Calibrating the Wavelength of the Spectrometer

The following describes how to calibrate the wavelength of your spectrometer. Though each spectrometer is calibrated before it leaves Ocean Optics, the wavelength for all spectrometers will drift slightly as a function of time and environmental conditions.

You are going to be solving the following equation, which shows that the relationship between pixel number and wavelength is a third-order polynomial . . .

$$\lambda_p = I + C_1 p + C_2 p^2 + C_3 p^3$$

. . . where λ is the wavelength of pixel *p*, *I* is the wavelength of pixel 0, C_1 is the first coefficient (nm/pixel), C_2 is the second coefficient (nm/pixel^2), and C_3 is the third coefficient (nm/pixel^3). You will be calculating the value for *I* and the three *C*s.

Setting Up

To re-calibrate the wavelength of your spectrometer, you will need the following:

- ♦ A light source that produces spectral lines. Ocean Optics' HG-1 Mercury-Argon lamp is ideal for this purpose. If you do not have an HG-1, you will need a spectral line source that produces several (at least 4-6) spectral lines in the wavelength region of your spectrometer.
- ♦ Your spectrometer.
- ♦ An optical fiber (for spectrometers without a built-in slit, a 50-µm fiber works best).
- ♦ Either a spreadsheet program (Excel or Quattro Pro, for example) or a calculator that performs third-order linear regressions. If you are using Microsoft Excel, choose **Tools | Add-Ins** and check **AnalysisToolPak** and **AnalysisToolPak-VBA**.

Calibrating the Wavelength of your Spectrometer

1. After placing OOIBase32 into Scope Mode, take a spectrum of your light source. Adjust the integration time -- or the A/D card conversion frequency -- until there are several peaks on the display screen that are not off-scale.
2. Move the cursor to one of the peaks and carefully position it so that it is at the point of maximum intensity. Record the pixel number that is displayed in the status bar (located beneath the graph). Repeat this step for all of the peaks in your spectrum.
3. Using your spreadsheet, create a table like the one shown on the next page.
   - ♦ In the first column, place the exact or true wavelength of the spectral lines that you used. Most calibration line sources come with a wavelength calibration sheet. If you do not have a wavelength calibration sheet for your light source, you can probably find the wavelengths for your spectral lines (assuming that they are being produced by pure elements) in a Chemistry or Physics textbook or handbook, such as the *CRC Handbook of Chemistry and Physics*.
   - ♦ In the second column of this worksheet, place the observed pixel number.
   - ♦ In the third column, calculate the pixel number squared.
   - ♦ In the fourth column, calculate the pixel number cubed.

Independent Variable — Dependent Variables — Values computed from the regression output

True Wavelength (nm)	Pixel #	Pixel # ^{2}	Pixel # ^{3}	Predicted Wavelength	Difference
253.65	175	30625	5359375	253.56	0.09
296.73	296	87616	25934336	296.72	0.01
302.15	312	97344	30371328	302.40	-0.25
313.16	342	116964	40001688	313.02	0.13
334.15	402	161604	64964808	334.19	-0.05
365.02	490	240100	117649000	365.05	-0.04
404.66	604	364816	220348864	404.67	-0.01
407.78	613	375769	230346397	407.78	0.00
435.84	694	481636	334255384	435.65	0.19
546.07	1022	1044484	1067462648	546.13	-0.06
576.96	1116	1245456	1389928896	577.05	-0.09
579.07	1122	1258884	1412467848	579.01	0.06
696.54	1491	2223081	3314613771	696.70	-0.15
706.72	1523	2319529	3532642667	706.62	0.10
727.29	1590	2528100	4019679000	727.24	0.06
738.40	1627	2647129	4306878883	738.53	-0.13
751.47	1669	2785561	4649101309	751.27	0.19

4. Now you are ready to calculate the wavelength calibration coefficients.In your spreadsheet program, find the functions to perform linear regressions.
   -- if using Quattro Pro, look under **Tools | Advanced Math**
   -- if using Excel, look under **Tools | Data Analysis**
5. Select the true wavelength as the dependent variable (Y). Select the pixel number, pixel number squared and the pixel number cubed as the independent variables (X). After you execute the regression, an output similar to the one shown below is obtained.

Regression Statistics	
Multiple R	0.999999831
R Square	0.999999663
Adjusted R Square	0.999999607
Standard Error	0.125540214
Observations	22

intercept

	Coefficents	**Standard Error**
Intercept	190.473993	0.369047536
X Variable 1	0.36263983	0.001684745
X Variable 2	-1.174416E-05	8.35279E-07
X Variable 3	-2.523787E-09	2.656608E-10

first coefficient

second coefficient

third coefficient

6. The numbers of importance are indicated in the above figure. You will need to record the Intercept as well as the First, Second, and Third Coefficients. Also, look at the value for R squared. It should be *very* close to 1. If it is not, you have probably assigned one of your wavelengths incorrectly.
7. Select **Spectrometer | Configure** from the menu and choose the **Wavelength Calibration** page to update the wavelength coefficients within OOIBase32.
8. Repeat this process for each channel in your setup.