*High Sensitivity Luminescence Measurements of Materials – The St Andrews Luminescence Facility by Adrian A Finch, Yafang Wang, Peter D Townsend, Martin Ingle*

# Supplementary Information 3 – Data Formatting from the RLTLCL System Time-Independent Spectral Data

## 1. How are Raw Data Formatted?

The RLTLCL software takes your sample name and creates a new DIRECTORY into which several files are deposited. The files within the directory share the same stem as the directory itself so they can be identified even if they part company with the directory that hosts them. Many of these files are present only to allow debugging in the event of an error and are subsequently not of use.

Please note that the processing software assumes that the files within the directory have the same stem as the host directory and will crash if that is not the case. For that reason, ***you cannot rename the directory without renaming all the files within it***. ***All text files are ASCII text with TAB delimiting.***

### Raw Data

The raw data are images from the detectors and can be saved in one of 6 formats. The save routines are switched on and off by flags within the software. Four of those are images of the detector plate in different image formats, i.e. PNG, JPEG, TIFF, BMP. The fifth is in Photek's own image format which incorporates not just the image itself, but also technical information such as the integration time. The sixth format is a simple text file with an integer to represent the intensity at each pixel of the image plate. These files are produced by IMAGE32 – Photek's own software – in response to commands issued by the instrument control software.

The image files are large (MB each) and so it has been our procedure NOT routinely to save the individual image files, leaving only the (relatively) small TXT file. The first file in any run is given the number 0; subsequent files (e.g. collected at different temperatures) have the number 1 and so on. The programme captures data from both detectors, generating separate files with a suffix B (for UV-Blue), R (for Red-IR) and RB for a single file that includes both datasets. Hence the first integrations generate files called SAMPLE_0_B.TXT and SAMPLE_0_R.TXT and so on. These files are only useful if the routine crashes during analysis and you want to reconstruct data before the error (see below), or if you want to revisit the wavelength calibrations.

When a run completes, the software exports two more files that summarise the data. These files are generated by the instrument software after image processing and calibrate distance on the detectors to particular wavelengths. The files SAMPLE_B_XY.TXT and SAMPLE_R_XY.TXT are text tab-delimited files where the first row is wavelength, the first column is temperature and the individual intensities are represented by raw counts. All the individual files (e.g. SAMPLE_0_B.TXT) are now redundant since the data are summarised in SAMPLE_B_XY.TXT. Note that sometimes wavelengths are presented in reverse order, with the longest wavelengths first.

The program also saves screen dumps of the software windows (these have cryptic numerical names based on the time) and a SAMPLE.HTML file which summarises technical data and sample information, including the temperatures at which each file was collected. The sample information presented to the software during the run is in the HTML file.

## 2. System Corrections

The data are kept as close to raw, unprocessed images as possible. This is a conscious decision so that a) data collection is as fast as possible, b) we can retrospectively process data in different ways, and/or c) revisit older data with better processing methods. All the system corrections are done offline.

I have written a LabVIEW program that takes raw data, performs background and system corrections and then amalgamates the data into a single output for the wavelength range 200-800 nm. The program's input is the directory (in these examples: SAMPLE) and the program finds and reads automatically the appropriate files within it. The correction routines NEVER overwrite raw data, although they can overwrite earlier versions of processed data. The outputs are both simple corrected data (*_corr.DAT) and 'rebinned' data (*_rebin.DAT) which are the products of a running mean in wavelength.

The program generates two new directories within SAMPLE called 'ORIGIN' and 'MATLAB'. The data in these directories are in formats that import painlessly into either program. If you want to save a version of the corrected data while you explore better corrections, rename the ORIGIN/MATLAB directories to e.g. ORIGIN1/MATLAB1.The MATLAB directory contains four files:

| FILENAME | Description |
|---|---|
| SAMPLE_MATLAB_RB_TEMP.DAT | Temperatures for each data point |
| SAMPLE_MATLAB_RB_WAV.DAT | Wavelengths for each data point |
| SAMPLE_MATLAB_RB_XY_corr.DAT | Corrected intensity data without a running mean |
| SAMPLE_MATLAB_RB_XY_rebin.DAT | Corrected intensity data with a n point running mean |

Most users find the ORIGIN directory most useful. This contains two files: SAMPLE_ORIGIN_RB_XY_corr.DAT and SAMPLE_ORIGIN_RB_XY_rebin.DAT. These are tab-delimited text of the data in an XY matrix format, amalgamating the data from both detectors into a single file. The first row of the data includes the wavelength labels, the first column are the temperature labels and each cell contains the intensity at that wavelength and temperature. corrected for system response. There is also a "rebin" file which is corrected AND has smoothed a running mean in wavelength based upon the numbers of points given during correction (the default is 3). These files will import straight into ORIGIN.

For plotting data in EXCEL, use the ORIGIN files. Open these as TEXT, TAB delimited files in EXCEL ***and delete the 0 in cell A1***. You can then plot this successfully as 2D temperature or wavelength slices.

Some programs require 3D data as three columns corresponding to x, y and z coordinates. Origin can convert XY matrix data (the default output in the ORIGIN directory) to XYZ but we have also written a conversion routine.

## 3. Data – What you need to know

- Never RENAME directories!
- Correct the raw files using our in-house software,
- Look for your corrected data in the ORIGIN or MATLAB sub-directories created within your sample directory.

## 4. Data – The Future

We are always looking to improve the correction routines, and at present we are developing exporting directly into ORIGIN to create ORIGIN PROJECT (*.opj) and EXCEL (*.xlsx) formats. These may be present in your ORIGIN directory by the time you read this and can be opened directly.

Irvine Building, North Street, St Andrews, Fife KY16 9AL
Tel: 01334 462384 Fax: 01334 463949 Email: Adrian.Finch@st-andrews.ac.uk

University of St Andrews

Facility for the Luminescence of Minerals

# How to Plot RLTLCL Data in Origin
# LONG VERSION

## 1. How Do I import into ORIGIN?

*All of the following is done using Origin 2015*

a) Normally on opening Origin, a new blank workbook is created called Book1. If this is not present, create it using the ‘New Workbook’ icon (third from the left, Figure 1).

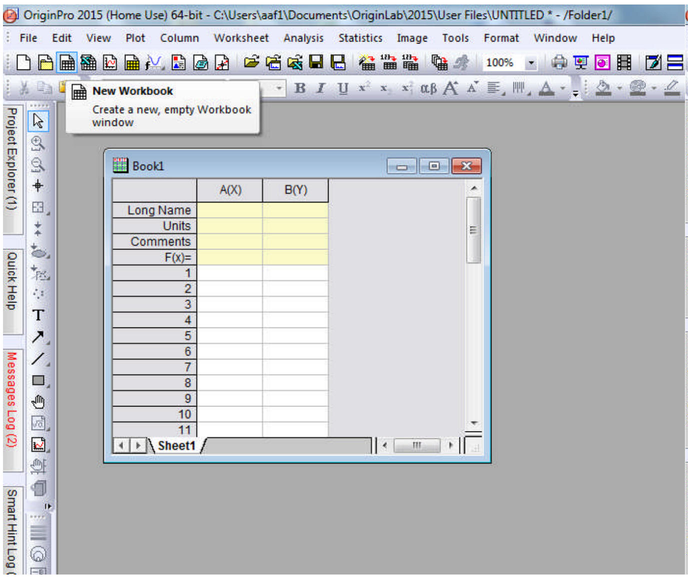



**Figure 1: Creating an New Workbook.**

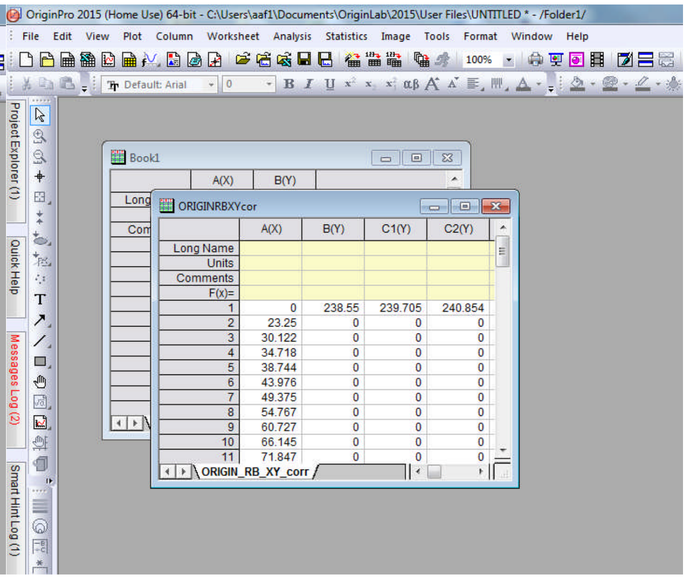



**Figure 2: Data Imported to the Worksheet**

b) Go to File >> Open >> and set the file type to ASCII *.DAT. Point to your data file within the Origin Directory. Double click and the data are imported to the Worksheet (Figure 2).

Irvine Building, North Street, St Andrews, Fife KY16 9AL
Tel: 01334 462384  Fax: 01334 463949  Email: Adrian.Finch@st-andrews.ac.uk

c) Click Right Mouse over the first row and click on ‘Set as Comment’ (Figure 3).

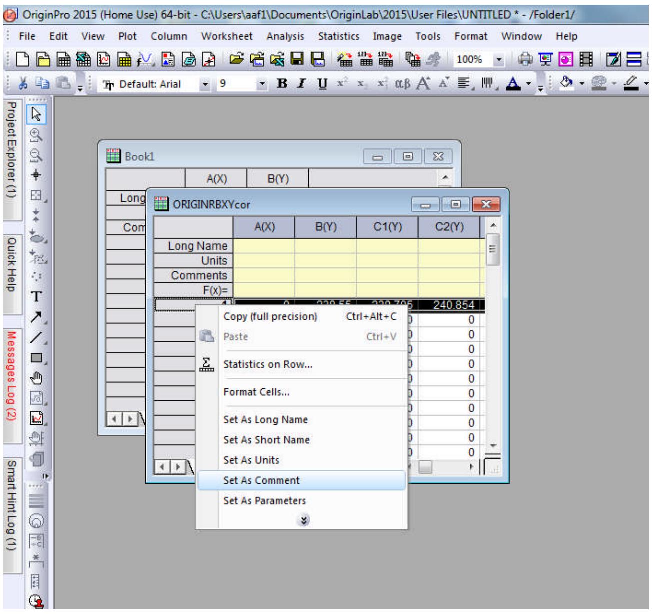



Figure 3: Set Wavelengths to a Comment

The data need to be converted to an XYZ format for 3D graphing. More recent versions of our processing software generate an XYZ file directly, so if a file *_corr-XYZ already exists, then you can import this straight away without the need to go through steps d-e.

d) Click Worksheet >> Convert to XYZ >> Open Dialog… (Figure 4).

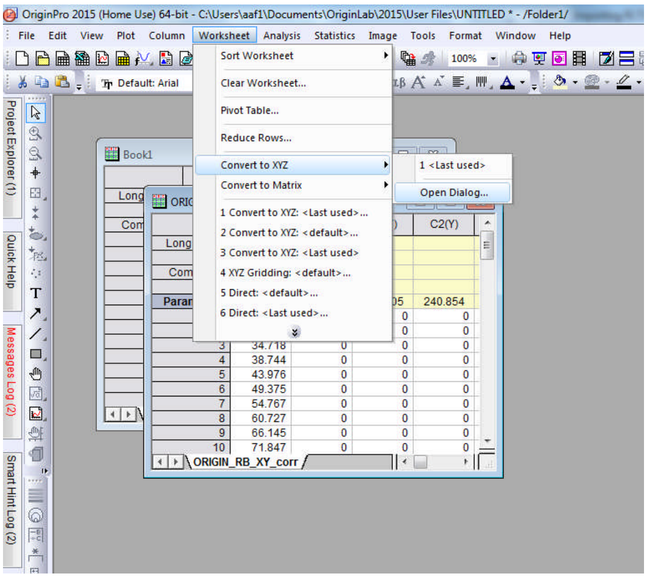



Figure 4: Creating an New Workbook

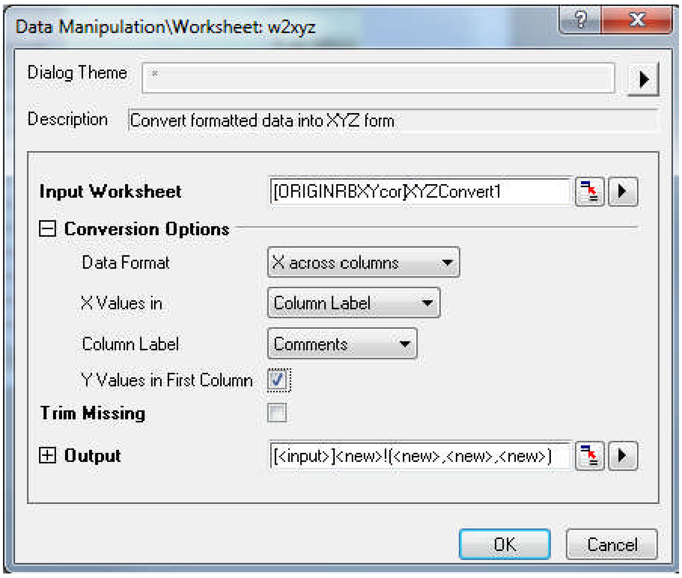



Figure 5: XYZ dialog box

e) In the resultant dialogue box, Click the options:
***Data Format:*** *X across Columns;*
***X Values in:*** *Column Label*
***Column Label:*** *Comments*
And check the tick box that says ‘***Y values in First Column***’ (Figure 5).
Click << OK >>

Irvine Building, North Street, St Andrews, Fife KY16 9AL
Tel: 01334 462384 Fax: 01334 463949 Email: Adrian.Finch@st-andrews.ac.uk

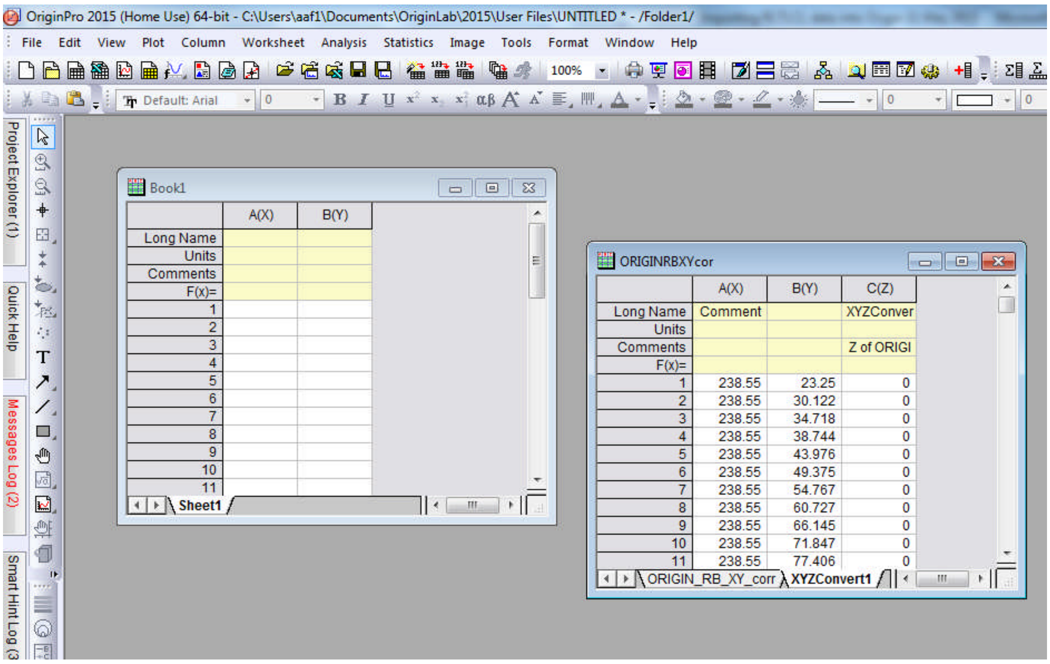


**Figure 6: Data now in XYZ Format**

f) Change the Labels of X, Y and Z columns, adding the appropriate wavelengths. To allow access for editing, double click on each of the cells.

*For the ° symbol, press and hold ALT, then type 248 on the numerical keypad. Release ALT and the ° symbol appears.*

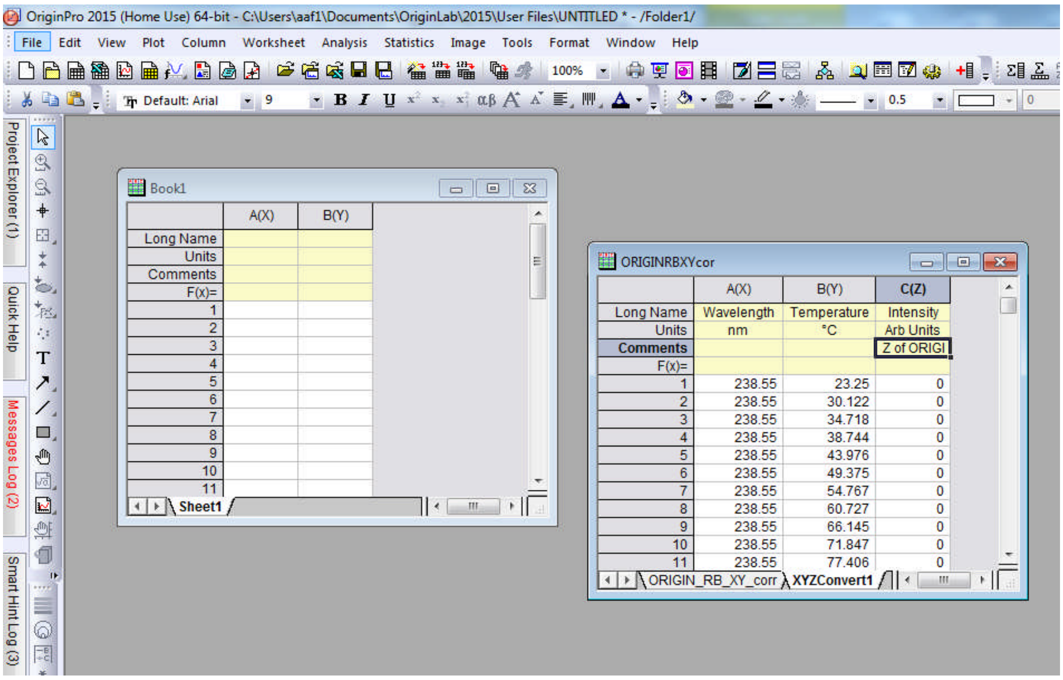


**Figure 7: Data now in XYZ Format with Correct labels**

## 2. Plotting a NEW 3D Surface

***NB If you have a ready-made template, go to 4.***

With XYZ data, 3D graph formats can be plotted. First a 3D graph:

g) Click Plot >> 3D Surface >> Colour Map Surface (Figure 8).

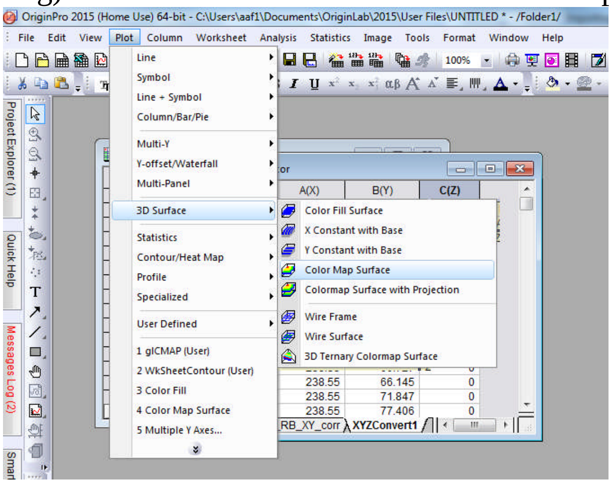



**Figure 8: Plotting a 3D Surface**

h) Check the tick boxes to link the X, Y and Z columns to the A, B and C inputs that create the graph (Figure 9). Then click << Add >> and a new source the graph (Figure 10). Press << OK >>.

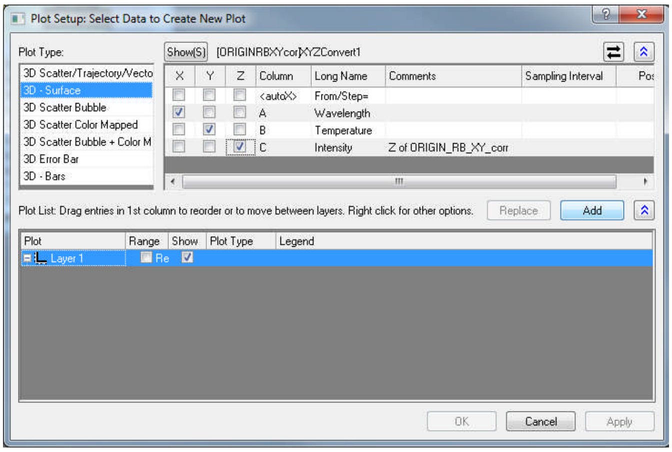



**Figure 9: Tick boxes to link XYZ & ABC; press << Add >>…**

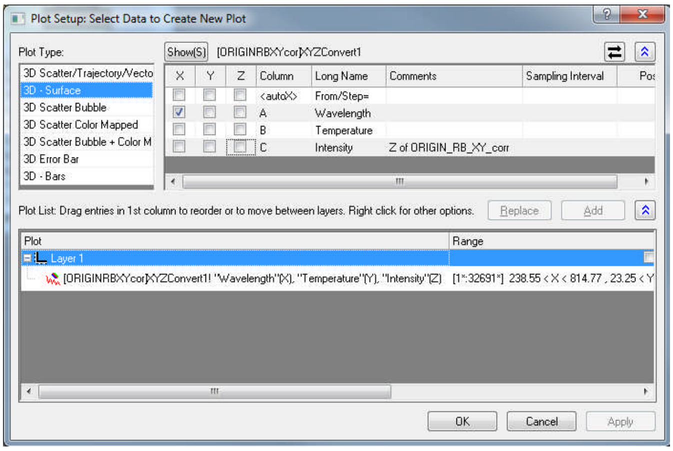



**Figure 10: … and a new source appears..**

i) A 3D surface graph is created. For details on how to manipulate that, see accompanying sheet.

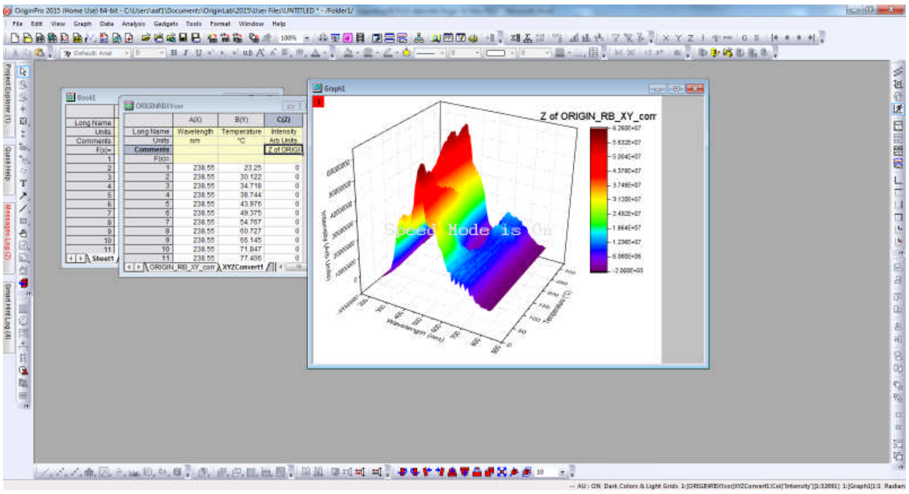



**Figure 11: A 3D Surface**

## 3. Plotting a NEW Contour Graph


Irvine Building, North Street, St Andrews, Fife KY16 9AL
Tel: 01334 462384 Fax: 01334 463949 Email: Adrian.Finch@st-andrews.ac.uk

j) Click on the Worksheet Window at the top – make sure that that window is in the foreground on top of all others.
k) Click Plot >> Contour/Heat Map >> Colour Fill (Figure 12).

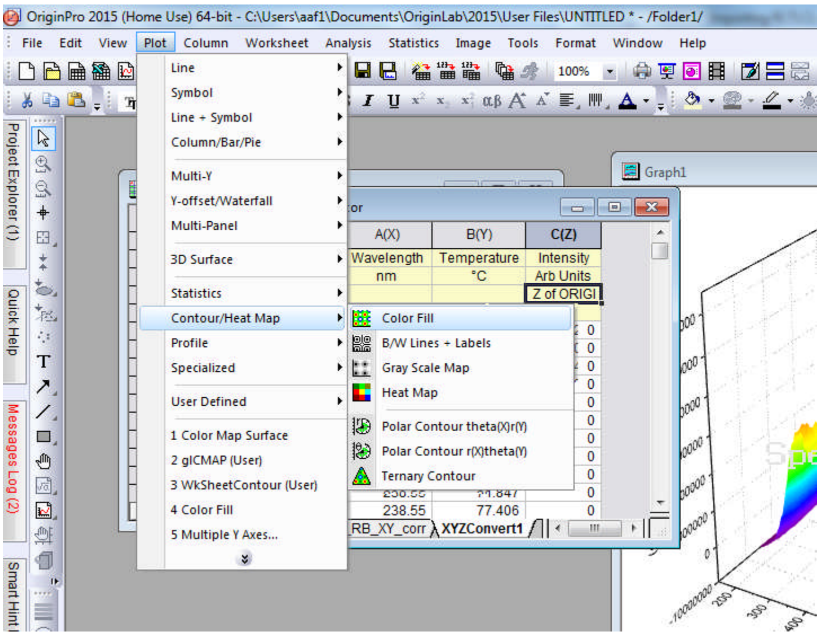


**Figure 12: Plotting a Contour Surface**

l) Check the tick boxes to link the X, Y and Z columns to the A, B and C, click << Add >> and a new source the graph appears. ***This section is identical to Figure 9 and 10.*** Press << OK >>.
m) A 3D contour map is created (Figure 13). For details on how to manipulate, see separate sheet.

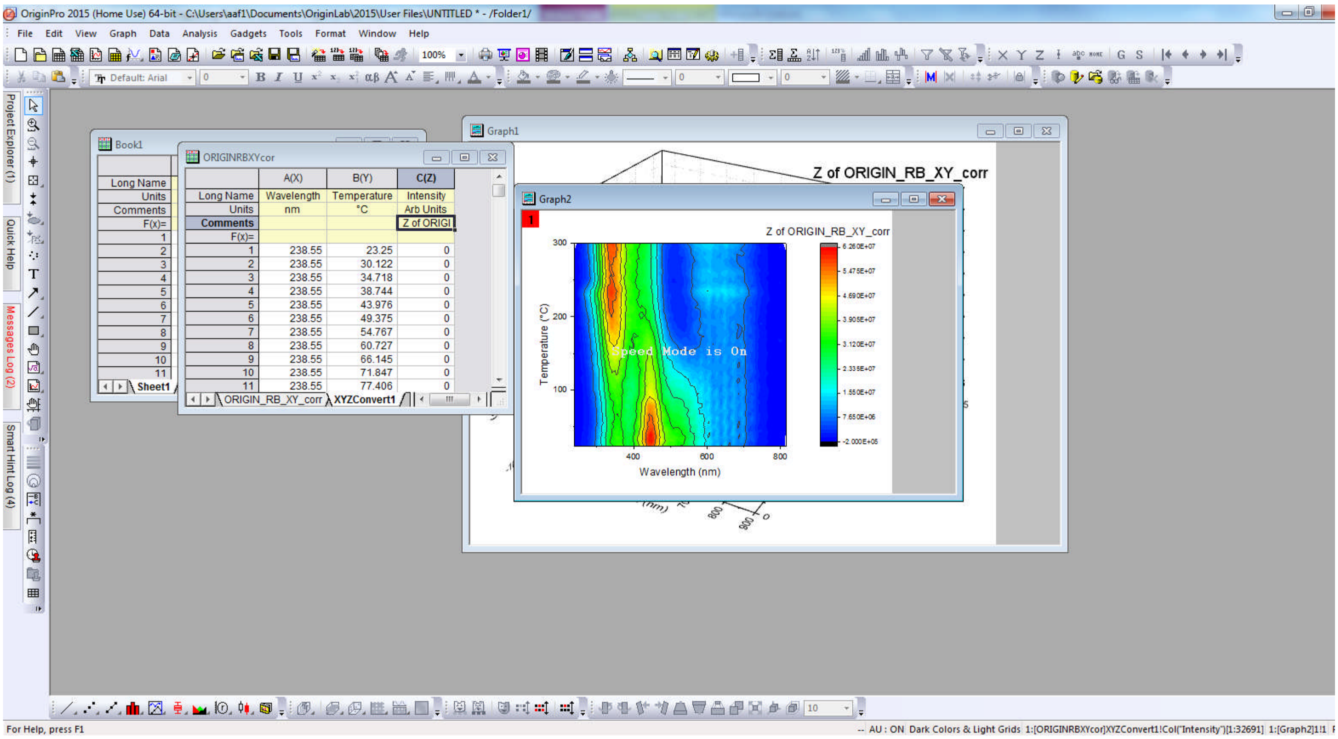


**Figure 13: A Contour Map is added to the 3D Surface**

n) >>> Go to 5.

## 4. Plotting Using Templates

Templates are ways of storing graph formats so that new data can be plotted in the same way as an old graph. The facility can supply Graph Template Files, or you can create your own. If you have Templates on disc, you can skip a lot of the tedious reformatting. To create a graph using Templates:

o) Click on the Worksheet Window at the top – make sure that that window is in the foreground on top of all others.
p) Click Plot >> User Defined >> gICMAP (for 3D graphs) or >> WkSheetContour for Contour maps (Figure 14).

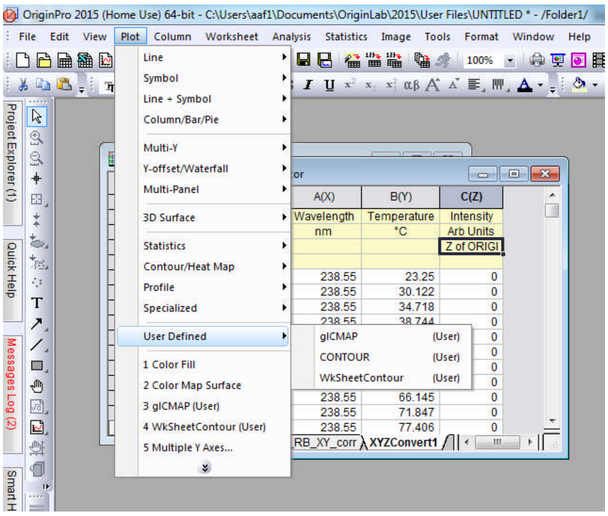
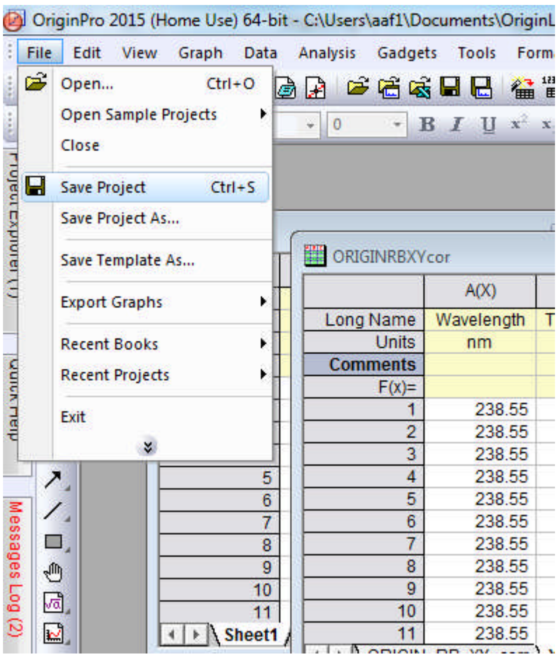



**Figure 14: Plotting using Templates**

## 5. Saving your work

It is a good idea to save the Origin file as an Origin Project. To save:

q) Click File >> Save Project and provide a filename. I suggest you save this back into the ORIGIN directory of the directory of your raw data.




Saving the Project will allow you to recall both the worksheet and the graphs formed from it.

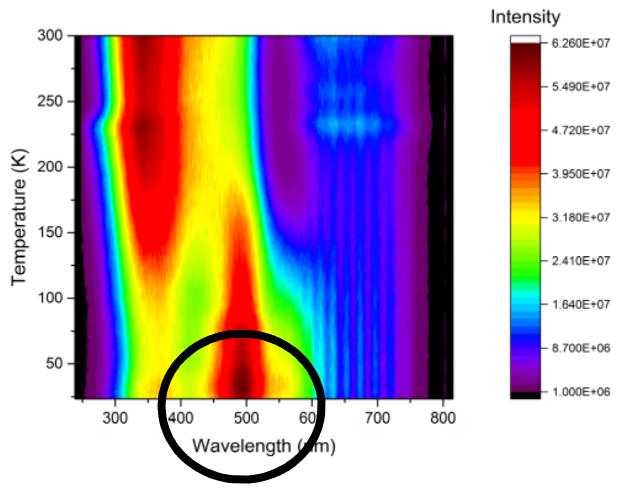
**Figure 15: Save the Origin Project**

University of St Andrews
Facility for the Luminescence of Minerals

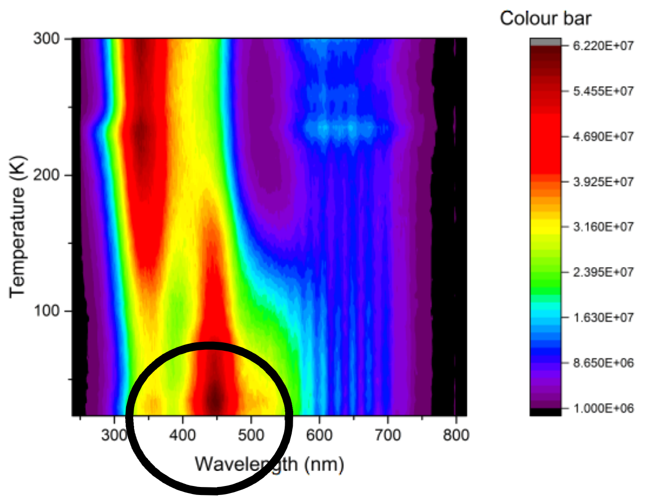
# Using Origin 3D Plotting – A Warning

Originally we plotted using the simpler Origin MATRIX facility to give 3D and contour graphs. However it has become clear that to do that, Origin resets the data spacing in both T and λ. This is usually less noticeable in T, but it causes the centre of the data to move slightly to higher wavelengths in λ. This is because the wavelength spacing in the UV-Blue detector is smaller than that in the red. When origin imports the data as a Matrix, it averages the data intervals between the two detectors, shifting data in the Blue region to the right. At its worst, this is a shift of 40 nm. Hence the maximum at 20 K in these data plotted on the left is actually at 450 nm.

**ORIGIN MATRIX PLOT (INACCURATE!)**




**ORIGIN VIRTUAL MATRIX PLOT (ACCURATE!)**




The solution is to employ an Origin Virtual Matrix plotting XYZ data, rather than the way we were first advised. We import the data as an X-Y matrix with the x data (wavelengths) as labels in the top, and the Y data (Temperature) in the first column. You then create an XYZ format (Origin does this for you) and plot these. Now the data spacings are ***uneven and accurate***.

Irvine Building, North Street, St Andrews, Fife KY16 9AL
Tel: 01334 462384  Fax: 01334 463949  Email: Adrian.Finch@st-andrews.ac.uk