. Aside from the wavelengths around 2.1 μm where the zero order "spectrum" of another source is contaminating the extracted spectrum, the ratio values from the best background subtraction are consistent with 1.0 within about ±1% where the spectrum is not affected by bad pixels causing the signal to drop. Deviations down by about 1% are more common than deviations up by 1%.

Looking at orders 2 and 3, the order 2 spectrum is close to the expected spectrum for wavelengths less than about 0.9 μm and deviates high for longer wavelengths whereas order 3 is too high by about 20-40% over the wavelength range of better signal. This is shown in Figure 17 below. Although the pattern of the ratio values is broadly similar to what is seen for BD+60°1753, the deviations are larger than for the brighter standard. The results for order 2 and 3 may indicate that there is some systematic effect present that is a function of the spectral type of the standard in these higher orders.

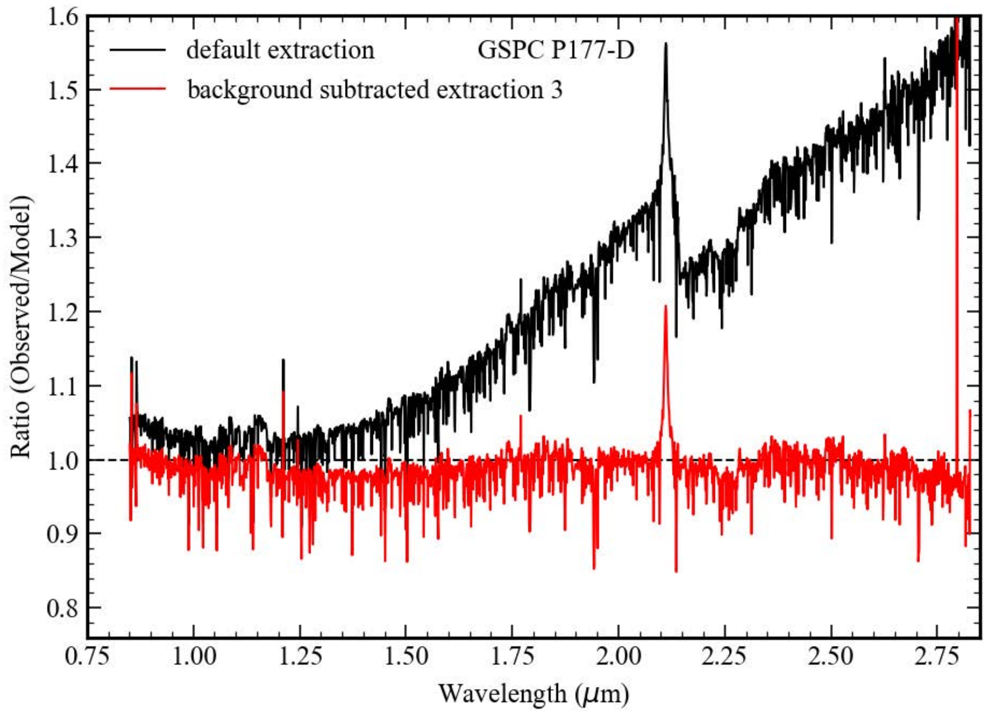

Figure 16: The ratio of the extracted spectra for GSPC P177-D to the CALSPEC model for the raw observation (black curve) and for the best background subtraction that was found (red curve). The narrow peak at about 2.1 μm is due to an order zero "spectrum" contaminating the extraction.

3.5 Observations of 2MASS J17430448+6655015

This star is a fainter A-type photometric standard, spectral type A8III. It was observed in program 1536 observation 9. The output mean rate image from the JWST data reduction pipeline is shown in Figure 18 below. Clearly there is a contamination issue in that a second fairly bright spectrum is seen on the left side of the image, which is a problem for the long wavelength part of order 1. It is also an issue for order 3 and the longer wavelength part of order 2; but in the latter case the S/N would have been very low anyway.

Figure 19 shows the Sloan Digital Sky Survey image of the field of the standard with the SUBSTRIP256 sub-array overlaid at the orientation of the observation. The epoch of observation turned out to be unlucky because of the presence of another star in the sub-array. In retrospect this orientation should have been excluded in the APT file.

The star that is causing the contamination problem appears to be star SDSS J174253.95+665341.8 = 2MASS J 17425395+6653418 = WISE J174253.93+665341.8 = Gaia DR3 1634280277840964864. The Gaia DR3 astrophysical parameters for this star are T=5415 K (range 5407-5429 K) and $\log_{10}(g)$ = 4.173 (range 4.152-4.187). These suggest that the star is mid-G type and may be of luminosity class IV. The available

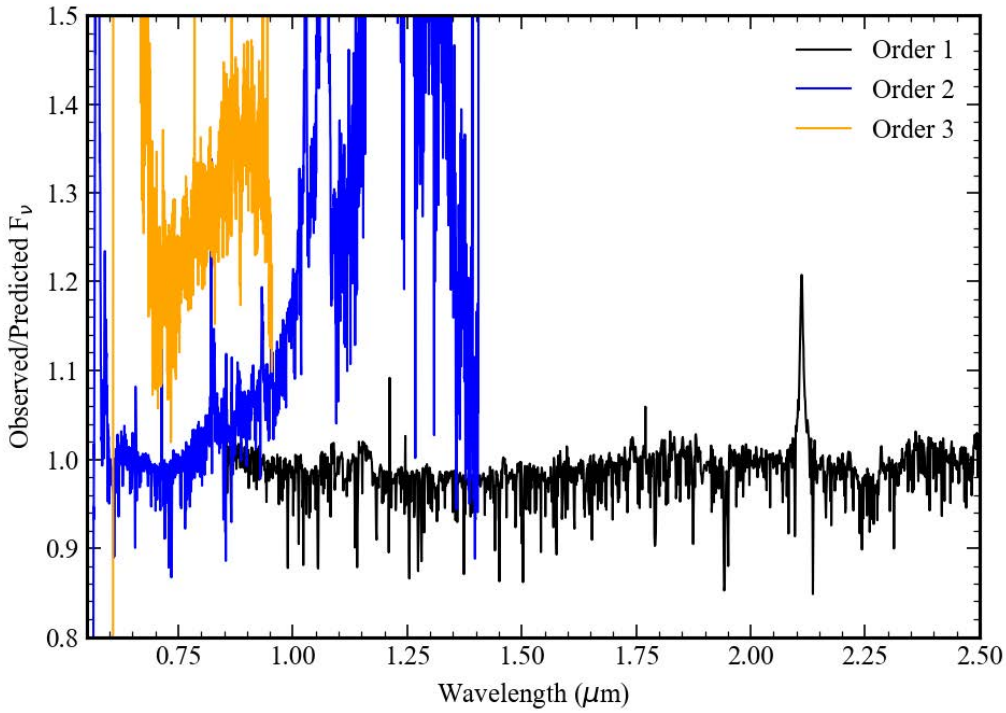

Figure 17: The ratio of the extracted GSPC P177-D spectra in the three orders to the CALSPEC model. The calibration is clearly off for order 3 over the entire wavelength range, while for order 2 the calibration is reasonable at wavelengths less than 0.9 µm but clearly fails at longer wavelengths.

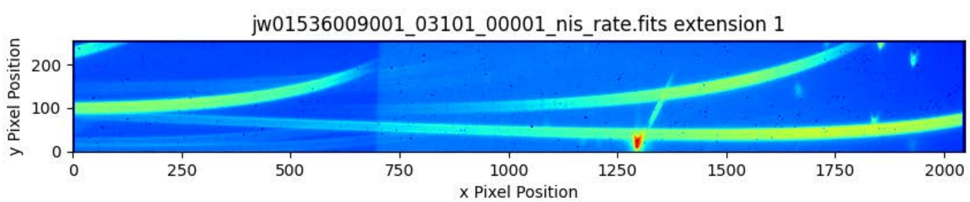

Figure 18: The mean rate image for the observation of standard 2MASS J17430448+6655015 in program 1536. The display is using an IRAF-style logarithmic display to show the background component. One sees a contaminating order 1 spectrum at left overlapping with the science target spectrum, and there is an order 0 spectrum close to the bottom of the sub-array near x pixel 1275.

photometry for the star is presented in Table 3 along with the values for the photometric standard star.

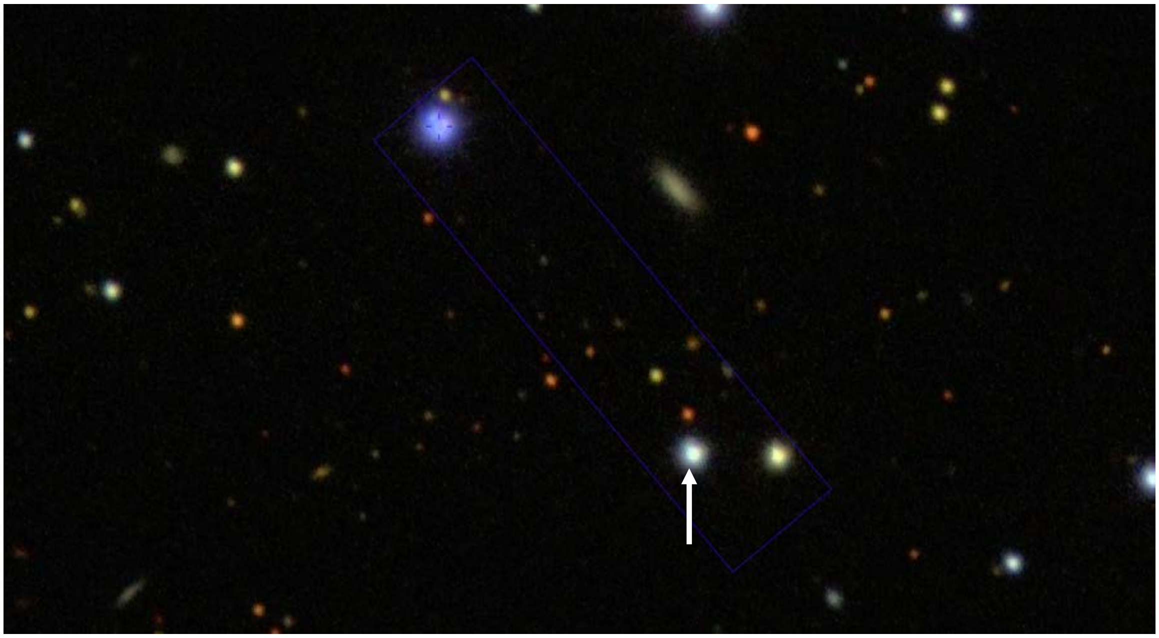

Figure 19: The Sloan Digital Sky Survey image of the field of G 191-B2B with the orientation of the SUBTRIP256 subarray for observation 9 of program 1536 overlaid. This orientation turned out to be bad for the observation, and should have been excluded from consideration. The star marked by the arrow is the main contaminating source seem in Figure 18.

As was the case for GSPC P177-D there is a clear need for background subtraction in the rate image for the observation of 2MASS J17430448+6655015. Figure 20 shows the ratio of the extracted order 1 spectrum to the CALSPEC model 1743045_stisnic_007.fits, both in the original extraction from the raw rate image (black), from the background-subtracted rate image with a scaling value of 0.8593 and offset 0.0 for the commissioning zodiacal background template (blue), and from a further scaling down to 0.8 again with offset 0.0 (green). The usual discontinuity in the spectrum at about 2.15 μm is seen in the raw rate spectrum ratio, and this is absent in the corrected spectrum ratio for both scaling values. There is also a large feature near 1.55 μm due to an order 0 contamination.

It is unusual for the ratio values to start to decrease significantly for wavelengths above 2.5 μm when one sees in Figure 18 that there is a contaminating order 1 spectrum overlapping on the standard star order 1 spectrum at these wavelengths. It seems that this must be some type of issue in the pipeline spectral extraction, although it is difficult to attempt to track down why or how this is taking place. As the spectrum is unreliable at these wavelengths in any case, this has not been investigated further.

Table 3: Photometry for the marked contaminating star in Figure 19 and for the photometric standard star.

Filter	SDSS J174253.95+665341.8 Magnitude	2MASS J17430448+6655015 Magnitude
SDSS u	16.805±0.007	14.761±0.004
SDSS g	15.168±0.003	13.545±0.002
SDSS r	14.627±0.003	12.494±0.003
SDSS i	14.475±0.003	14.083±0.006
SDSS z	14.420±0.004	13.362±0.003
Gaia DR3 G	14.6828±0.0002	13.4711±0.0002
Gaia DR3 G_{BP}	15.0591±0.0008	13.6078±0.0006
Gaia DR3 G_{RP}	14.1488±0.0007	13.2368±0.0004
2MASS J	13.357±0.026	12.979±0.022
2MASS H	13.248±0.028	12.880±0.024
2MASS K_S	13.092±0.035	12.772±0.028
WISE W1	13.128±0.023	12.822±0.022
WISE W2	13.171±0.023	12.846±0.022
WISE W3	13.048±0.312	12.663±0.227
WISE W4	>9.791	>9.692

Although the corrected spectrum ratio is relatively flat and shows no evidence of the discontinuity, there is some structure in the ratio spectrum from short wavelengths out to 2.5 μm at the few percent level. This structure is likely to be due to limitations in the background template shape in detail, although it is also possible that there is some issue with the CALSPEC model at this level of accuracy.

As was seen for standard BD+60°1753, the line profiles in the model are not a good match to the line profiles in the extracted spectrum. The Paschen series line wavelengths need to be shifted by a factor of 1.0037 to match the model line wavelengths, and even when this is done there are residual line shape variations between the CALSPEC spectrum and the SOSS spectrum. A simple scaling of this sort may not be sufficient to describe the wavelength issue over all of order 1, as there seem to be some much smaller discrepancies between the shifted wavelengths of the higher series lines at wavelengths above 2 μm after this scaling is applied.

In Figure 21 the ratio values from Figure 20 are replotted with the y axis range from 0.9 to 1.1 to show the detailed deviations with wavelength. From 0.8 5 to 2.0 μm the deviations from 1.0 are limited to within ±2.5% for the general upper envelope of values, with the usual "drop-outs" from bad pixels. Beyond 2 μm the ratio values are larger than 1 and show several local peaks. The two local peaks near 2.1 and 2.3 μm seem to correspond to two very faint contaminating order 1 spectra visible in Figure 18. However, the two spectral traces are very faint in the rate image and it was not expected that these would cause a 10%-15% change in the extracted spectral signal. Nonetheless, it appears that the ratio values are not reliable for wavelengths beyond 1.9 μm.

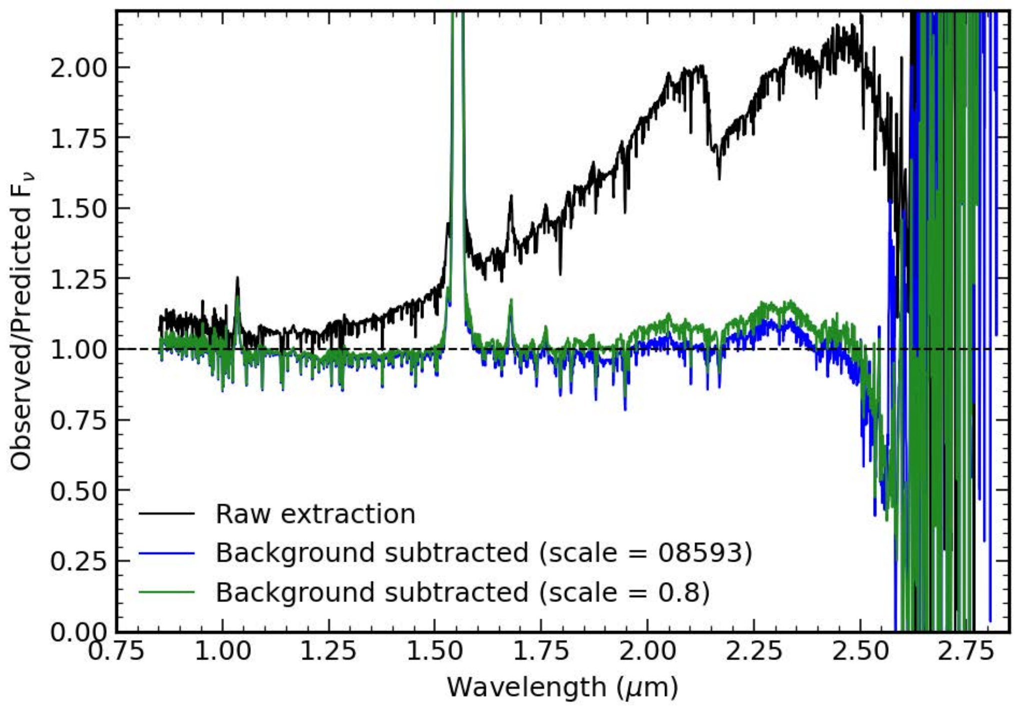

Figure 20: The extracted order 1 spectrum for 2MASS J17430448+6655015 without and with the background correction. The results of two different background scalings are shown for reference. The scaling of 0.8 appears to produce a reasonable result for most of the short wavelength part of the order 1 spectrum.

The standard star 2MASS J17430448+6655015 is close to the same brightness as GSPC P177-D and G 191-B2B at these wavelengths, but the end result for 2MASS J17430448+6655015 is about a factor of 3 worse in the ratio value deviations than for the other two cycle 1 standard stars. It would be useful to re-check this standard star in SOSS mode at some point in the future, possibly using a longer exposure and also taking a dedicated background exposure to reduce the uncertainties caused by the background subtraction.

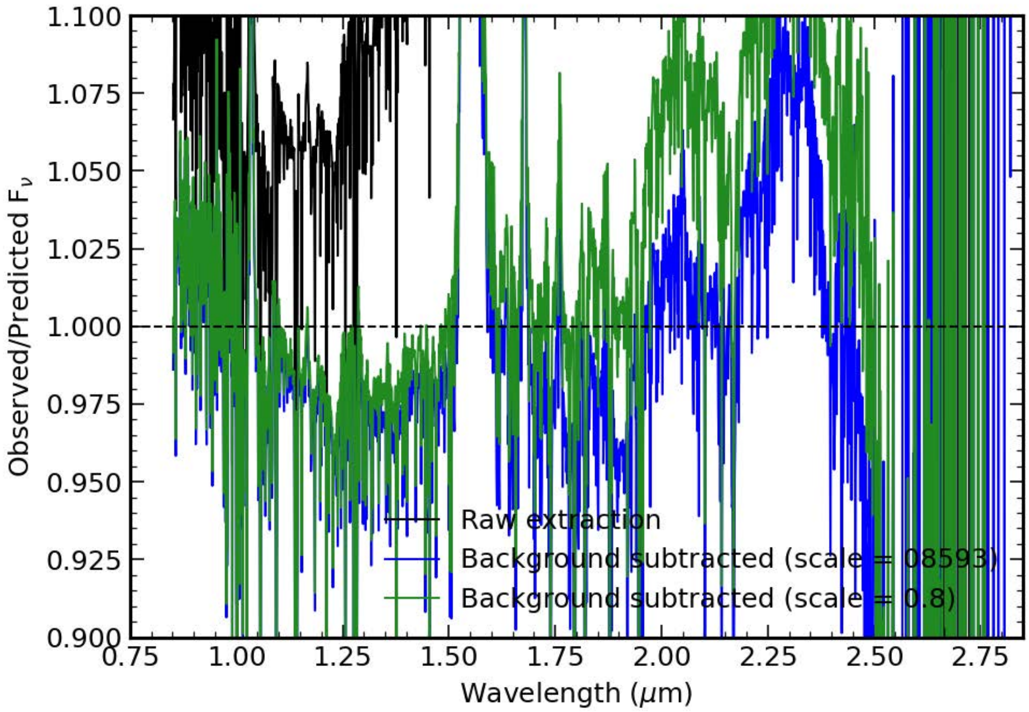

Figure 21: The short wavelength part of Figure 20 for comparison with Figure 6 and Figure 12.

3.6 SOSS Photometric Calibration Revision

Based upon the results for standards BD+60°1753, G191-B2B, GSPC P177-D, and 2MASS J17430448+6655015 in Figure 6, Figure 12, Figure 16 and Figure 21 the photometric calibration in order 1 is consistent with the CALSPEC models to an accuracy of about ±1% for BD+60°1753, G191-B2B and GSPC P177-D, while for 2MASS J17430448+6655015 the agreement is at the ±2.5% level.

The revision of the SOSS photometry file for the correction described in section 3.2.1 and for a preliminary revised fit to the ATOCA spectrum for BD+60°1753 was delivered to CRDS on 7 November 2023. The new file jwst_niriss_photom_0045.fits replaced the commissioning file jwst_niriss_photom_0034.fits at that time. The reductions shown in this report using pipeline version 1.14.0 are using this revision of the photometric scaling values. The latest reduction for BD+60°1753 and for P177-D may indicate that another 1% reduction is needed for order 1, whilst the results for G 191-B2B for order 1 argue against any further revision. The revisions to the order 2 and 3 response values discussed in section 3.2.2 produce reasonable results for the commissioning observation of BD+60°1753 (see Figure 7) but there are issues for the other standards in those cases where a comparison can be made. This is particularly the case for order 3, which deviates by 10-30% from the model prediction in two of the standard star observations. More work is needed to understand what the issue is in the order 3 calibration, and also for the long wavelength part of order 2. Since the long wavelength part of order 2 is redundant with the wavelength coverage of order 1 and has relatively low S/N for part of this wavelength range this is not vital to SOSS observations but it is still desirable to get a better calibration.

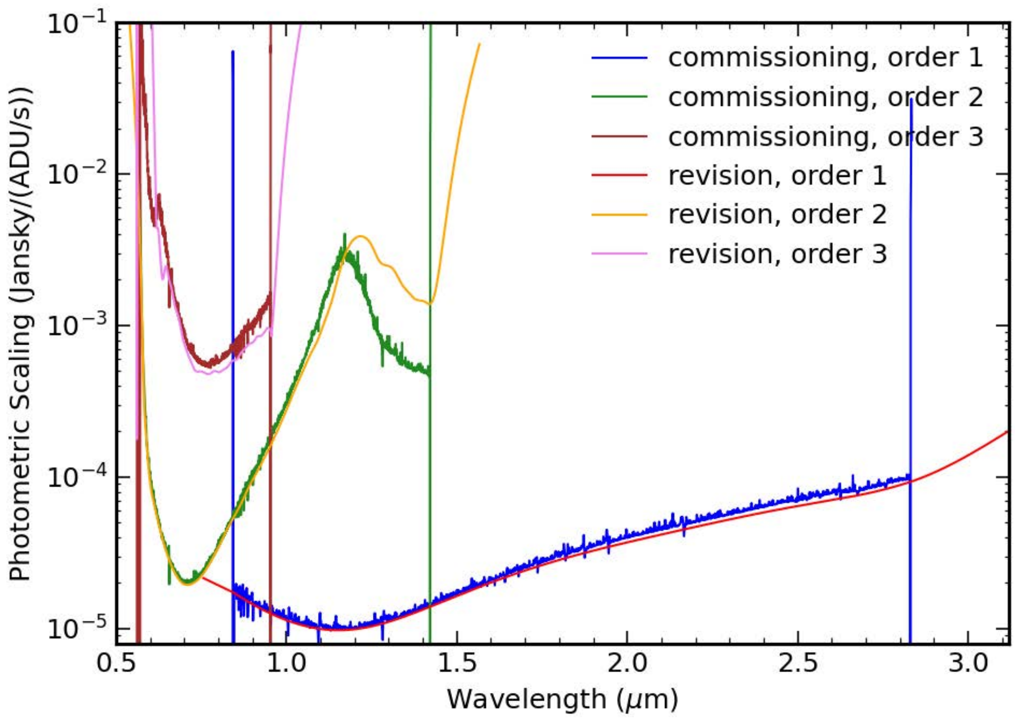

Figure 22: Illustration of the changes to the NIRISS SOSS photometric scaling function between commissioning and the cycle 1 revision.

Figure 22 and Figure 23 show a comparison of the commissioning SOSS photometry values in file jwst_niriss_photom_0034.fits and in file jwst_niriss_photom_0045.fits. Note that the units were changed between the commissioning file, where the scaling was in units of MJy/(ADU/s), to the cycle 1 revision file, where the scaling is in units of Jy/(ADU/s). In the plots the commissioning values are scaled by a factor of 10^6 for the change in output units from MJy to Jansky. The reason for the change in units is that the JWST pipeline documentation at the time of commissioning stated that the reference file needed to have conversion values to MJy but the values in the header of the output file indicated that the units out are Jansky.

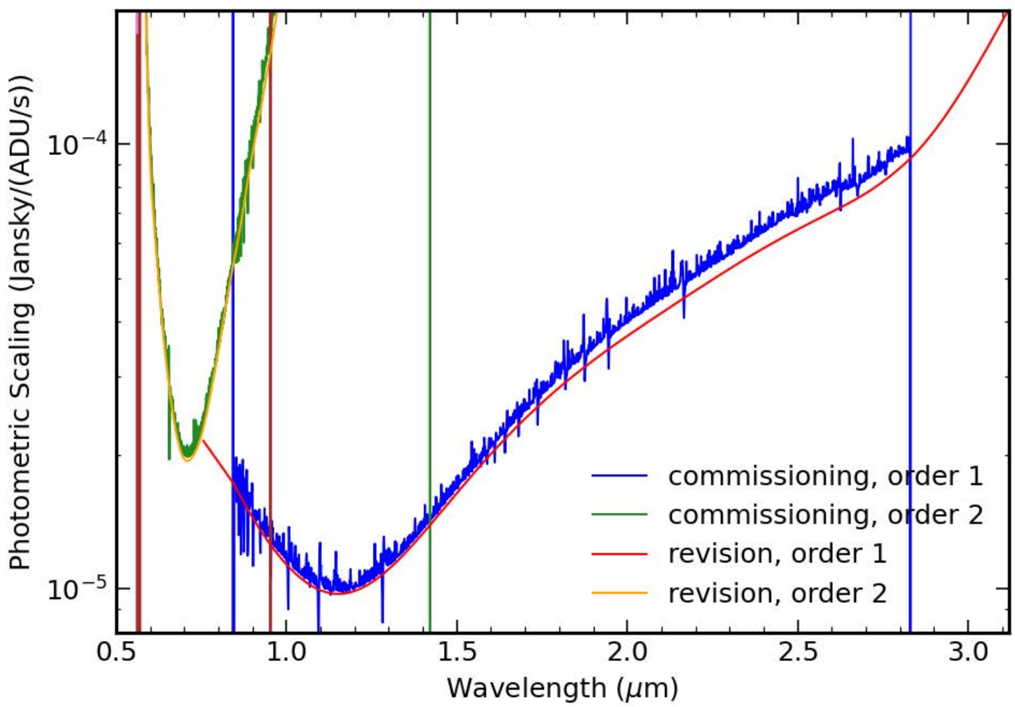

Figure 23: As in Figure 22, but with a restricted y axis range to show the changes in order 1 and order 2.

In Figure 22 the changes in the fitting of the order 2 and order 3 functions in the regions of lower signal are obvious. There are also small changes in the values around the peak response, where the values are the lowest, due to small changes in the extraction and fitting in the re-reductions.

In the revised reference file, there was also a change of the F277W order 1 response function to use the smoothed functional fit rather than the raw noisy values, but since the ATOCA code does not currently extract the F277W order 1 spectrum this change is not shown in the plots. There was no additional work done for the extraction or fitting of the F277W SOSS mode based on the cycle 1 observations and there was no re-reduction of the commissioning data in this case. Such analysis will only be done if the JWST pipeline is changed to extract the F277W SOSS spectrum.

4.0 Conclusions

Analysis of the cycle 1 SOSS photometric calibration observations in cycle 1 programs 1536, 1537, 1538, and 1539 along with a re-reduction of the commissioning SOSS photometric calibration observation in program 1091 has been carried out. In these newer reductions of the spectra the ATOCA algorithm is used to extract the spectral orders, leading to some changes in the output spectra for the commissioning observations. There are also some changes in the spectral results from changes in the ramp fitting part of the JWST pipeline, although these are generally small. The change to using ATOCA for the extractions led to a 1% reduction of the commissioning photometric calibration values for all orders. As well, an error in the commissioning photometry file adopted at the end of commissioning which led to some noise being imprinted on the JWST pipeline spectra was corrected. These changes were submitted to CRDS on 7 November 2023. That set of revised photometric scaling values is used in the most recent reductions shown in this report.

There is indication of issues with the order 2 and order 3 photometric calibrations at some wavelengths from the observations of GSPC P177-D in cycle 1. The largest discrepancies between the order 2 extracted spectra and the CALSPEC model spectrum are seen in the wavelength ranges where these orders have low signal, and hence the largest uncertainties, but there are also indications of smaller discrepancies at short wavelengths. For order 3 there remain discrepancies at the 10%-30% level between the extracted spectra and the CALSPEC model spectrum, which may be the result of the ATOCA extraction algorithm for this order, or the generally lower S/N of the observations, or be in part because of the effect of the background subtraction. More work is needed in the calibration of SOSS order 3. The cycle 2 program 3279 is specifically intended to improve the calibration of SOSS order 3.

For the cycle 1 calibration observations the background subtraction was found to have a strong effect on the output spectra from the JWST pipeline. Background subtraction was done for each source using a “standard” zodiacal light background template derived from observations in commissioning in a two-parameter model with an offset and a scaling value. This model can produce reasonable results, but the reason for needing an offset term in some cases is not understood. It is not straightforward to carry out the background subtraction in the general case where one does not know the absolute shape and level of the object spectrum. Work is underway in cycle 2 and cycle 3 calibration programs to see if the background can be characterized better to aid in the correction. In cases where the output spectral shape accuracy is required to be of the highest fidelity it is probably necessary to have a background observation in addition to the main science observation. The background scaling compared to the commissioning template derived in these reductions varies from 0.8 to 1.25.

Given the issues with the background subtraction it may be future photometric calibration observations should include a dedicated background measurement. The possibility that the detailed background shape is a function of time as well as the specific ecliptic coordinates of the observation may mean that the current idea of using a two-parameter shift and scaling of the “standard” zodiacal light templates observed in the SOSS background calibration program 4479 may be insufficient to allow 1% or better photometric calibration observations. If the background variability cannot be accurately modelled then this type of observation will be required for any SOSS mode observations for which the background subtraction is a concern for the quality of the extracted spectra.

Some of the cycle 1 observations have spectral overlap from other sources in the field. This is particularly of concern for the observations of G191-B2B and 2MASS J17430448+6655015, where the order 2 and order 3 spectra are heavily affected by contamination and where the long wavelength part or order 1 was also affected by contamination. We do not have a method for correcting observations for contaminating sources in SOSS mode, such as is used in wide-field slitless spectroscopy on the Hubble Space Telescope and which is also under development for the NIRISS and NIRCam wide-field slitless spectroscopy mode. The complexity of the SOSS PSF along with the absence of direct images at the wavelengths covered by the GR700XD grism to go along with the grism images makes this type of correction much more difficult than is the case for the wide-field slitless spectroscopy modes.

Another issue with the standard star observations in general is the effect of bad pixels on the extracted spectra. As is seen in the various figures in this report, the extracted spectra are all subject to numerous "drop-outs" where the signal is reduced by up to 20% in individual spectra elements. There is no dithering in the SOSS mode observations so we cannot use dithers to replace these bad pixels. In the longer term some method to correct for these bad pixels is needed to improve the general S/N of the photometric calibration results.

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