Spectrometer Configuration Impact on Spectrum Measurement Accuracy

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Introduction:

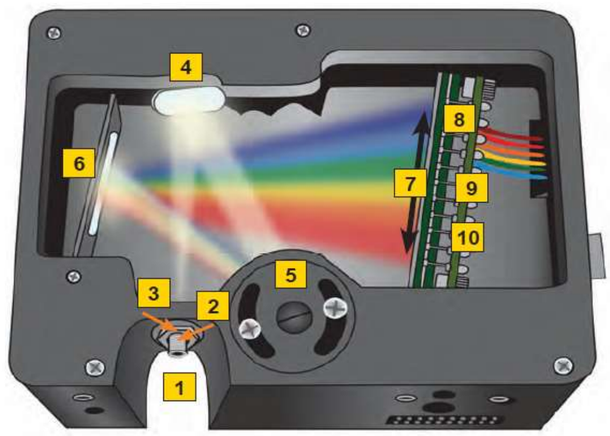
USB spectrometers are wonderfully useful devices. In a very compact package, and at a reasonable price, one can have the ability to measure the detailed spectrum of a light source. There are innumerable applications of this capability, from medical diagnostics to product design to quality control. My main application of the technology is the measurement of astronomical filter transmission spectra. I have been using a used Ocean Optics (now Ocean Insight) USB4000 spectrometer (see Figure 1) that I purchased on Ebay for this task since December 2012. It wasn't until recently however that I learned of the limitations imposed on my spectrum measurements by the physical configuration of my device. This report documents my investigation of how spectrometer resolution impacts spectrum measurement accuracy, and the steps I took to improve the resolution of my USB4000.

Figure 1 Image of Ocean Optics USB4000 Spectrometer

Background:

A schematic view of the interior of the USB4000 is presented in Figure 2. The device works by first passing the sampled light source through a small entrance slit, and then directing it through a glass diffraction grating. The diffraction grating spreads the sampled light out according to wavelength just like a prism does, and then that pattern is projected onto a CCD sensor for measurement. The device is actually relatively simple, however it requires high precision components and calibration to be able to deliver repeatable high accuracy spectrum measurements.

The ability of the spectrometer to resolve a spectrum accurately depends on a number of things, including: the resolution of the CCD sensor, the groove density of the diffraction grating, and the width of the entrance slit. The sensor in the USB4000 is a Toshiba TCD1304AP linear CCD array, with 3648 pixels of size 8µm wide by 200µm tall. For the wavelength range my spectrometer is designed to work in, from 350 to 1000nm, the resulting minimum resolution that should be resolvable by the sensor is 0.18nm. The resolution of the spectrometer is also affected by the groove density of the diffraction grating. My device has a grating with 600 lines per millimeter. Changing the groove density changes the angle at which the diffracted light spreads out from the grating. Thus a grating with a higher groove density would spread the spectrum out more across the sensor, reducing the overall wavelength measurement range but increasing resolution.



(1. SMA905 connector, 2. Slit, 3. Optional filter, 4. Collimating mirror, 5. Diffraction grating, 6. Focusing mirror, 7. L4 detector collecting lens, 8. CCD detector, 9. Optional OFLV filters, 10. Optional UV4 detector upgrade)

Figure 2 Schematic View of USB4000 Spectrometer Interior

The final characteristic affecting spectrometer resolution is the entrance slit width. The spectrum image that is projected onto the sensor is in fact an image of the entrance slit that has been spread out according to wavelength. A wide entrance slit permits more light to enter the device, allowing the measurement of faint light sources, but it also blurs the spectrum that is projected onto the sensor. This blurring effect detrimentally impacts the resolution of the spectrometer. Thus, to achieve a high resolution the entrance slit must be narrow. The original entrance slit of my USB4000 was 100µm (i.e. not narrow).

The overall resolution reported by Ocean Insight for my device in its original configuration is 3.9nm. To better understand how spectrometer resolution impacts the accuracy of a spectrum measurement, I set up a simple mathematical model of an ideal filter spectrum and simulated numerically what the measured spectrum would look like using different spectrometer resolutions. I repeated this calculation assuming filters with different full width half maximum (FWHM) bandwidths. The resulting comparison plots are presented in Figures 3 to 5 for theoretical filters with FWHM values of 12, 7, and 3nm respectively. In each plot the black line is the actual filter spectrum, and the coloured lines are what would be measured using different spectrometer resolutions. For a filter with 12nm FWHM the spectrometer resolution can be quite large and still accurately measure the filter's spectrum (see Figure 3). For the 7nm FWHM filter (Figure 4) the effect of spectrometer resolution on the measured spectrum is more obvious. The ability to resolve the peak transmission is detrimentally affected by increasing spectrometer resolution, as well as the steepness of the cut-off on either side of the pass band. For a 7nm FWHM filter my USB4000 is likely still not bad at measuring the peak transmission, the

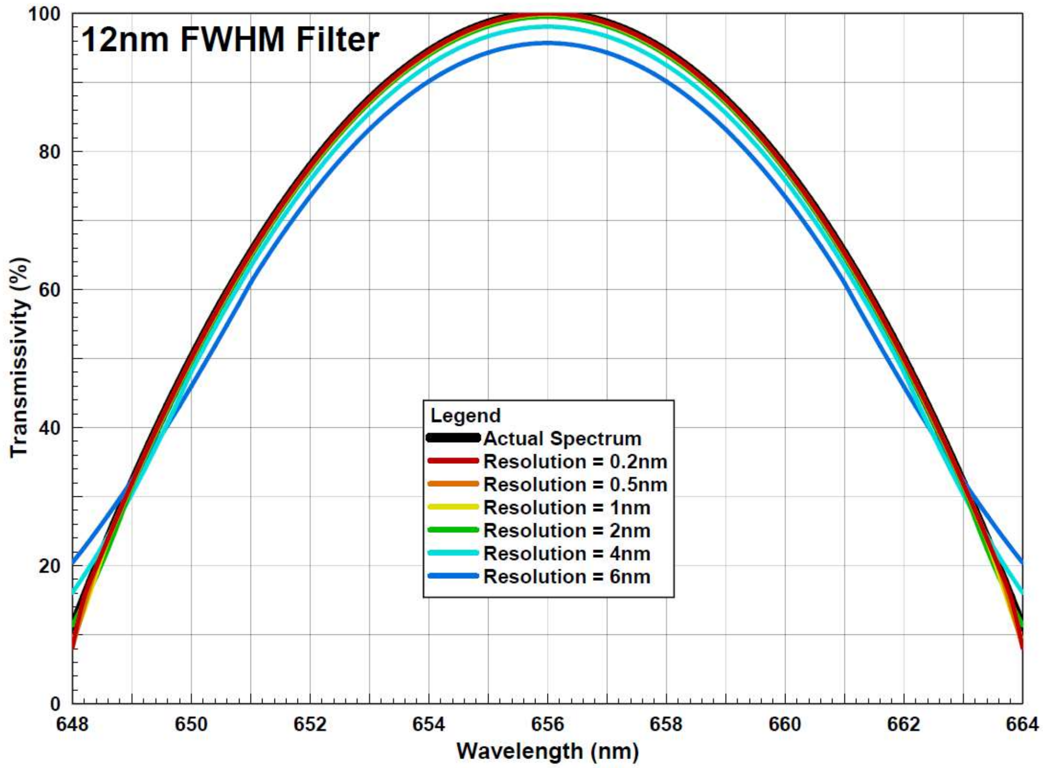


Figure 3 Simulation of Measured Spectrum vs Spectrometer Resolution, 12nm FWHM Filter

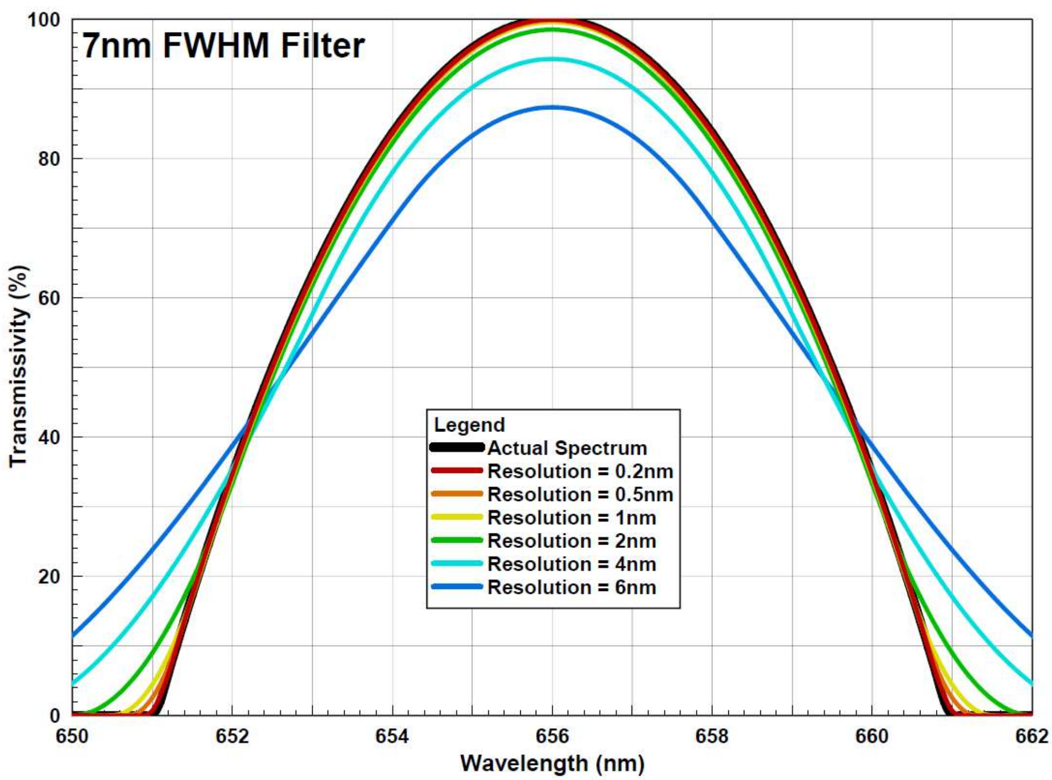


Figure 4 Simulation of Measured Spectrum vs Spectrometer Resolution, 7nm FWHM Filter

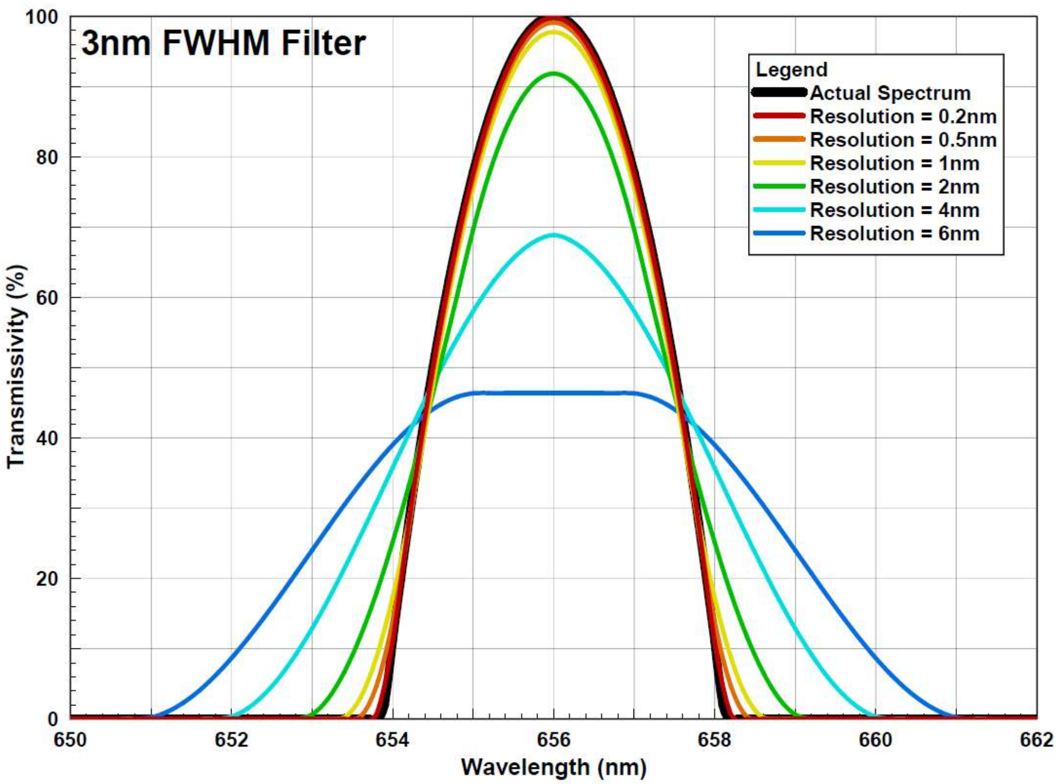


Figure 5 Simulation of Measured Spectrum vs Spectrometer Resolution, 3nm FWHM Filter

measurement being estimated from my simulation to be approximately 94% of the actual transmission. When measuring a filter as narrow as 3nm FWHM (Figure 5), the impact of spectrometer resolution is severe. My USB4000 can only hope to measure 69% of the actual peak transmission for such a narrow filter, and the measured FWHM will be significantly larger than actual. Based on this simulation, my spectrometer in its original configuration is not suitable for measuring filters narrower than 7nm. From these calculations a spectrometer resolution better than 1.5nm is required if I want to measure the peak transmission of a 3nm FWHM filter to within at least 95% of the actual. Fortunately for me, the USB4000 is designed to have modular components that are relatively easy to change. Using the tools available on the Ocean Insight website I was able to determine the spectrometer resolution I could expect for variously sized entrance slits. To help me choose which slit to go with I plotted the ratio of measured peak transmission to actual versus spectrometer resolution as predicted by my numerical simulation. The resulting graph is shown in Figure 6. I have included several vertical lines corresponding to different USB4000 entrance slit widths. Based on this plot I needed to swap the original 100µm slit for one 25µm or narrower to be able to measure the peak transmission of a 3nm filter to within 95% of the actual.

The narrowest entrance slit available for the USB4000 is 5µm. With that slit width a spectrometer resolution of about 1nm can be achieved. To achieve better resolution than this requires the diffraction grating to also be changed. Changing to a 1200-line per mm grating cuts the resolution in half, so around 0.5nm for a 5 or 10µm entrance slit. It turns out that is exactly what I did as I will explain next.

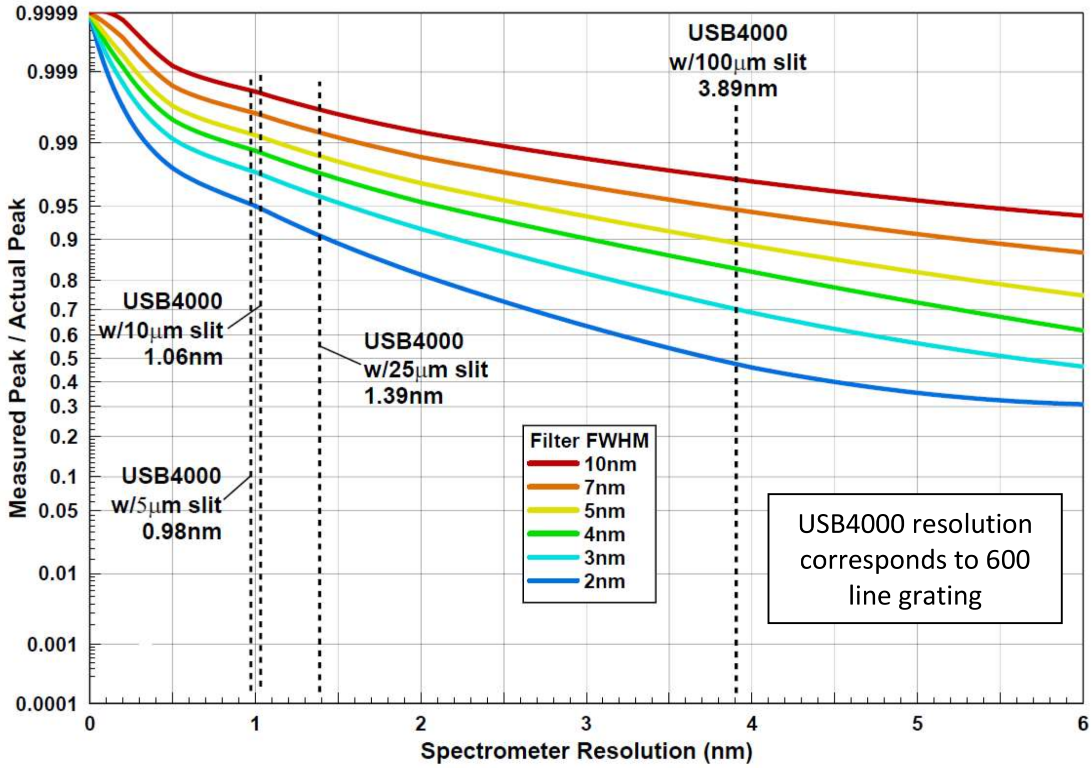


Figure 6 Simulated Impact of Spectrometer Resolution on Measured Peak Transmission

Spectrometer Upgrades:

The USB4000 I own is a relatively old device; it was originally manufactured in 2009. I was initially concerned about finding spare parts for my unit but was fortunate to find a reseller on eBay (spectrophoton) who has a large inventory of old Ocean Optics spectrometers and parts. From this supplier I was able to purchase a narrower entrance slit for $100. While combing eBay for used parts I also found some refurbished USB4000s for sale. For risk reduction reasons I purchased one of these units to use in my experimental parts swap exercise – if things went downhill, I would at least still have my original unit in working order. The used unit I purchased was configured with the same diffraction grating but a 25µm entrance slit. A view of the second USB4000 and replacement entrance slit is provided in Figure 7.

Changing the entrance slit consisted of removing the cover plate held on by four screws, removal of the main circuit board also held on by four screws, and removal of the retaining nut holding the SMA-905/entrance slit assembly in place. Figure 8 illustrates the views encountered during the work. The most challenging aspect of the job was breaking the circuit board free of the enclosure as it is sealed against light and dust ingress with an adhesive around all of the connectors. A significant amount of force was required to break the board free, resulting in several moments of me thinking: "Gah! What the heck am I doing?" In the end the entrance slit replacement was completed without incident and all that remained was to re-calibrate the spectrometer, a process that will be discussed later in this report.

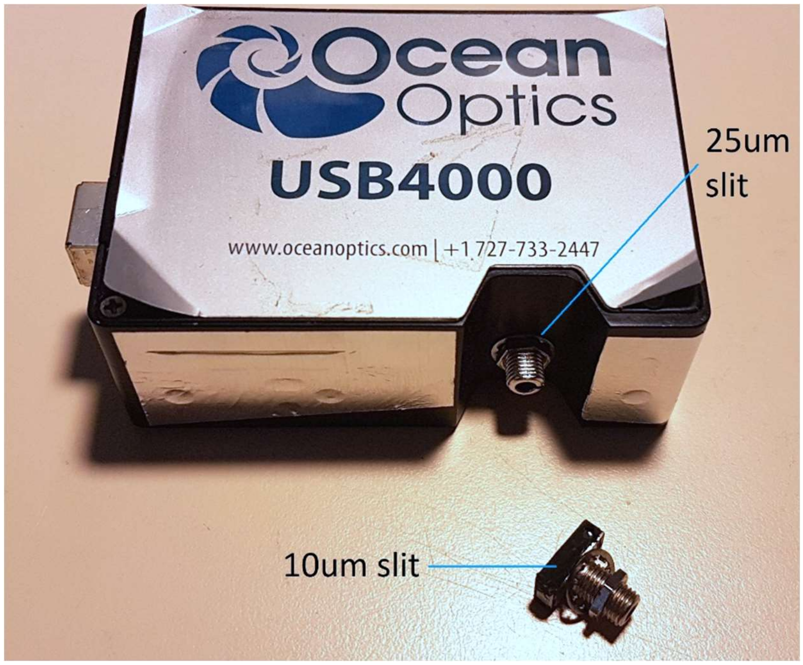
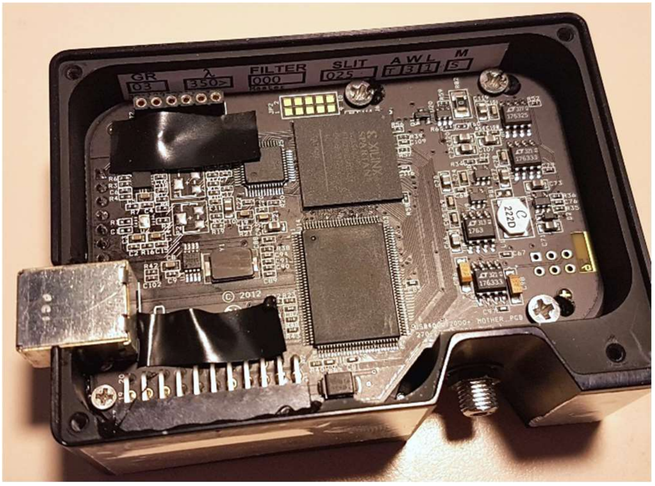


Figure 7 Second Used USB4000 w/ Replacement Entrance Slit

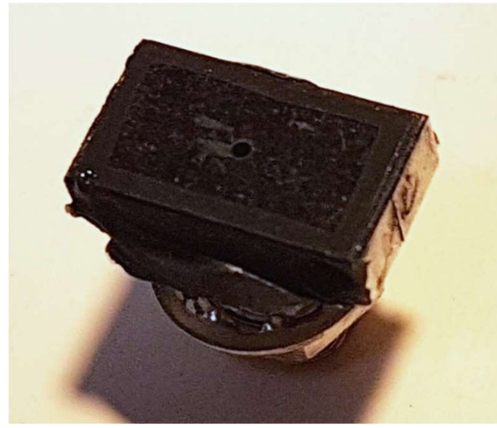
Before performing the slit replacement, I made some spectrum measurements using reference filters for which I had high resolution spectrum data from the filter manufacturer. I compared this before data to the results after changing the entrance slit. The improvement in spectrum accuracy was evident, but there was still room for improvement. That is why I next considered changing the diffraction grating groove density. I was able to source a replacement 1200-line grating from the same eBay supplier, but at the same time I came across an exceptional deal on a third USB4000 that already had a 1200-line grating installed. I also saw this as an opportunity to explore wider entrance slits so that measurements of lower light levels would be possible (i.e. night sky measurements). At the end of all my refurbishment activities I was left with three USB4000 units having the following configurations:

1. 600-line grating, no slit, wavelength range 350-1000nm, resolution fibre dependant;
2. 600-line grating, 5µm slit, wavelength range 350-1000nm, 0.98nm resolution; and
3. 1200-line grating, 10µm slit, wavelength range 414-746nm, 0.50nm resolution.

My original USB4000 is now configured with no entrance slit, so the diameter of the fibre optic patch cable I am using defines what the entrance slit size is and therefore the resolution of the spectrometer.

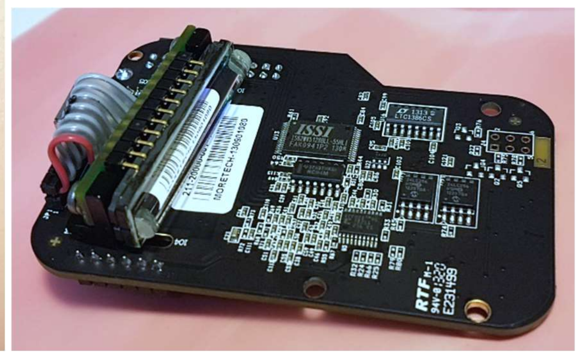


USB4000 w/ cover plate removed



Close-up of entrance slit

Circuit board removed, exposing optical bench



Circuit board showing side with sensor

Figure 8 Images Taken During Entrance Slit Replacement

Calibration:

The act of removing components from the spectrometer and putting them back unavoidably results in the CCD sensor position changing relative to the projected spectrum. The change may be small, but it is still enough to significantly affect the wavelength accuracy of the device. In the case of the unit with the 1200-line grating I also adjusted the grating's orientation so that the desired wavelength range was projected onto the sensor (it was originally configured for a wavelength range of 573-883nm). This adjustment also resulted in the need to re-calibrate the spectrometer once all the physical changes were completed.

To accomplish the wavelength calibration of each modified spectrometer, I made use of three IDAS brand filters from my library for which I already had detailed spectrum data supplied by the manufacturer. I have to thank the engineers at IDAS for supporting me in this effort, and supplying me the necessary data, captured using their laboratory-grade spectrometer, an Agilent

Cary 6000i. A graphical view of the spectrums provided by IDAS for use as my calibration reference is shown in Figure 9.

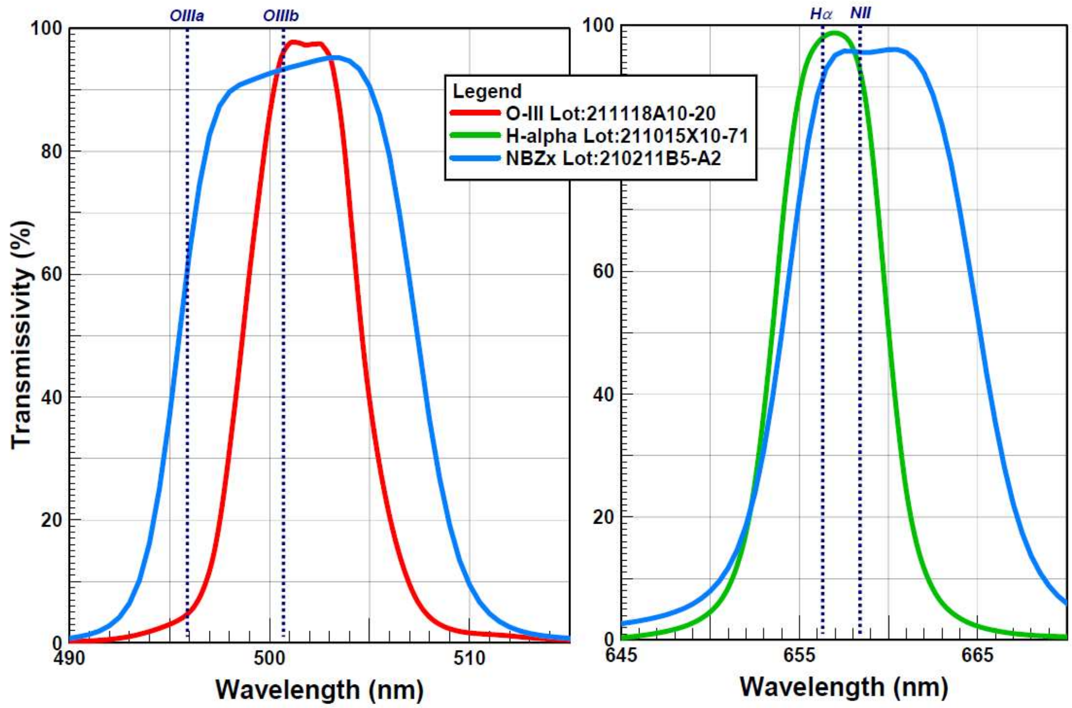


Figure 9 IDAS Supplied Filter Transmission Spectrum Data

The wavelength calibration process consisted of measuring the reference filter spectra with the USB4000 and comparing it to the manufacturer provided data. The amount of offset and scaling required to align the measured data with the manufacturer data was determined by trial and error. The coefficients of the resulting linear transformation were then noted as the new wavelength calibration for that particular spectrometer. Note that this only deals with calibration of the wavelength scale. Calibration of the amplitude (transmissivity) scale is handled during the spectrum measurement process through using a regulated light source and periodic recapturing of the reference light source spectrum. The results of the wavelength calibration process are shown in Figures 10 and 11, which present the measured spectra of each reference filter captured using a different spectrometer configuration. There is still some band widening observed in my measurements, which I believe is due to my measurement apparatus setup (see Figure 12). The light passing through the filter into the receiving optical fibre of the spectrometer is not collimated, so I think there is a small amount of band shift resulting from this arrangement. Nonetheless the correlation between my measurements with the 1200-line grating spectrometer configuration and the IDAS data is very good.

Out of curiosity I also collected spectra through this process from a number of other filters, ones with bandwidths narrower than used for my wavelength calibration. My interest was in knowing the impact of improved spectrometer resolution on my spectrum measurements for these narrower filters. The results are presented in Figures 13 to 15. The extent to which the original spectrometer configuration fails to capture each filter's spectrum is progressively larger the narrower the filter's FWHM, as I predicted in my simulation.

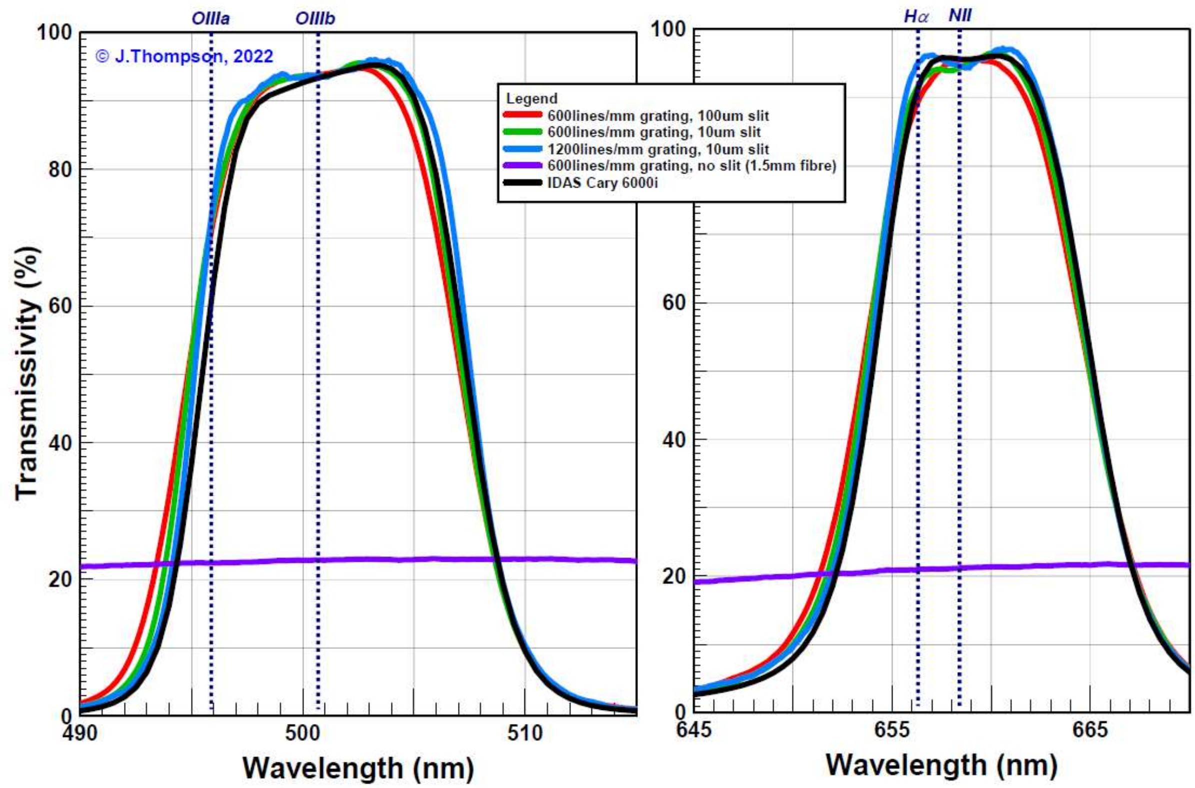


Figure 10 Post Calibration Spectra of Reference Filters, NBZx (Lot: 210211B5-A2)

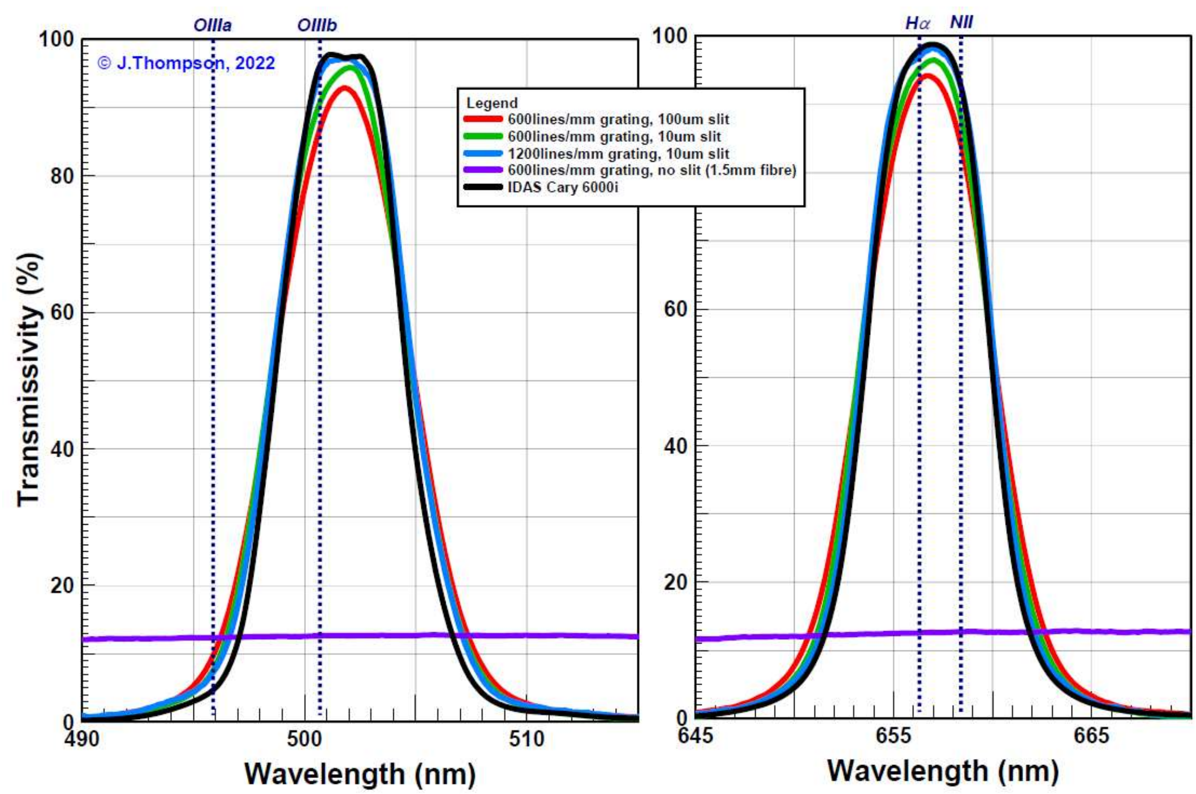


Figure 11 Post Calibration Spectra of Reference Filters, O-III (Lot: 211118A10-20) & H-α (Lot: 211015X10-71)

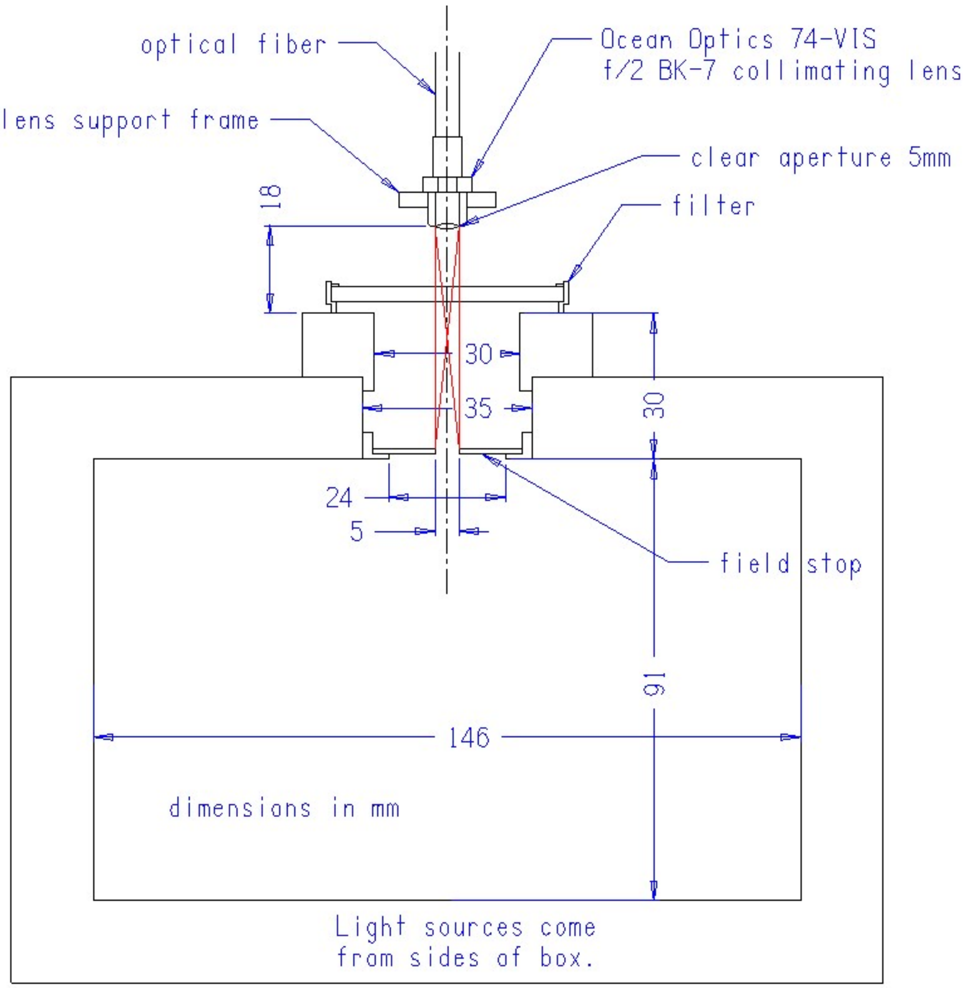


Figure 12 Schematic Cross-section of Filter Spectrum Measurement Rig

Conclusions:
The resolution of a spectrometer is affected by three things: sensor resolution, diffraction grating groove density, and entrance slit width. A spectrometer's resolution has a large impact on the device's ability to accurately capture a filter's spectrum, especially in the case of filters with narrow FWHMs. Through the use of aftermarket parts I was successful in upgrading my spectrometer to a resolution of 0.5nm, a resolution that is compatible with measuring the latest narrowband astronomical filters that have 3nm FWHMs. Calibration of my upgraded spectrometer was made possible through the use of sample filters with associated high resolution spectra provided by the filter manufacturer IDAS.

If you have any questions, please feel free to contact me.

Cheers!

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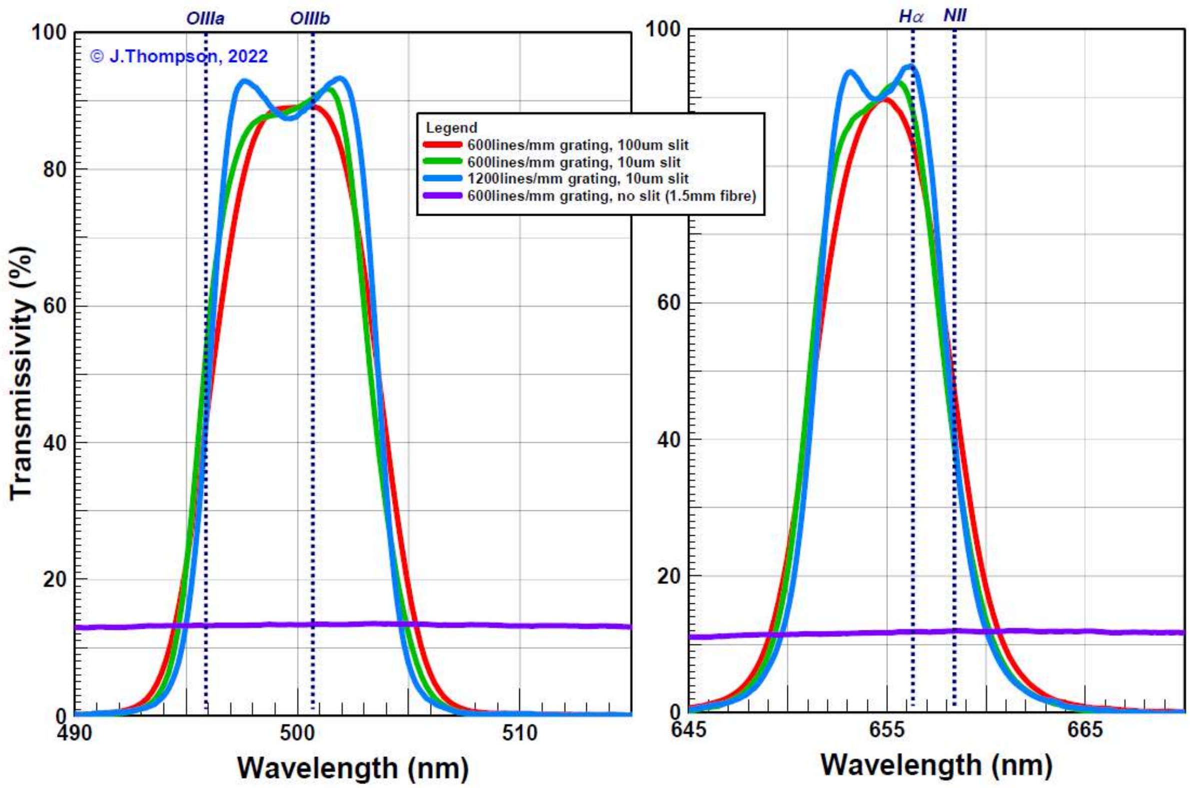

Figure 13 Post Calibration Spectra of Optolong L-eXtreme (dual 7nm bands)

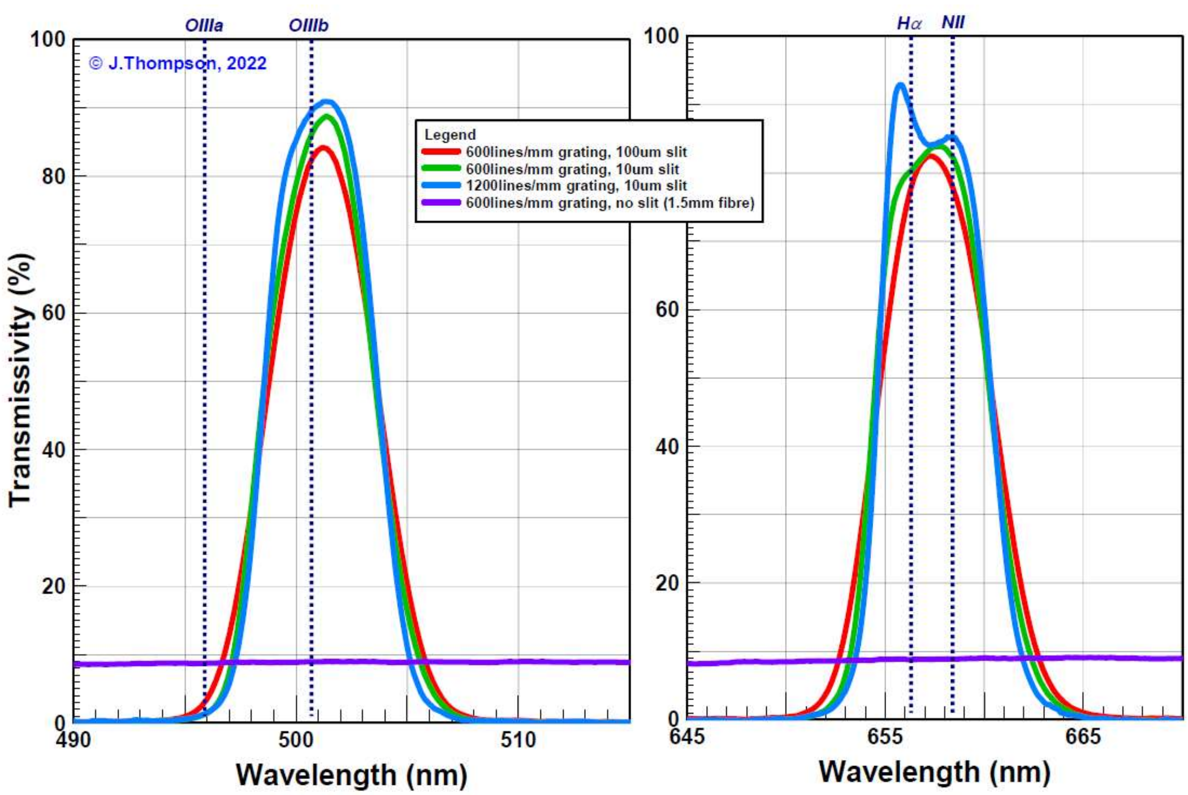

Figure 14 Post Calibration Spectra of Antlia ALP-T (dual 5nm bands)

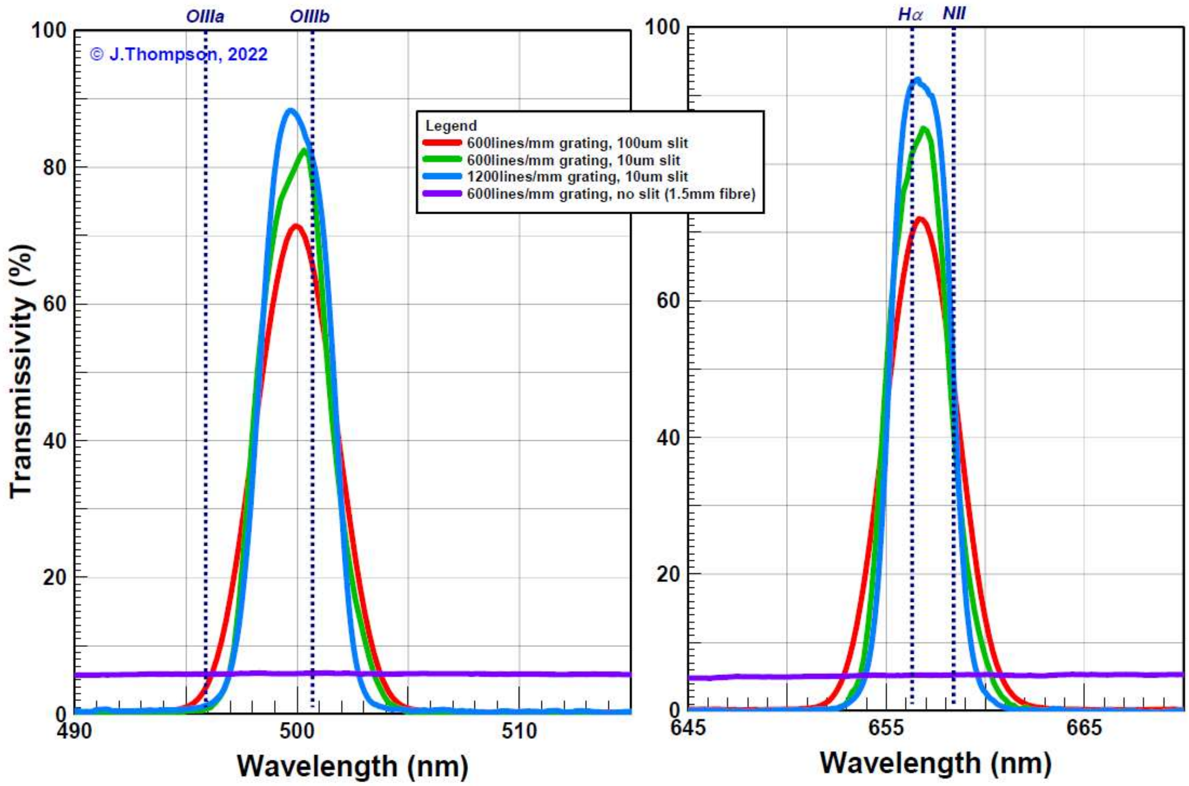

Figure 15 Post Calibration Spectra of Optolong O-III & H-α (both 3nm bands)