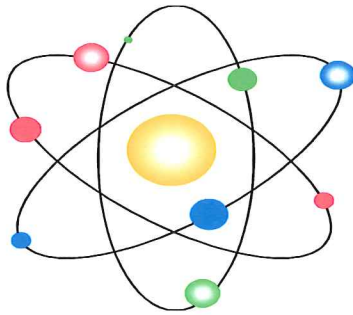


# Analysis





## **DATA ANALYSIS HIGHLIGHTS**

1.	Data Format	3
2.	Save and Recall of Analyzed Data	5
3.	Composition Table Generation	6
4.	Import from SSI DOS data system (Vectra)	7

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## **TOPICAL DESCRIPTION OF SOFTWARE**

1. Analyze Composition -Introduction
  - a. Auto find
  - b. Area Dialog Box
  - c. Area Spreadsheet
  - d. Scofield Editor
2. Data Presentation
  - a. Annotation and Editing labels
  - b. Customize Graphics
  - c. Changing scales
  - d. Removing Grids
  - e. Headers and Footers
3. Depth Profiles
4. Export
  - a. Spectra to Vamas and Excel
  - b. Spreadsheet to Excel
5. File menu
  - a. Open Source
  - b. Save
  - c. Save As
  - d. Compact Database
  - e. Export
  - f. Backup database

6. Manipulating Spectra
  - a. Change line type and color
  - b. Charging Spectra - Shift
  - c. Tools for manipulating spectra
    - i) Add
    - ii) Differentiate
    - iii) Integrate
    - iv) Smooth
    - v) Subtract one spectra from another
    - vi) Subtract satellites
  - d. Zoom and Pan
7. Peak Fitting
8. Print and Paste operations

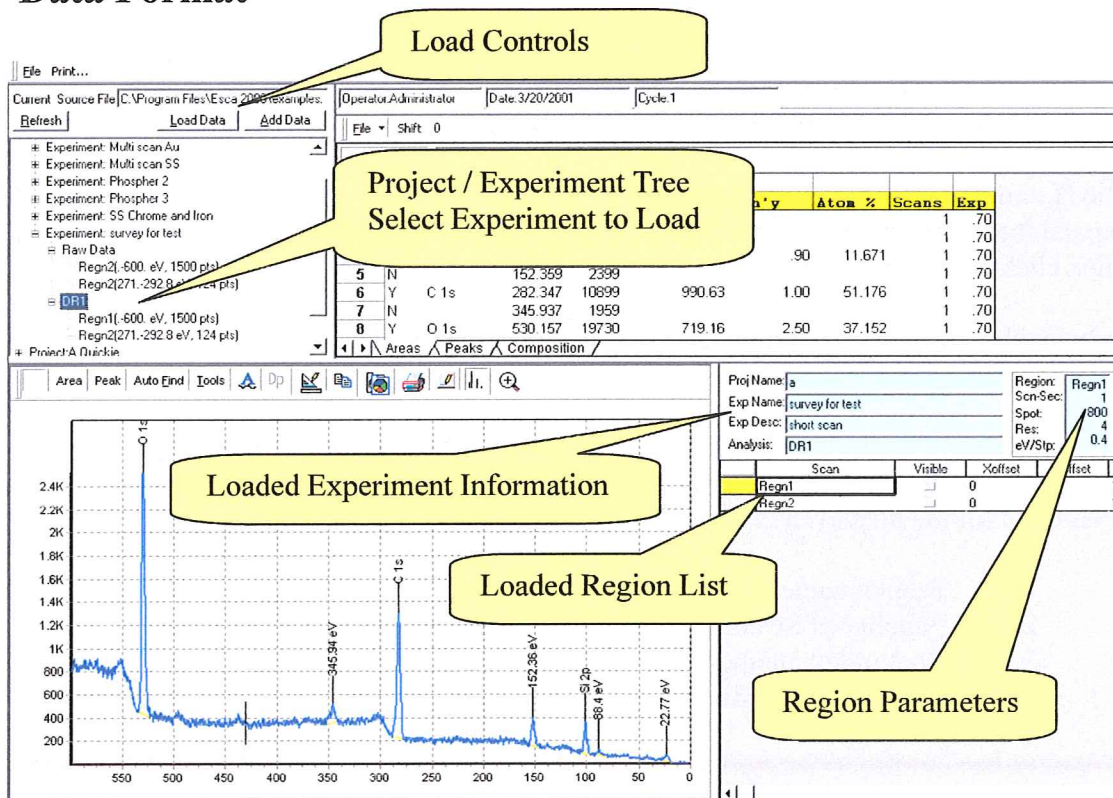
#### Software conventions

1. When text boxes are White they will accept data entry.
2. When text boxes are Blue they are read only.
3. Buttons or labels that are Red indicate something is turned off.
4. Buttons that are Green indicate something is turned on.
5. Buttons that are Yellow indicate something is turned on but temporarily not in a useable state.

#### Manual conventions

1. Buttons and other controls that respond to the mouse are enclosed in parentheses. For example the OK button in a dialog box will be typed as **(OK)**.
2. Keys on the keyboard are enclosed in square brackets. **[ENTER]** stands for the enter key.
3. Text that is required for input or displayed in a text box will be shown as **<This text displayed without the delimiting symbols>**.

## Data Format



The Project / Experiment Tree displays all experiments contained in the current database. The tree structure is used to locate the experiment that will be loaded for Analysis. The data stored by the capture program is listed as the **<Raw Data>**. The raw data is never exposed to modification. The Data Analysis program works with copies made from the raw data. After the copy is modified or analyzed the results may be stored under the original Project / Experiment name but with an additional descriptor. This new descriptor is the Analysis Name. In the tree shown above the Experiment: **<survey for test>** has a data set named **<Raw Data>** and one named **<DR1>**. DR1 is the Name for the analysis displayed in the graph and the spreadsheet. Stored reduced data may be recalled and further analyzed. The results of additional analysis may be saved as a new data set such as DR2 or copied over its source data set, DR1, as an incremental improvement.

This data structure provides for a high level of safety for the original data set. It also provides flexibility in saving multiple attempts at data analysis. Finally, the tree structure keeps the source data connected with the analyzed data.

The **(Load Data)** and **(Add Data)** buttons are used to initiate the load operation for the experiment selected in the tree. The load function copies over the currently displayed experiment. The user **MUST** use the file menu's Save or Save As operations to save the

analyzed data. The **(Add Data)** button allows data from a second, or additional, experiment to be added to the displayed data set. The regions for all loaded experiments will be listed in the Loaded Region List in the lower right quadrant of the display. However, the first loaded experiment will act as the primary experiment. This primary experiment's Project name, Experiment name and Experiment description will be displayed in the blue display boxes. The saved composite dataset will be found in the tree as a reduced data set under the primary experiment.

The **(Load Data)** and **(Add Data)** buttons can be used to load a single region. Simply expand the Experiment / Project Tree to the region level and select the region of interest. Then click on the **(Load Data)** or **(Add Data)** button.

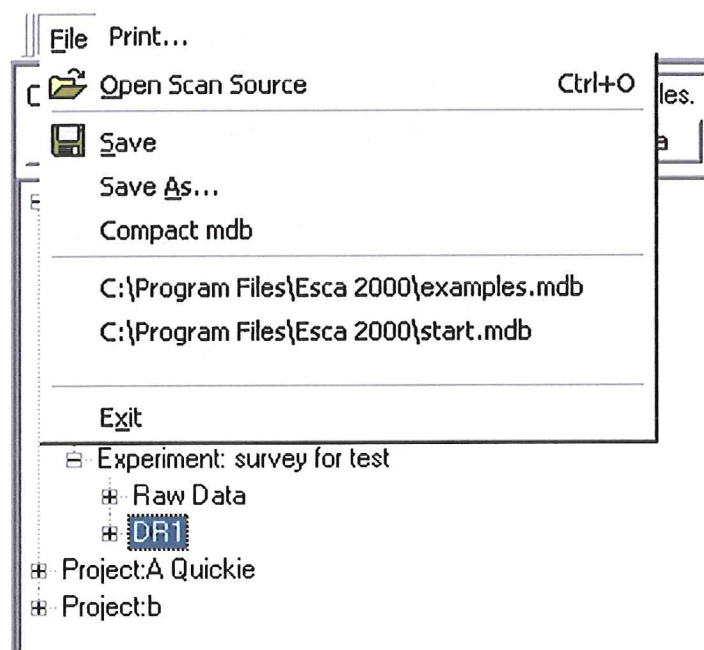
Individual Regions can be removed from the current Document. Click on the region in the Loaded Region List and then use the keyboard [**Delete**] Key.

You can select a Region to view by clicking its row button in the Loaded Region List. The spectrum will be displayed. The Parameter Table will display the collection conditions for the displayed region. The displayed parameters are:

1. Region name
2. Number of Scans or collection time in seconds
3. Spot index number
4. Resolution number
5. EV/Step

The **(Visible)** column in the Loaded Region List provides a check box that can be used to lock a row in the visible state. After one row is locked in the visible state it can be compared to another region by selecting a second region

## Save and Recall of Analyzed Data



The File menu shown above ONLY applies to the saving of Reduced Data. As stated above the Raw Data is not brought to the screen. Raw Data cannot be manipulated or resaved under a new name with Save As. Only a copy of the Raw Data is available. The Save and Save As command will store the copy along with any changes made to the copy as addendum to the original Project / Experiment.

This approach has a few properties worth noting.

1. If Raw Data is loaded and then saved you will be offered a default name. The default would be DR1 the first time you load the data. If you accept the default, you will then have two entries in the Project / Experiment tree. One will be the original Raw Data and one DR1.
2. If you have loaded Raw Data, performed some Analysis operations and then select Save you will again be offered a default of DR1. This will allow you to save the modified copy as DR1.
3. If DR1 is then reloaded and further analysis is performed then you have the choice of saving the changes over DR1 or saving the changes with a new name. To overwrite DR1 select the Save command in the file menu. To create a separate new analysis select the Save As command.

## Composition Table Generation

File ▾ Shift 0									
Z8		2.93							
1	Inc	XPS Lin	Adj'ed	Area	Norm Area	Sen'y	Atom %	Scans	Exp
2	N		22.770	635				1	.70
3	N		88.397	563				1	.70
4	Y	Si 2p	101.281	2240	225.93	.90	11.671	1	.70
5	N		152.359	2399				1	.70
6	Y	C 1s	282.347	10899	990.63	1.00	51.176	1	.70
7	N		345.937	1959				1	.70
8	Y	O 1s	530.157	19730	719.16	2.50	37.152	1	.70
9									

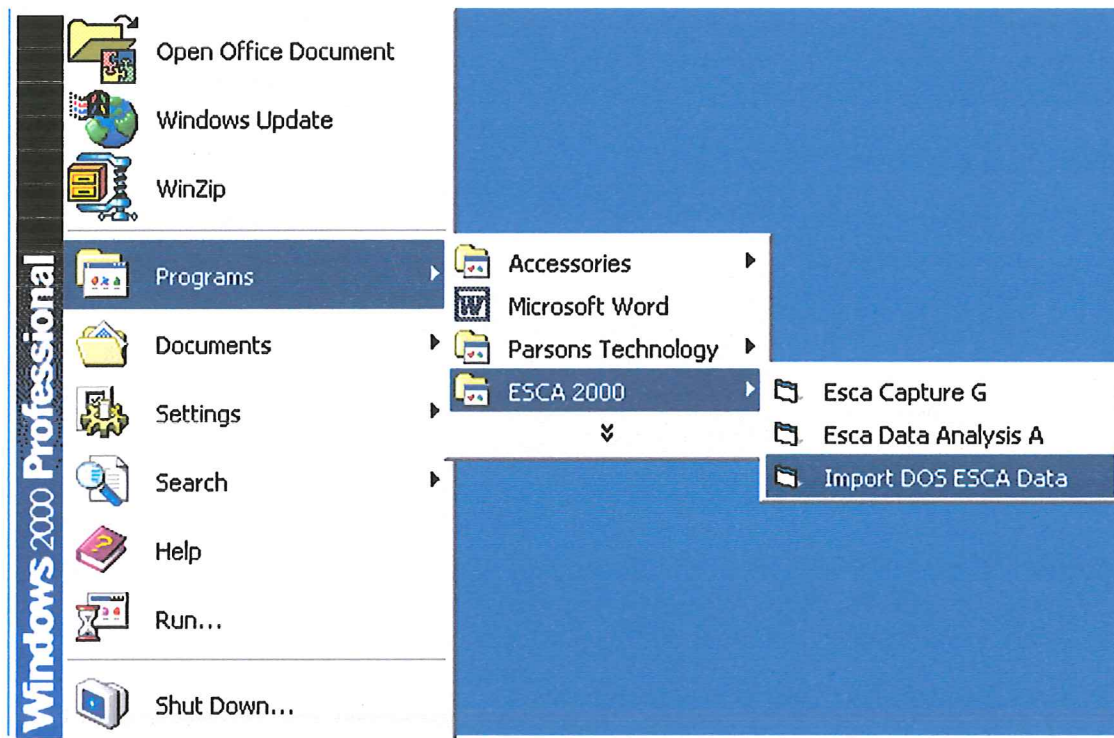
◀ ▶ ↖ ↗ Areas / Peaks / Composition /

The following improvements have been made to the table displays.

1. There is no Normalized Area, Sensitivity or Atom% field entries unless the peak has received an XPS Line assignment.
2. The Y symbol is automatically entered as a default value when the peak receives its XPS line assignment.
3. The ESCA 2000 V1.00 version was not picking up the sensitivity exponent from the calibration program. This is fixed.
4. The XPS Line assignments are reliably saved and recalled for all tables.



## Import of DOS ESCA Data (Vectra) for Analysis

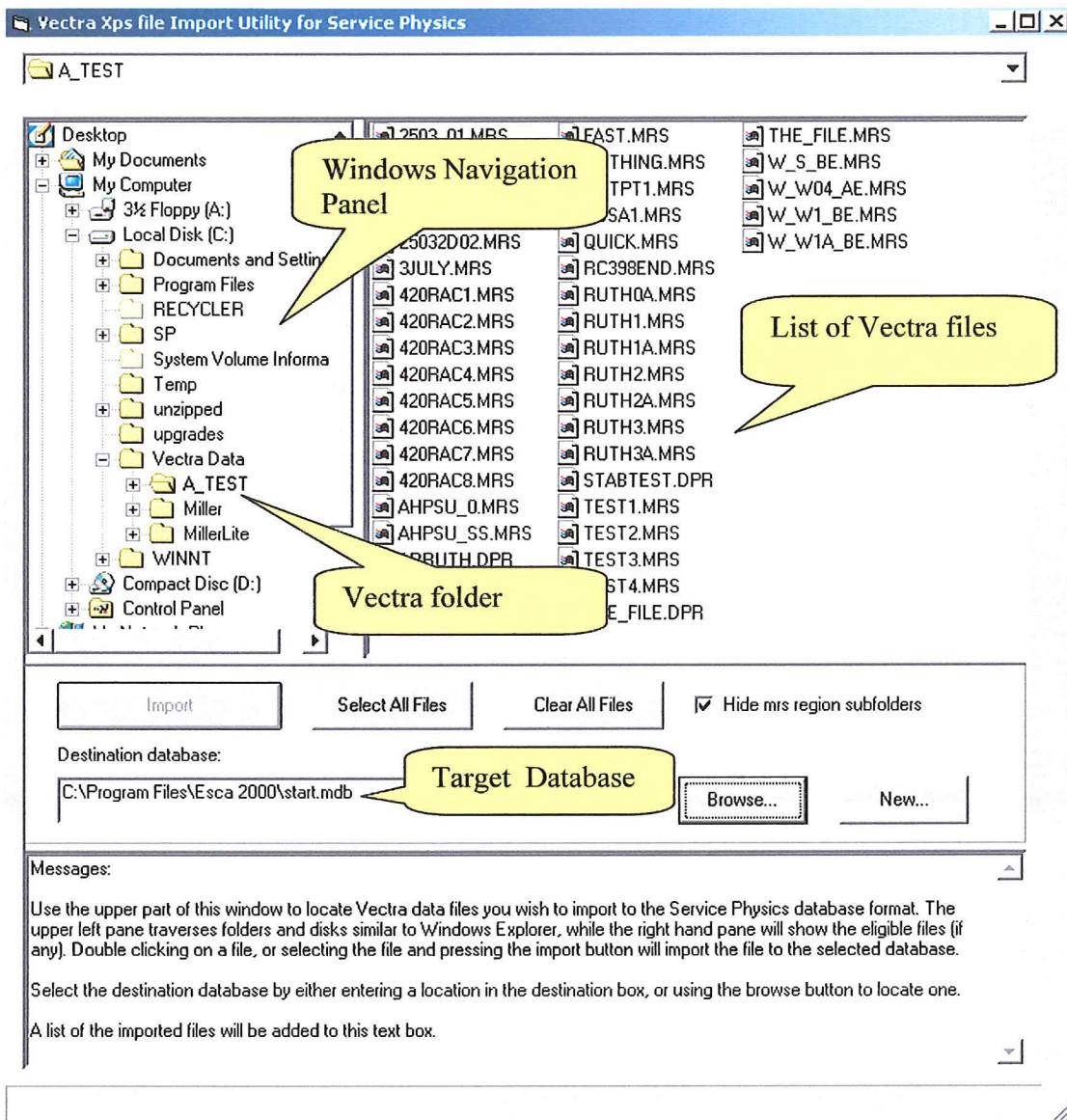


The “Import DOS ESCA Data” is a stand-alone program. This program will translate the data stored in the Vectra format (The “Vectra” ESCA program was a DOS based program developed by Surface Science Instruments that operated on early 386 and 486 PC’s) to the ESCA 2000 database format use by the ESCA 2000 Analysis program.

The translated data can be stored in any existing database that is currently in use with the ESCA 2000 Analysis program. The import program will also create a new database if desired.

The import program does not attempt to create the MRS tables that were used to capture the data. This program does recreate all analyzed data as well as the raw data contained in the Vectra files.

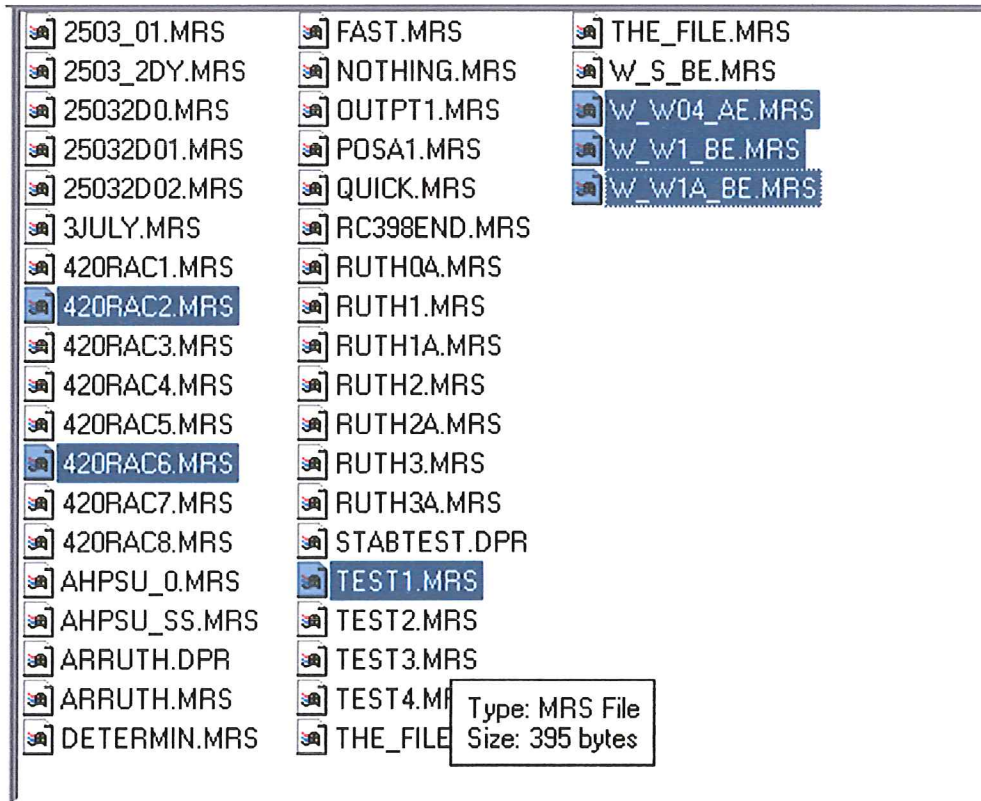
The Vectra file navigator will allow you to use all windows file navigation tools to find Vectra files anywhere on your hard drive, removable disc or Local Area Network. Once a Vectra file is found the import program will explode the Vecra file structure and display all internal components of the Vectra file. The MRS and DPR file will be identified.



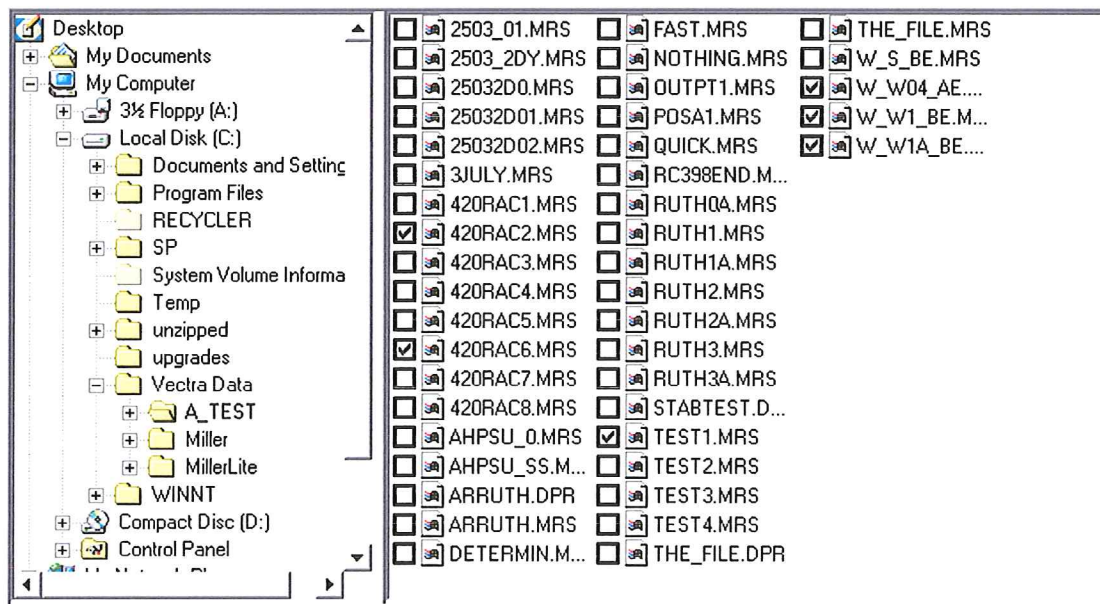
The **(Browse)** button is used to find the database you want to use to store your translated files. The **(New)** button is to create a new database to store the translated files.

The **(Select All Files)** button is used to mark all Vectra files in the Vectra File List for import. **(Import)** will enable as soon as at least one file is marked for import. The **(Import)** button starts the translation and import process.

If the **[Ct]** key is held down as files are selected with the mouse multiple files can be marked for import. The **(Clear All Files)** will remove the “marked for import” condition from all files in the list.



The above figure shows six files marked for import.



After the import is complete the box with checks show which files have been imported.

A\_TEST

<ul style="list-style-type: none"> <li>Desktop</li> <li>My Documents</li> <li>My Computer             <ul style="list-style-type: none"> <li>3½ Floppy (A:)</li> <li>Local Disk (C:)                 <ul style="list-style-type: none"> <li>Documents and Setting</li> <li>Program Files</li> <li>RECYCLER</li> <li>SP</li> <li>System Volume Informa</li> <li>Temp</li> <li>unzipped</li> <li>upgrades</li> <li>Vectra Data                     <ul style="list-style-type: none"> <li>A_TEST</li> <li>Miller</li> <li>MillerLite</li> <li>WINNT</li> </ul> </li> <li>Compact Disc (D:)</li> <li>Control Panel</li> </ul> </li> </ul> </li> </ul>	<table border="0"> <tr> <td><input type="checkbox"/> 2503_01.MRS</td> <td><input type="checkbox"/> FAST.MRS</td> <td><input type="checkbox"/> THE_FILE.MRS</td> </tr> <tr> <td><input type="checkbox"/> 2503_2DY.MRS</td> <td><input type="checkbox"/> NOTHING.MRS</td> <td><input type="checkbox"/> W_S_BE.MRS</td> </tr> <tr> <td><input type="checkbox"/> 25032D0.MRS</td> <td><input type="checkbox"/> OUTPT1.MRS</td> <td><input checked="" type="checkbox"/> W_W04_AE....</td> </tr> <tr> <td><input type="checkbox"/> 25032D01.MRS</td> <td><input type="checkbox"/> POSA1.MRS</td> <td><input checked="" type="checkbox"/> W_W1_BE.M...</td> </tr> <tr> <td><input type="checkbox"/> 25032D02.MRS</td> <td><input type="checkbox"/> QUICK.MRS</td> <td><input checked="" type="checkbox"/> W_W1A_BE....</td> </tr> <tr> <td><input type="checkbox"/> 3JULY.MRS</td> <td><input type="checkbox"/> RC398END.M...</td> <td></td> </tr> <tr> <td><input type="checkbox"/> 420RAC1.MRS</td> <td><input type="checkbox"/> RUTH0A.MRS</td> <td></td> </tr> <tr> <td><input checked="" type="checkbox"/> 420RAC2.MRS</td> <td><input type="checkbox"/> RUTH1.MRS</td> <td></td> </tr> <tr> <td><input type="checkbox"/> 420RAC3.MRS</td> <td><input type="checkbox"/> RUTH1A.MRS</td> <td></td> </tr> <tr> <td><input type="checkbox"/> 420RAC4.MRS</td> <td><input type="checkbox"/> RUTH2.MRS</td> <td></td> </tr> <tr> <td><input type="checkbox"/> 420RAC5.MRS</td> <td><input type="checkbox"/> RUTH2A.MRS</td> <td></td> </tr> <tr> <td><input checked="" type="checkbox"/> 420RAC6.MRS</td> <td><input type="checkbox"/> RUTH3.MRS</td> <td></td> </tr> <tr> <td><input type="checkbox"/> 420RAC7.MRS</td> <td><input type="checkbox"/> RUTH3A.MRS</td> <td></td> </tr> <tr> <td><input type="checkbox"/> 420RAC8.MRS</td> <td><input type="checkbox"/> STABTEST.D...</td> <td></td> </tr> <tr> <td><input type="checkbox"/> AHPSU_0.MRS</td> <td><input checked="" type="checkbox"/> TEST1.MRS</td> <td></td> </tr> <tr> <td><input type="checkbox"/> AHPSU_SS.M...</td> <td><input type="checkbox"/> TEST2.MRS</td> <td></td> </tr> <tr> <td><input type="checkbox"/> ARRUTH.DPR</td> <td><input type="checkbox"/> TEST3.MRS</td> <td></td> </tr> <tr> <td><input type="checkbox"/> ARRUTH.MRS</td> <td><input type="checkbox"/> TEST4.MRS</td> <td></td> </tr> <tr> <td><input type="checkbox"/> DETERMIN.M...</td> <td><input type="checkbox"/> THE_FILE.DPR</td> <td></td> </tr> </table>	<input type="checkbox"/> 2503_01.MRS	<input type="checkbox"/> FAST.MRS	<input type="checkbox"/> THE_FILE.MRS	<input type="checkbox"/> 2503_2DY.MRS	<input type="checkbox"/> NOTHING.MRS	<input type="checkbox"/> W_S_BE.MRS	<input type="checkbox"/> 25032D0.MRS	<input type="checkbox"/> OUTPT1.MRS	<input checked="" type="checkbox"/> W_W04_AE....	<input type="checkbox"/> 25032D01.MRS	<input type="checkbox"/> POSA1.MRS	<input checked="" type="checkbox"/> W_W1_BE.M...	<input type="checkbox"/> 25032D02.MRS	<input type="checkbox"/> QUICK.MRS	<input checked="" type="checkbox"/> W_W1A_BE....	<input type="checkbox"/> 3JULY.MRS	<input type="checkbox"/> RC398END.M...		<input type="checkbox"/> 420RAC1.MRS	<input type="checkbox"/> RUTH0A.MRS		<input checked="" type="checkbox"/> 420RAC2.MRS	<input type="checkbox"/> RUTH1.MRS		<input type="checkbox"/> 420RAC3.MRS	<input type="checkbox"/> RUTH1A.MRS		<input type="checkbox"/> 420RAC4.MRS	<input type="checkbox"/> RUTH2.MRS		<input type="checkbox"/> 420RAC5.MRS	<input type="checkbox"/> RUTH2A.MRS		<input checked="" type="checkbox"/> 420RAC6.MRS	<input type="checkbox"/> RUTH3.MRS		<input type="checkbox"/> 420RAC7.MRS	<input type="checkbox"/> RUTH3A.MRS		<input type="checkbox"/> 420RAC8.MRS	<input type="checkbox"/> STABTEST.D...		<input type="checkbox"/> AHPSU_0.MRS	<input checked="" type="checkbox"/> TEST1.MRS		<input type="checkbox"/> AHPSU_SS.M...	<input type="checkbox"/> TEST2.MRS		<input type="checkbox"/> ARRUTH.DPR	<input type="checkbox"/> TEST3.MRS		<input type="checkbox"/> ARRUTH.MRS	<input type="checkbox"/> TEST4.MRS		<input type="checkbox"/> DETERMIN.M...	<input type="checkbox"/> THE_FILE.DPR	
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<input type="checkbox"/> DETERMIN.M...	<input type="checkbox"/> THE_FILE.DPR																																																									

Hide mrs region subfolders

Destination database:

Messages:

Saved C:\Vectra Data\A\_TEST\420RAC2.MRS to C:\Program Files\Escra 2000\start.mdb:A\_TEST:420rac2

Saved C:\Vectra Data\A\_TEST\420RAC6.MRS to C:\Program Files\Escra 2000\start.mdb:A\_TEST:420rac6

Saved C:\Vectra Data\A\_TEST\TEST1.MRS to C:\Program Files\Escra 2000\start.mdb:A\_TEST:Test1

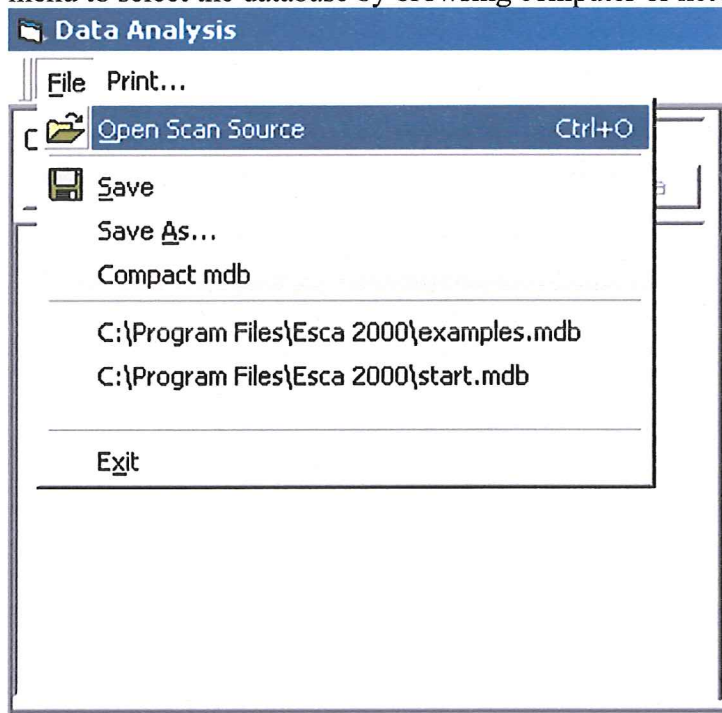
Saved C:\Vectra Data\A\_TEST\W\_W04\_AE.MRS to C:\Program Files\Escra 2000\start.mdb:A\_TEST:w\_w04\_ae

## ANALYZE COMPOSITION – Introduction

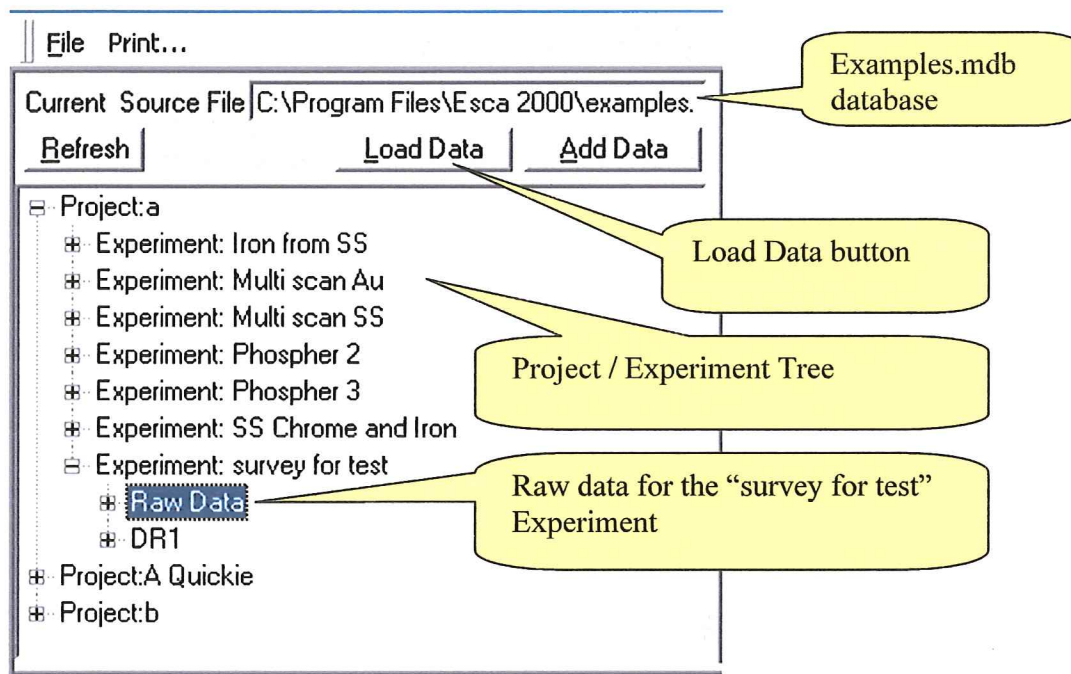
There are five steps to construct a compositional analysis from a survey spectrum. The compositional analysis is very common and typically part of the detailed analysis of a sample. The general steps are:

1. Find and measure the areas of the peaks in the spectrum
2. Identify the XPS emission line that produced the peak.
3. Compute the normalized area to account for the sensitivity factor associated with each emission line.
4. Choose the emission line used to represent each element in the composition table.
5. Compute Atomic percent

Before starting an analysis load a database. Use the (**Open Scan Source**) item in the file menu to select the database by browsing computer or network.



After the database is selected the Project / Experiment tree will be displayed.



Expand the tree to find the desired experiment and then expand to locate the Raw Data item. Click the (Load Data) button to load the regions that make up the Experiment List.

Proj Name:	a	Region:	1
Exp Name:	survey for test	Scn-Sec:	1
Exp Desc:	short scan	Spot:	800
Analysis:	Raw data	Res:	4
		eV/Stp:	0.4

	Scan	Visible	Xoffset	Yoffset	
	Regn1	<input type="checkbox"/>	0	0	1
	Regn2	<input type="checkbox"/>	0	0	1

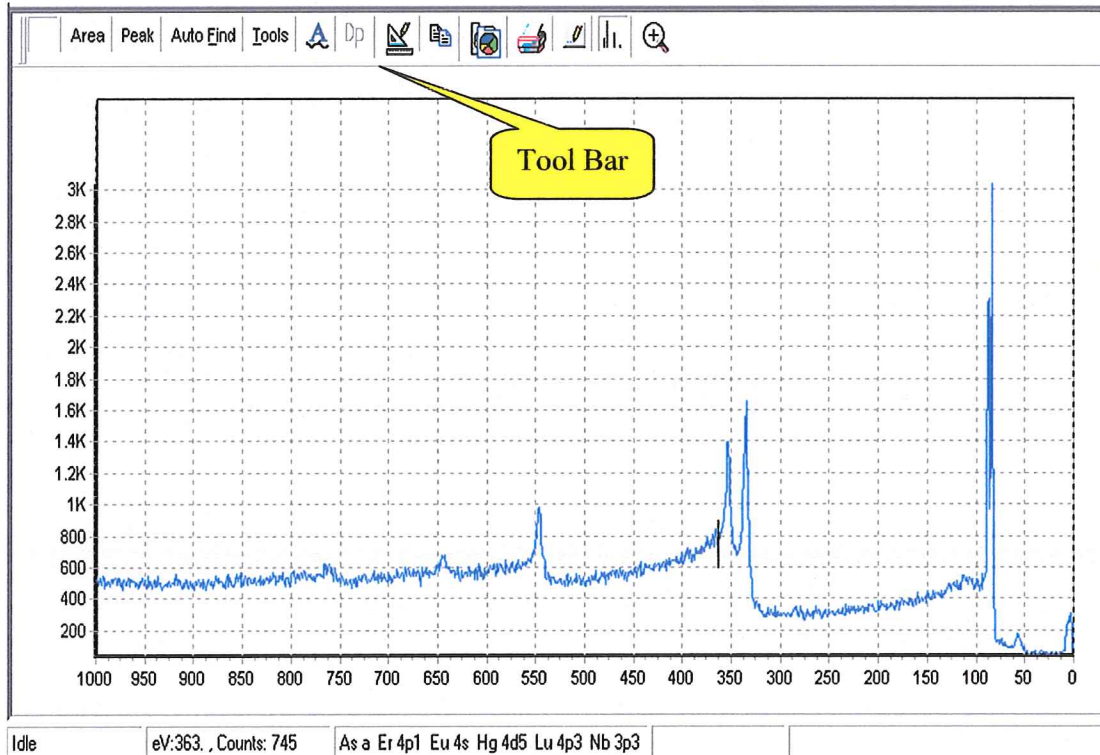
The Loaded Experiment review window will show the Project Name, Experiment Name, the Experiment Description and the Analysis Name. In the example above the Analysis Name shows <Raw Data> to indicate that no analysis has been performed and save yet. The small window summarizes the data collection parameters. Each region that is currently loaded for analysis is shown in the region list.

The spectrum for each region is made visible in the graphics viewer by clicking on the button at the left end of the row. The yellow button indicates that this region is currently the active region. All analysis operations will be performed on the active region.

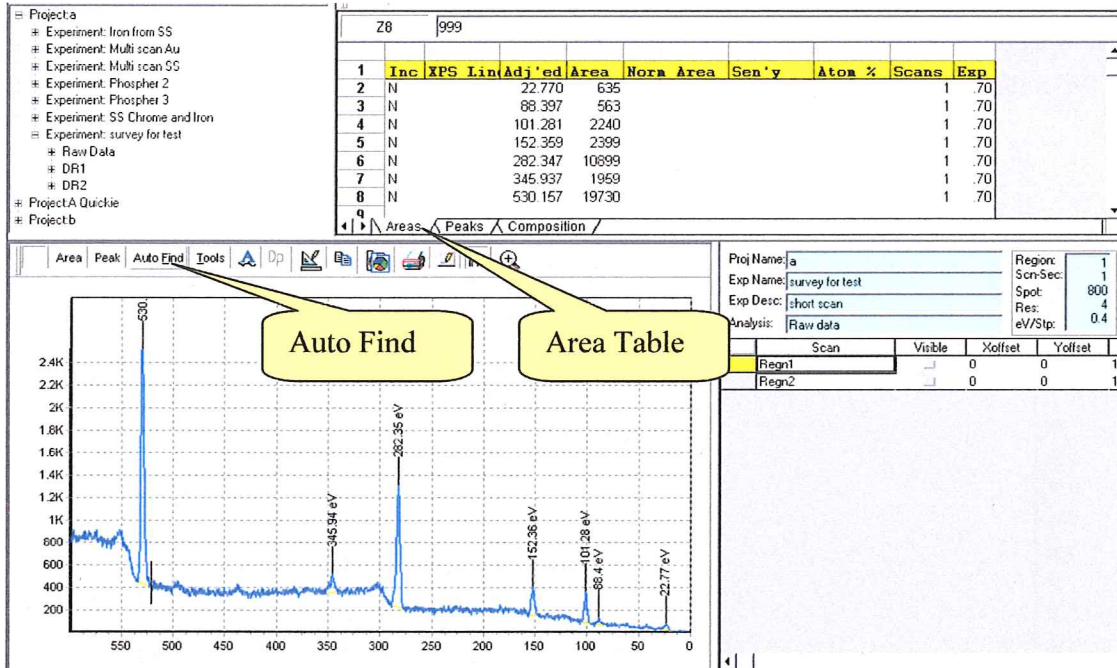
Regions can be made visible but not active by clicking the Visible checkbox in the column to the right of Scan Column.

The blue color is used for read only displays. No entries are made in the Project / Experiment display windows.

The Spectrum display window has a Tool Bar that provides the main controls necessary to carry out the data analysis.



# COMPOSITION – Auto Find



[Auto Find] locates all major peaks above a predetermined noise level. The base line for each peak is drawn and the area measured. The Area Table provides a list of the peaks that were found along with the peak location and Area. Each peak in the spectrum is labeled using the peak center binding energy.

This program does not attempt to identify the peaks. We have not found an algorithm that provides reliable identification. We have also noticed a troubling number of incorrectly labeled spectra in public and private reports. We feel that until an improved identification algorithm is developed it best to leave identification to the user.

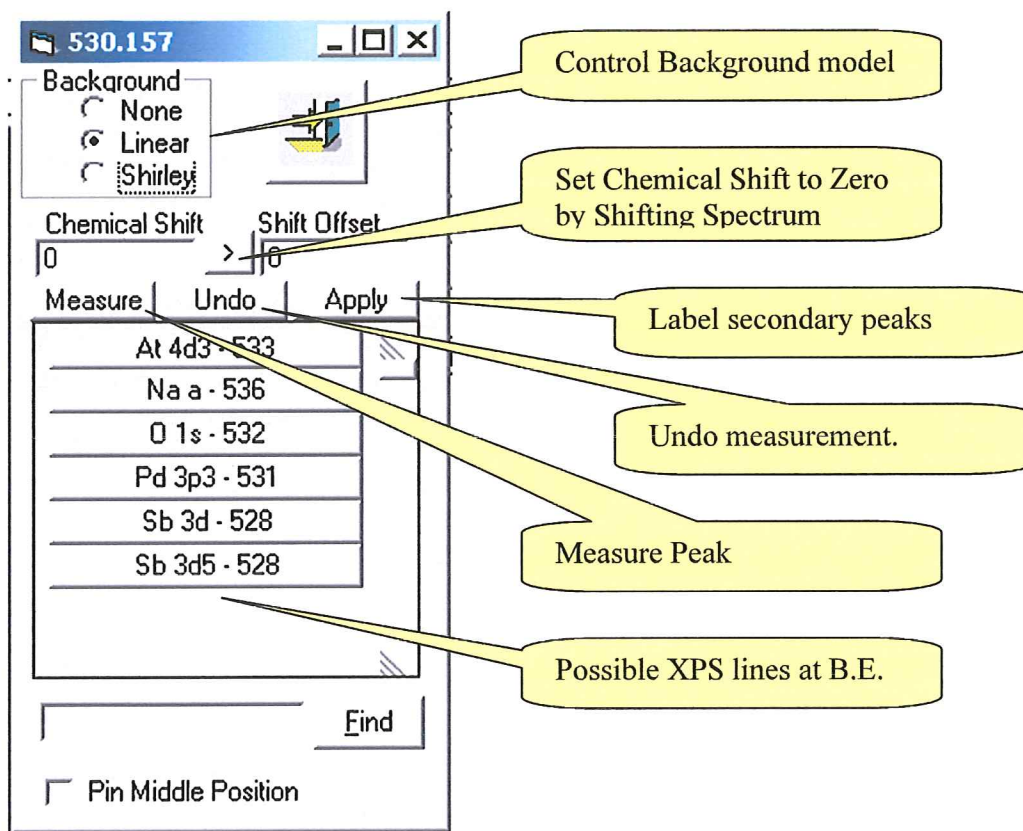


## COMPOSITION – Area Edit Dialog Box

We have provided a very fast and efficient identification procedure. The Area Edit Tool is launched when the [Auto Find] button is clicked. The [Area] button will also open the Area Edit Tool to aid in editing and identification of peak measurements. Manual area measurements can be made using the Area Edit Tool.



### Dialog Box



There are two activities that need to be mastered to identify peaks quickly. First is the editing and identification dialog shown above and second is spectrum manipulation. We will first cover the dialog box shown above.

After the (Auto Find) function has been performed the spectrum will be displayed and the peak at the highest B.E. will be selected. The selection is notified by changing the background line to black instead of yellow. The dialog will be displayed with the header

## COMPOSITION – Area Edit Dialog Box – Continued

(Blue band at the top) showing the BE for this peak. The correct assignment will most likely be found in the list of possible XPS lines. Click an XPS Line in the list to make a trial assignment. A set of markers will be displayed along the BE axis to show the location of all other emission lines for this choice. Evaluate how well the spectrum matches the emission lines for the selected element. You can click on a second choice. This choice will completely replace the previous one. When you determine the correct assignment you are ready to go on to the next emission line. Activate the next line by clicking the next peak of interest.

NOTE: You do not need to start with the default peak as described above. It is often best to start with the peak you want to use for the binding energy reference. See details on spectrum shifting below.

HINT: If you have trouble activating a peak try clicking inside the peak about 1/3 of the way up from the background line. Another approach is to click the B.E. label above the peak. The cursor is very busy trying to decide what you are going to do. If the cursor gets near either end point of the background line or near the stem of the label the cursor may become a hand. This indicates the program has changed into the edit mode. This mode is described below. You must avoid the edit mode when trying to send an unambiguous message that you want to select the peak.

In the simple cases you will be selecting a peak and then selecting the obvious element from the list. In cases where the assignment is not clear you will try various entries in the list to find the correct assignment. When many XPS lines are present for one element it is necessary to decide on the **Primary Peak** that will represent the element in the Composition Table. You may choose the primary peak by putting a “Y” in the “INC” column for the XPS line you wish to use and a “N” for all secondary entries.

The Area Edit Dialog provides a number of additional features to handle situations beyond these straightforward operations.

1. **Baseline selection.** The default baseline for a survey spectrum is the linear line. The baselines can be changed to Shirley by selecting the peak and then selecting the Shirley model. The “None” background model is useful for calculating the noise contained in the background over a specified range of binding energy. See the section: Calculating Detection Limits.
2. **Chemical Shift, Shift Offset and Global Shift.** The primary problem addressed by these three controls is charging. Insulating samples do not have an absolute reference for the Binding Energy scale. For conductors this reference is the Fermi edge. For insulators it is necessary to create a reference in order to judge the goodness of an element assignment.

## COMPOSITION –Area Edit Dialog Box - Continued

It is best to choose an XPS line that is unlikely to have any chemical shift. If this XPS line is in the selection list choose it. Click the (>) button. This sets the chemical shift to zero by creating a shift offset of the spectrum. Now all binding energies are “referenced” to the selected XPS line. The shift offset is also entered into the global (**Shift**) box in the Spreadsheet Toolbar.

If the XPS line is not presented in the selection list, then you need to provide a rough estimate of the shift offset that would bring this line into the range of the selection search. This estimate must be entered into the global (**Shift**) box and press [**Enter**] on the keyboard. (The Shift Offset in the dialog will not accept a complete number.) The XPS line should now appear in the list. Select the line. Now click the (>) button to refine the adjustment of the Binding Energy Reference.

The global (**Shift**) applies to all entries in the table.

3. **Editing Background endpoints.** The Auto Find will have problems with endpoint selection in parts of the spectrum where there is extensive shake up structure, interference between peaks and on some transition metals. The endpoints may be edited using the Area editing tools. The procedure is:
  - a. Click inside peak to activate the background line. It will turn black.
  - b. Move the cursor to the end point. The cursor will turn into a hand with the index finger as a pointer. Right mouse click and drag the endpoint to a new location. Repeat this procedure for the other endpoint if necessary.
  - c. Click on the (Measure) button to re-measure the area under the peak using the new endpoints.
  - d. Select the XPS line.

Note: The endpoints can be nudged one data point at a time. Activate the baseline. Place the cursor near the endpoint of interest. Hold the shift key down and tap right or left arrow key.

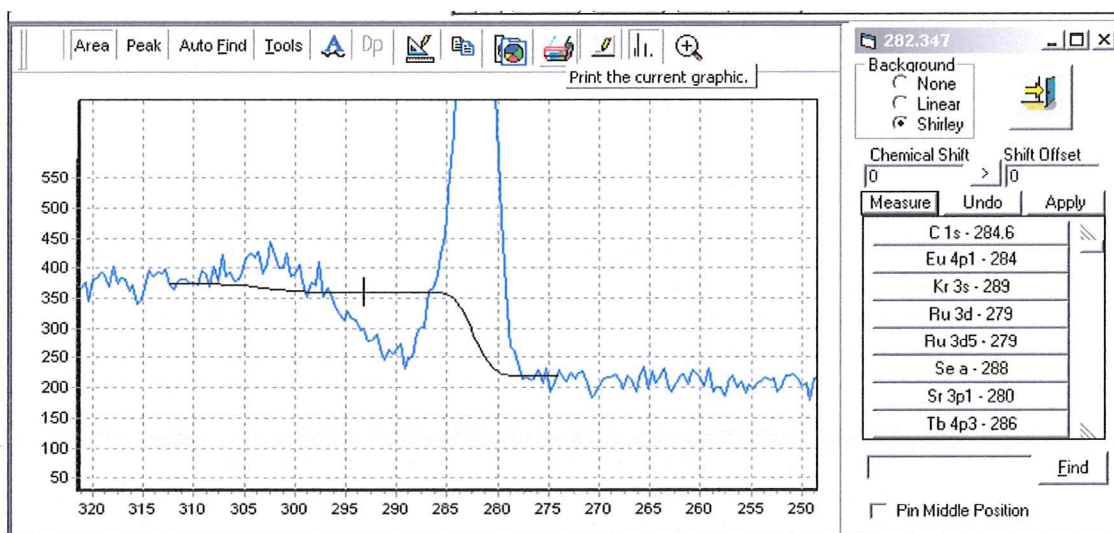
4. **Measure Area of Peak.** To measure the area of a peak from scratch move the cursor to one side of the peak where you want to start the background line. Put the cursor at the junction of the binding energy marker and the spectrum. Left click and drag to the other side of the peak. The background line will be drawn as you drag to the second endpoint. The type of background line will depend on the type selected at the top of the dialog box in the background group.

There are two competing actions when the left mouse button is clicked. One is the Zoom feature, which will be discussed below, and the other is the drawing of the background line. In order to get the background to draw it is

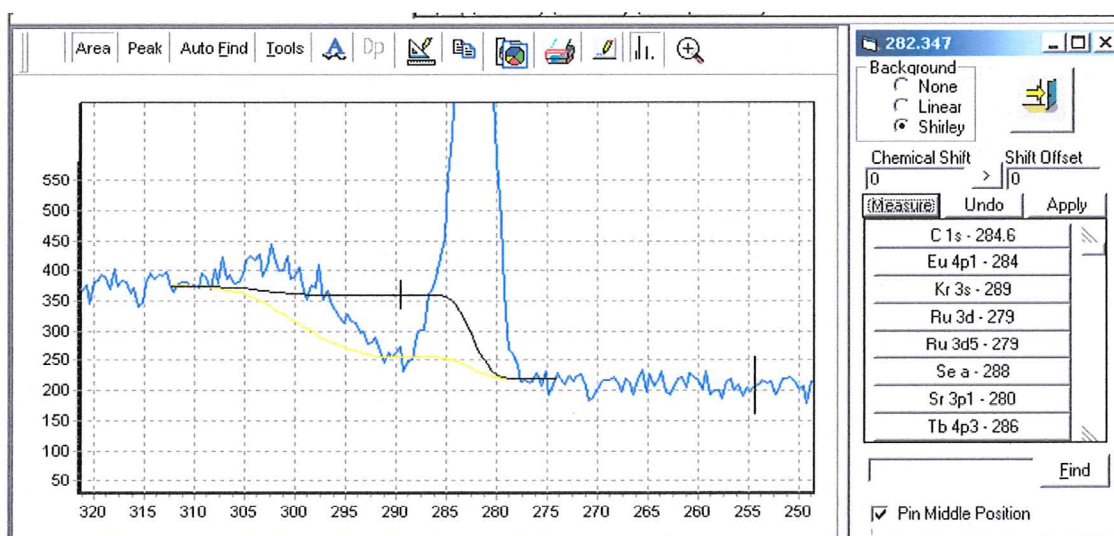
## COMPOSITION – Area Edit Dialog Box - Continued

important to place the pointer on a spectrum data point. The distance you can be from the data point is adjusted in the Preference dialog. This is the pencil. After the background is drawn then click the **(Measure)** button. Select the XPS line in the list.

- 5. Mid-Point pinning.** It is some times useful to include two parts of a peak with one background line. But, in some cases the Shirley background does not interest with the spectrum at a minimum point near the center. See example below.



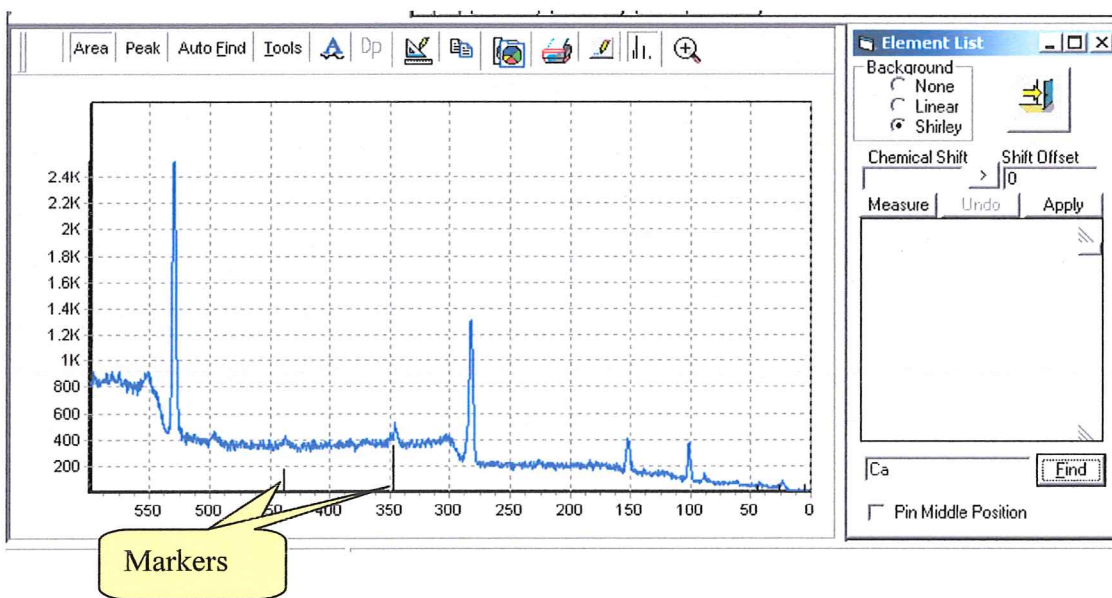
This problem can be solved using the mid-point pinning feature.



## COMPOSITION – Area Edit Dialog Box – Continued

The first step is to move the small vertical marker to the binding energy that needs to be pinned as shown above. (The yellow line would be in the unpinned position.) Put the cursor on the marker and left clicking, then drag the marker to the desired location. Click the check box at the bottom of the dialog. Click the **(Measure)** button. At this point the display should look as shown above. To remove the black line, click anywhere away from the spectrum.

6. **Checking a spectral region for the presents of other elements.** Some times it is convent to input an element name or symbol and display its XPS line markers. This can be done using the find tool at the bottom of the dialog. Enter an element symbol or full name and click **(Find)**.

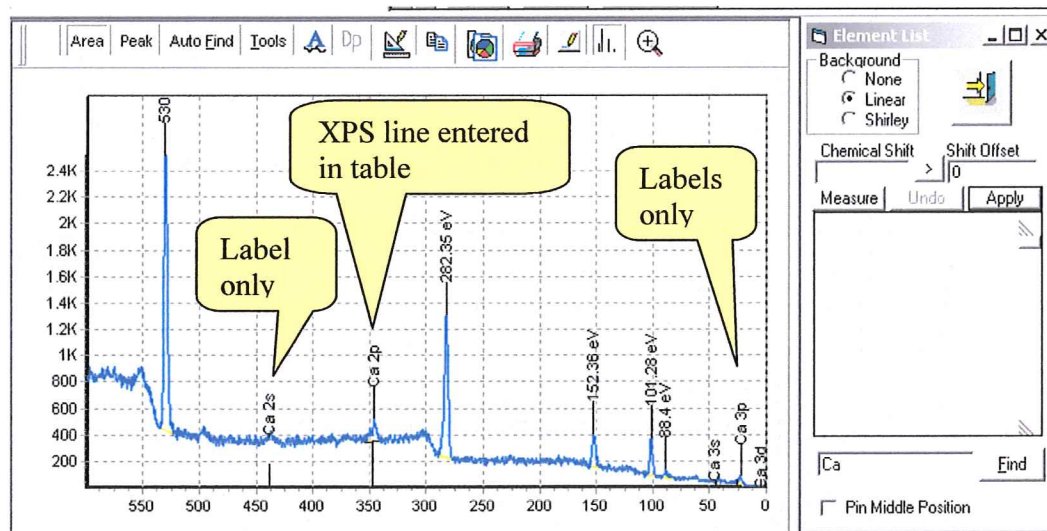


7. **(Apply) button labels all secondary peaks.** As described above it is generally useful to identify the most prominent peaks first. In this process it is often necessary to decide which XPS line will be the primary peak. The primary peak will represent the element in the composition table. If many peaks are present it is helpful to label the secondary peaks. Then as the identification process continues it is easy to see which peaks remain unlabeled.

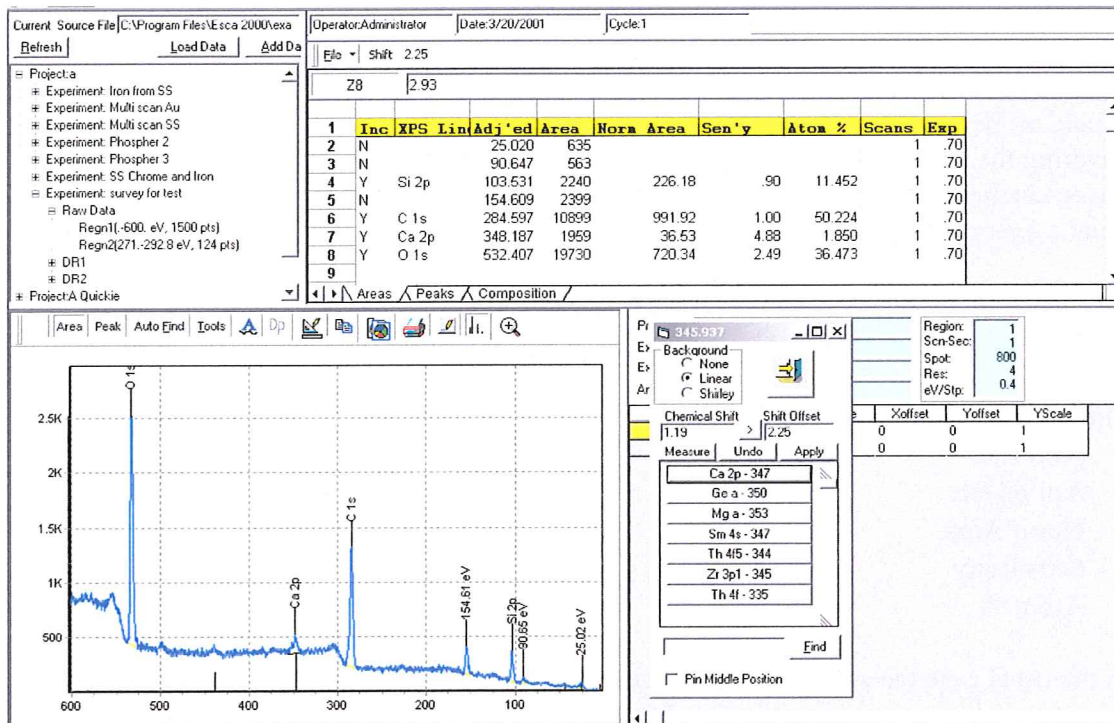
The **(Apply)** button will label all secondary peaks without computing their normalized areas. After selecting the XPS line assignment for the primary peak click on the **(Apply)** button. The XPS line assignment will enter the Primary line assignment into the Area Spreadsheet. The **(Apply)** button will place a label at the binding energy where each additional XPS lines should be found. The Apply process does not make entries into the spreadsheet.

## COMPOSITION – Area Edit Dialog Box - Continued

After using (Apply) button to label spectrum



# COMPOSITION – Area Spreadsheet



As the peaks are identified using the Area Edit dialog tool four tasks are automatically accomplished.

1. XPS Line assignment is entered into the table and the spectrum peak is labeled.
2. The photoelectron emission crosssection is looked up in the Scofield Table and the sensitivity factor is calculated. The sensitivity factor takes into account the variation in escape depth as a function of kinetic energy. The adjustable parameter is the Sensitivity Factor Exponent. This exponent is displayed as Exp in the table.
3. The Area is normalized to account for variations in Ev/Step, Detector Width, Scanned versus Unsanned and Dwell Time/Step. This normalization allows a very wide variety of operating conditions to be inter-compared in one Composition Table.

Note: The change in transmission function versus pass energy (RES #) and the change in x-ray flux versus spot size are not accounted for in the normalization process.

4. The Include (Inc) cell for the assignment is marked Yes (Y) so this assignment will be included in the Summary Composition Table found using the Composition tab.

## COMPOSITION – Area Spreadsheet - Continued

It is often useful to assign more than one XPS line for the same element and review how the various lines vary in their estimate of the Atom percent. Ideally all lines would provide the same estimate. If you had a pure sample and assigned three XPS lines they should all be displayed as 33.3%. In practice this is not observed. If a thin film is covering the sample then the higher binding energy lines will be depressed because the lower kinetic energy electrons are more like to be scattered by the film than the high kinetic energy electron.

The composition sheet of the NOTEBOOK summarizes the AREA and PEAK sheets for ALL Regions in the REGION LIST. **This is powerful and dangerous. See following.**

The parameters summarized are:

- XPS Line
- Adj'ed BE
- Norm Area
- Sensitivity
- Atom %

In the usual case the survey is used to generate the data used in the composition table and the Composition spreadsheet is simply a summary that is useful for printing or copy and pasting to other programs.

In special cases high sensitivity scans may be used to detect trace elements or peak fitting may be used to resolve overlapping emission lines. If the data from either of these cases is combined into one composition table with data from a survey scan then the data must be taken with the same Resolution setting and Spot Size setting. The ev/step, number of scans and scan width can be mixed. Scanned and unscanned can also be mixed

When a number of different regions are combined then you must keep track of the source of the data sent to the summary table. Any number of regions in the region list can send data to the summary composition table. Both area measurements and peak fits can be included. The include parameter controls what is included. The “Y” symbol includes the data for an XPS line and an “N” symbol will cause the assignment to be skipped. Any XPS emission line in either the area sheet or peak sheet that has a “Y” in the include column will be included. The Area sheet and the Peak sheet act independently. The Composition Sheet is the summary for all regions and the summary displayed does not depend on which region is active.



## COMPOSITION – Area Spreadsheet - Continued

Consider the example that a survey has been taken on a steel sample and a composition table generated. However, on review you are concerned there may be a small silicon signal at about 150 ev. A high sensitivity scan in res 4 with 0.4 ev/step is taken from 90 ev to 160 ev binding energy. This experiment is added to the region list. The area of a small peak at 150ev is measured using the area tool in the edit mode. When the XPS line assignment is made for Si 2s the include column will have a “Y” entered. If you go to the Composition Sheet you will find this assignment along with the assignments made from the survey.

You could also peak fit the Si 2p region to resolve the silicon and iron interference. You would enter Si 2p for the component at 100 ev and Fe 3s for the component at 95 ev. Notice that the include parameter is not automatically changed to “Y” in the peak fit mode. After entering “Y” for each component you will go to the survey and set the include parameter for the Fe 2p peak to “N”. Now review the Composition summary.

## COMPOSITION - Scofield Editor

The Scofield table use to store the XPS crossections, line positions and line position ranges can be edited to add additional lines, modify crossections, and adjust line position ranges. To open the editor, use the (**Settings**) button of the Analysis Toolbar. Select the [Edit Scofield Table] menu item.

The controls at the bottom of the spreadsheet provide tips on their use. When the table is close it will save the changes and resort new entries in alphabetical order.

We provide no provision for multiple tables at this time.

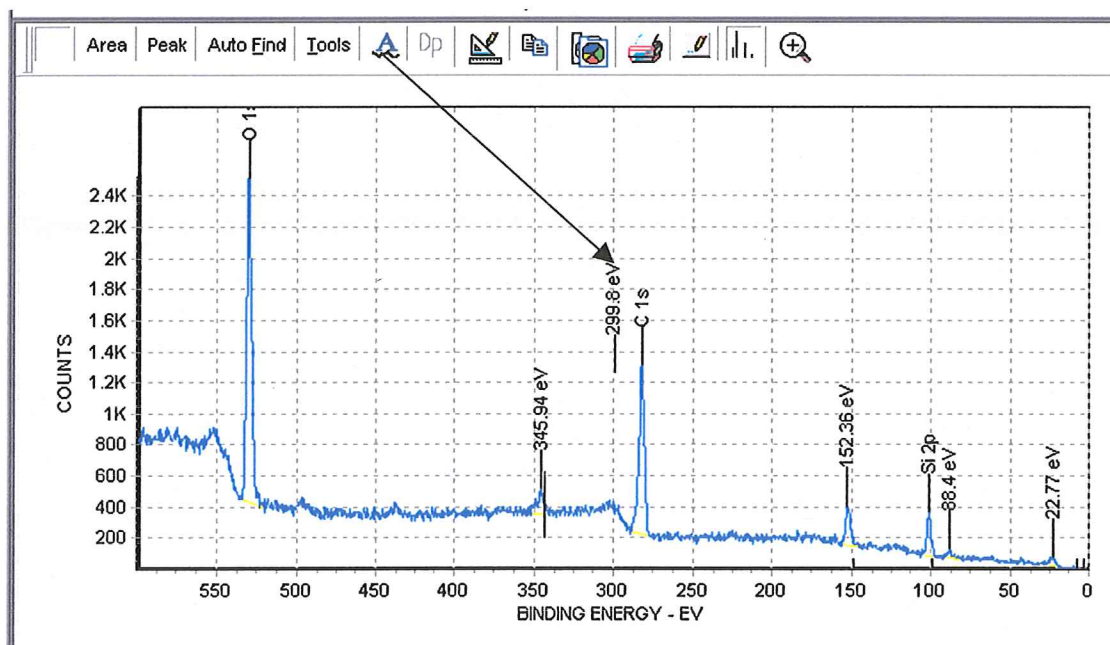
## Data Presentation

Data presentation is divided into two parts, composing the graphic and output. The tools covered in this section for composing the graphic are:

- a. Annotation and Editing Labels
- b. Customize Graphics
- c. Changing scales
- d. Removing Grids
- e. Headers and Footers
- f. Special Graphic formats

The tools for output are covered under the Print and Past section of this manual.

### Data Presentation – Annotation and Editing Labels

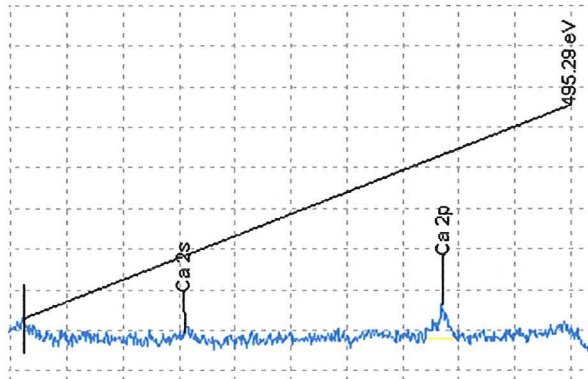


The Annotation button on the toolbar presents a stem and label at the center of the graphics window as shown above. This initial label has some interesting properties. You may use the mouse to drag the lower end of the stem to any location. The label will report the exact binding energy of the endpoint of the stem. The label may likewise be moved to any location. If the label is activated using the mouse it may be fully edited.

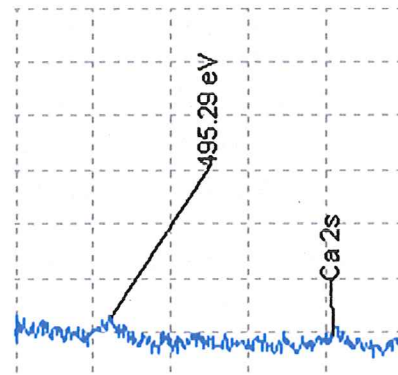
To move the stem or label, approach the bottom of the object until the cursor changes into a hand. Left mouse click and drag the stem or label. To edit the label approach

## Data Presentation – Annotation – cont

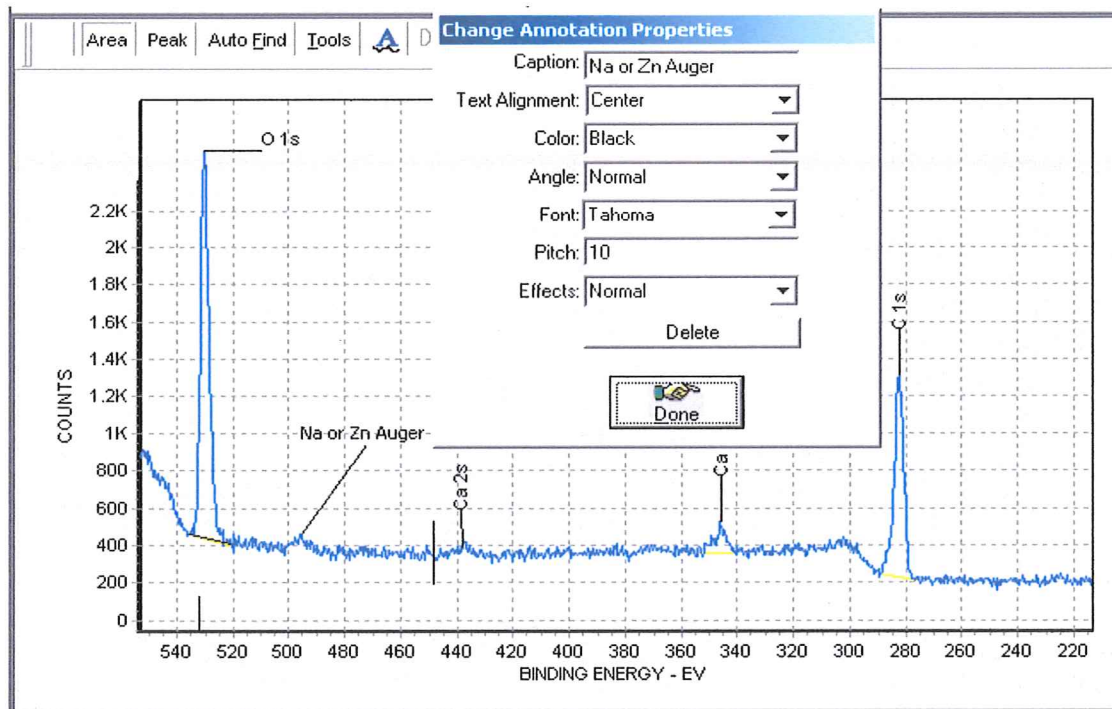
the bottom of the label with the mouse until the cursor becomes a hand. Right mouse click to open the Change Annotation Properties dialog. You may change the label making an entry into the caption box. The orientation and alignment may be changed. These operations are displayed in the following screen captures.



Move stem to new location



Move Label



Edit the Caption, Angle and Font then click done.

Any annotation, including those applied using by the Area or Peak Dialogs, may be edited using the Change Annotation Properties dialog.

A selected Annotation may be deleted using the delete button.

## Data Presentation - Customize Graphics

The graphics window can be converted into a number of formats and made available to other programs. It is useful to customize the graphic image to meet your needs before you export it in some format because after the translation into an export format you lose flexibility. The tools available in the toolbar vary in complexity. The tools are:



Graphic Editor

1. Panel fill color
2. Min / max scale
3. Remove grids
4. Headers / footers
5. Titles

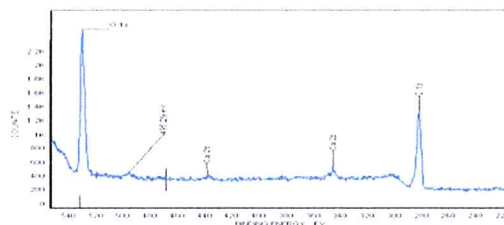
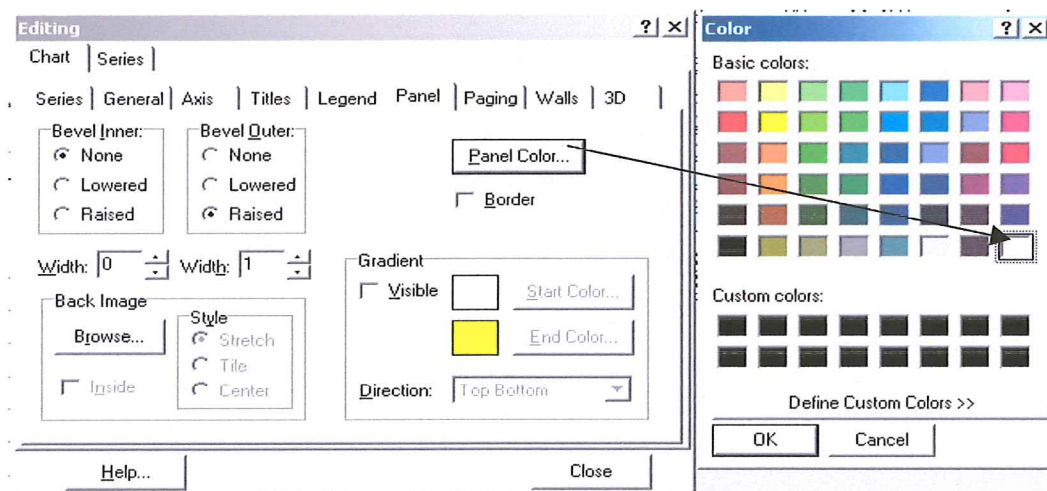
Change region color

1. Control spectrum color

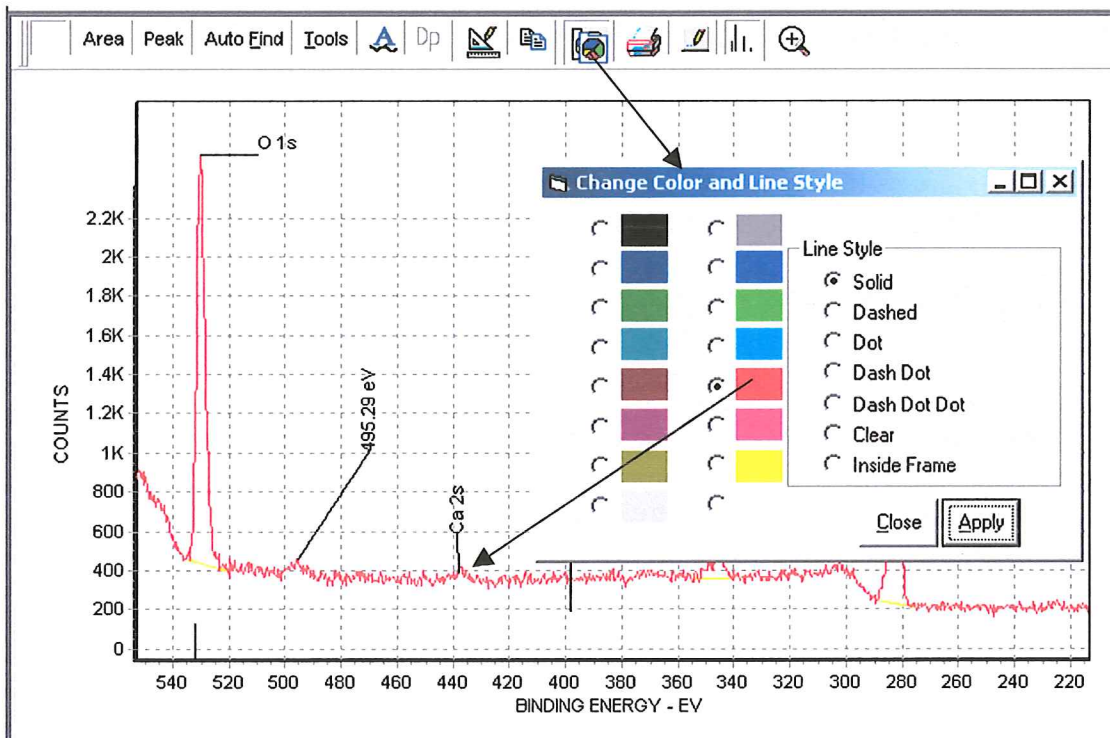
Preferences

1. Whole numbers on axis
2. Axis increment
3. Background color

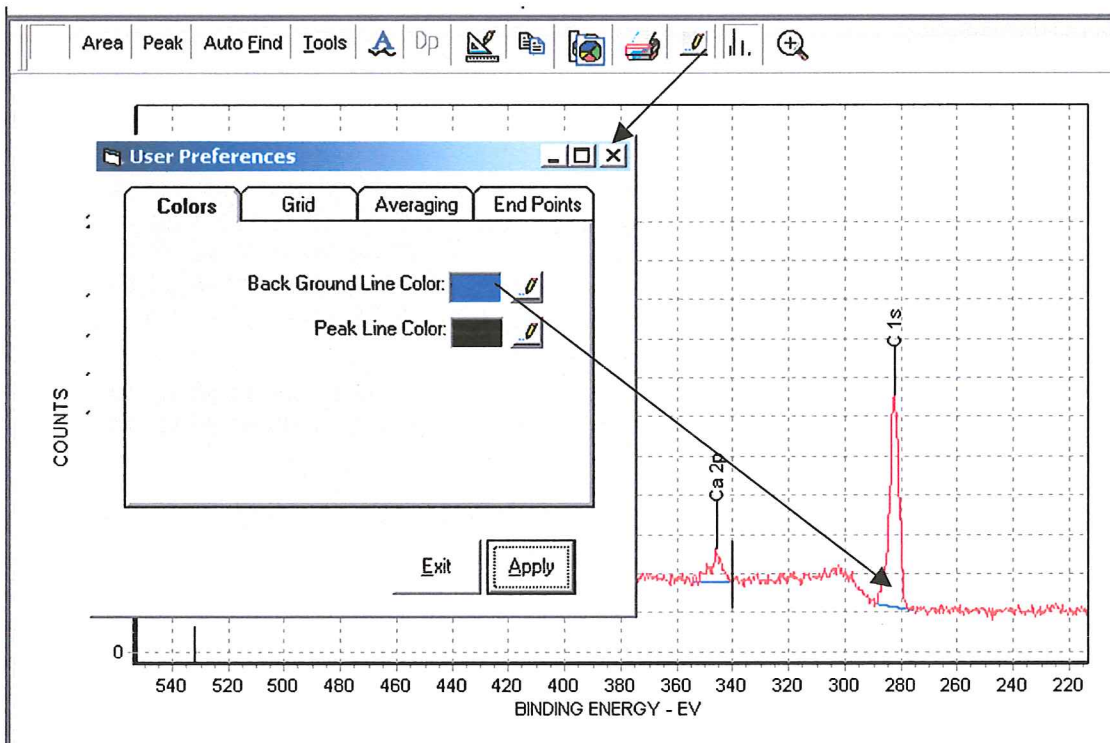
To remove the gray panel color Select the (**Chart Editor**) button on front page of the Graphic Editor. Select the (**Panel**) tab and then the (**Panel Color**) button. To set the background to white click the white color patch. Use the OK button to back out of the Color dialog, Close to back out of the Editing dialog and Done to close the 3D View properties dialog.



Graph with white background

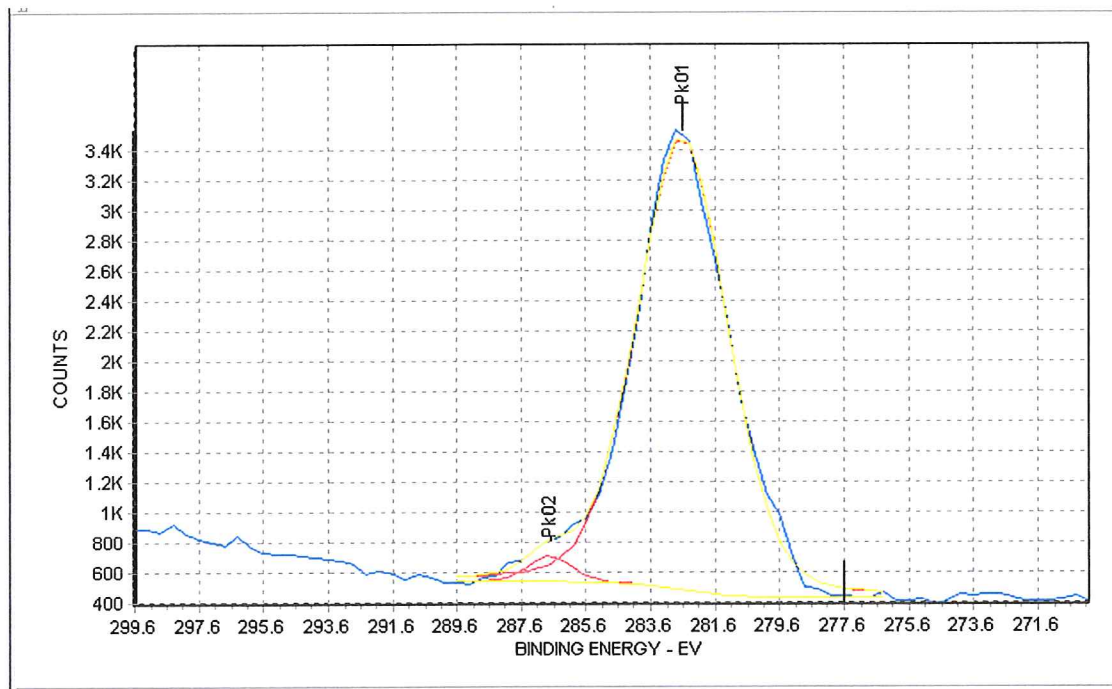


Change spectrum color.

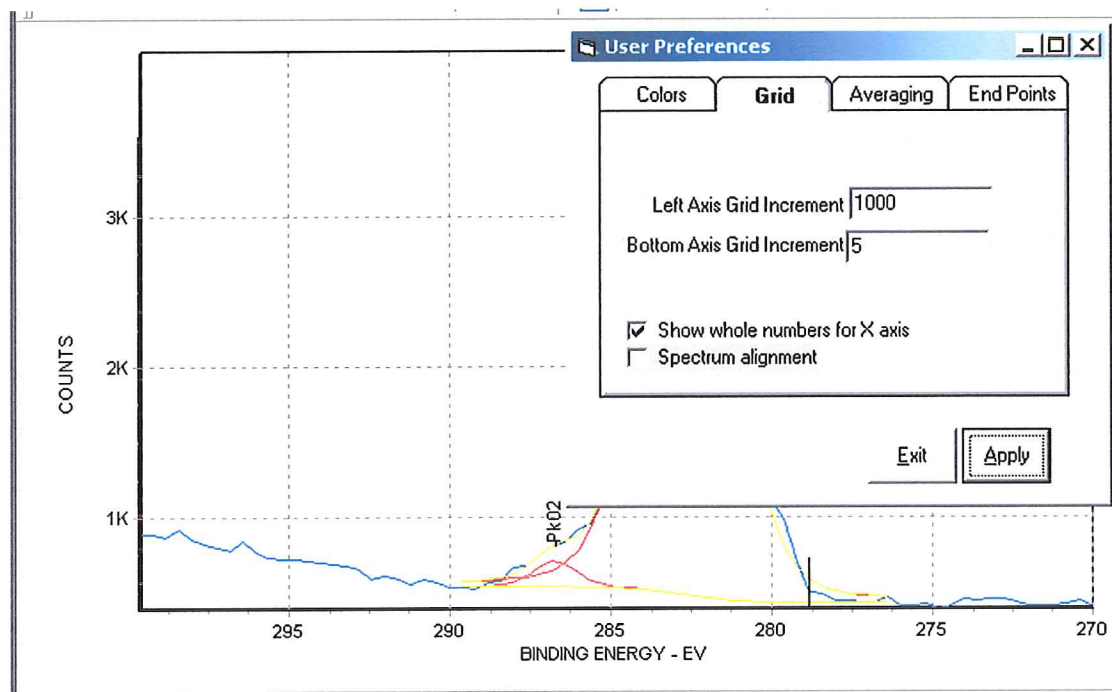


Change Back Ground Line color.

## Data Presentation - Changing scales



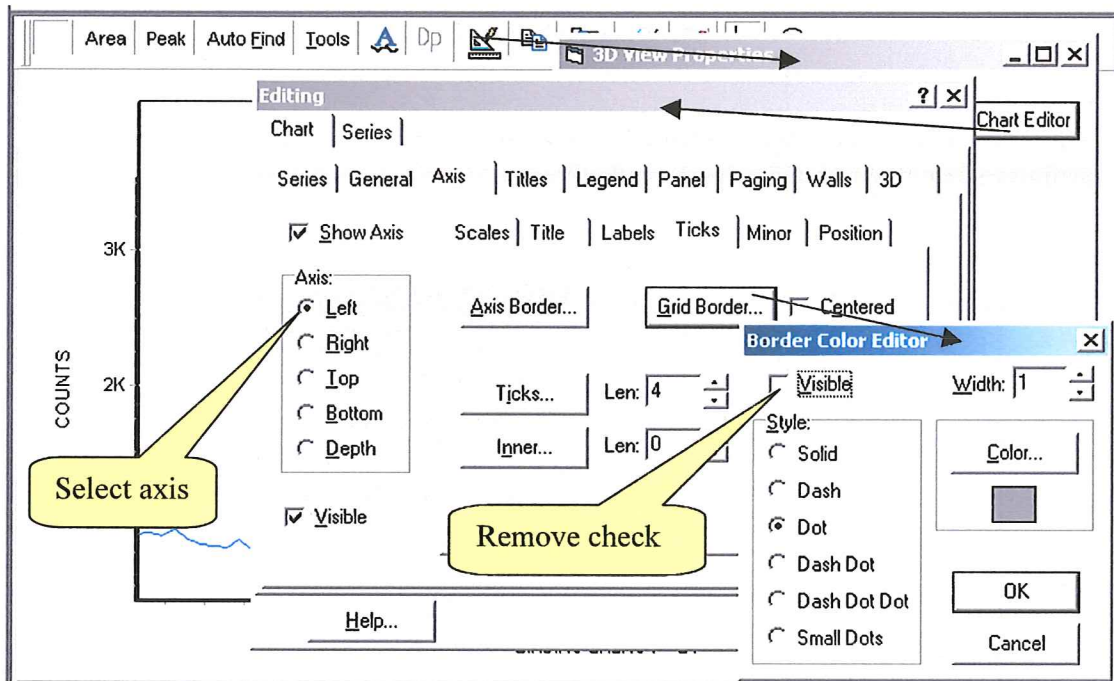
Use the Preferences to change from fractional numbers on x axis and the increment control to reduce the number ticks on both axes.



## Data Presentation – Remove grids

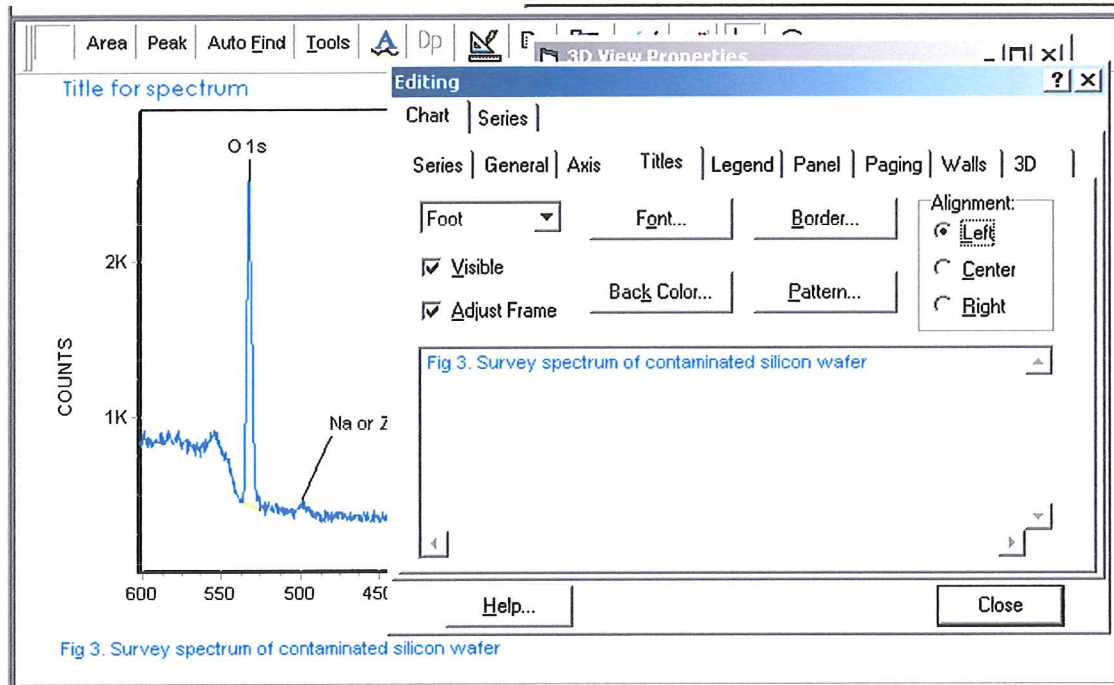
The remove grid operation involves a number of steps and demonstrates the extensive control over the graphic window. The steps to remove the grid are:

1. Open Graphic Editor (3D View Properties)
2. Open Chart Editor
3. Select Axis Tab
4. Choose the [Left] Axis as the active axis
5. Open the Grid Border Color Editor
6. Remove the check from the [Visible Box]
7. Select [OK] on Border Color Editor
8. Choose the [Bottom] Axis as the active axis
9. Open the Grid Border Color Editor
10. Remove the check from the [Visible Box]
11. Select [OK] on the Border Color Editor
12. Select [Close] on the Editing dialog
13. Select Done on the 3Dview Properties



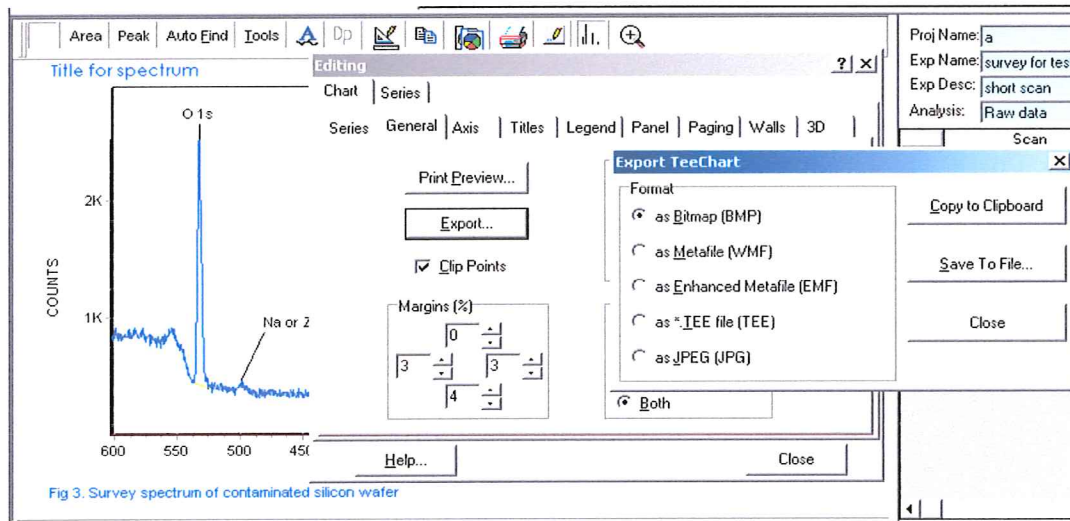


## Data Presentation – Headers and Footers



The Graphic Editor was used to create a header, or Title, and a footer that can be used to provide figure descriptions. The Title Tab on the Chart Editor provides control of the fonts, title alignment, borders for the titles and background colors or patterns.

## Data Presentation – Special Graphic Formats



The [General] Tab provides for Export of the graphic to 5 different formats and to Clipboard or file. The exported graphic can be imported to many other applications.

## Data Presentation – Special Graphic Formats – cont.

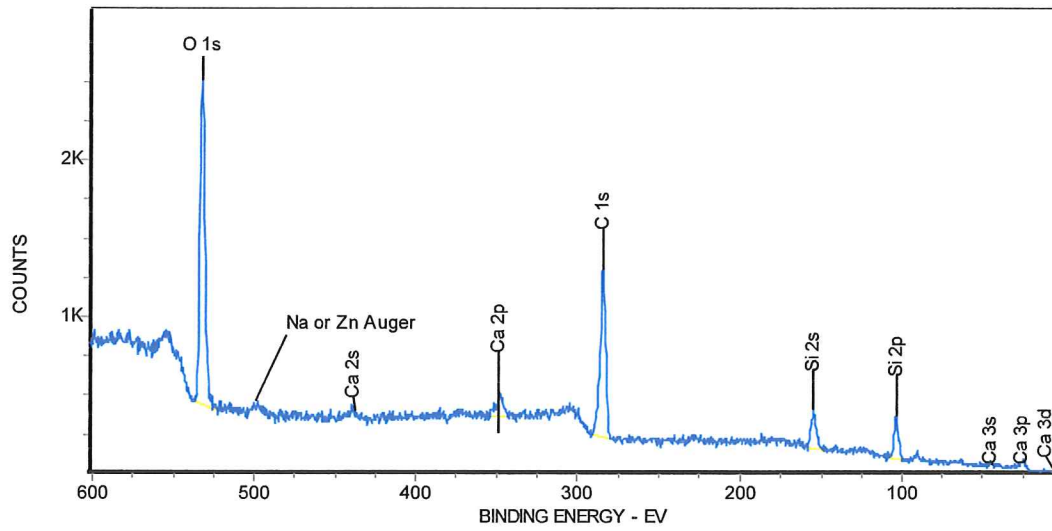
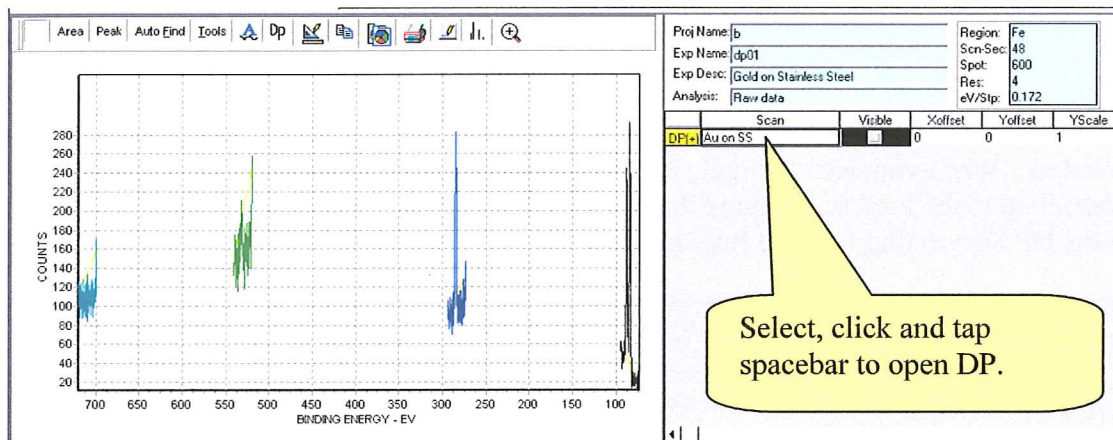


Fig 3. Survey spectrum of contaminated silicon wafer

The clipboard on the toolbar was used to copy and past this spectrum into Word.

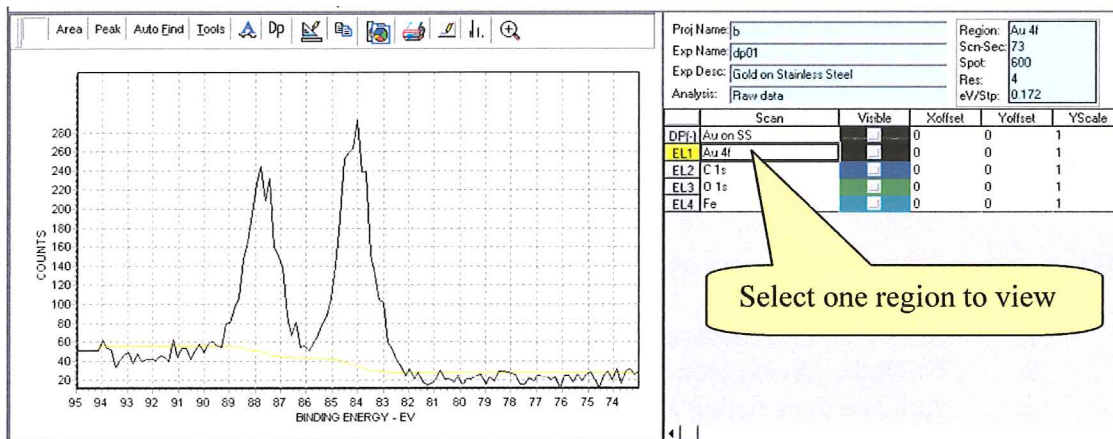
## DEPTH PROFILES

When a Depth Profile is loaded a preview is presented that shows all the regions of the depth profile on the same binding energy scale. The Region List only reports that a Depth profile is loaded but does not list the region in the preview.



### Depth Profile Preview

To open the Depth Profile you need to place the cursor in the white box under the Scan column of the Region list and click the left mouse button. This box will show the name of the Depth Profile. After clicking the mouse button hit the space bar on the keyboard. Then select a region of interest in the Region list.

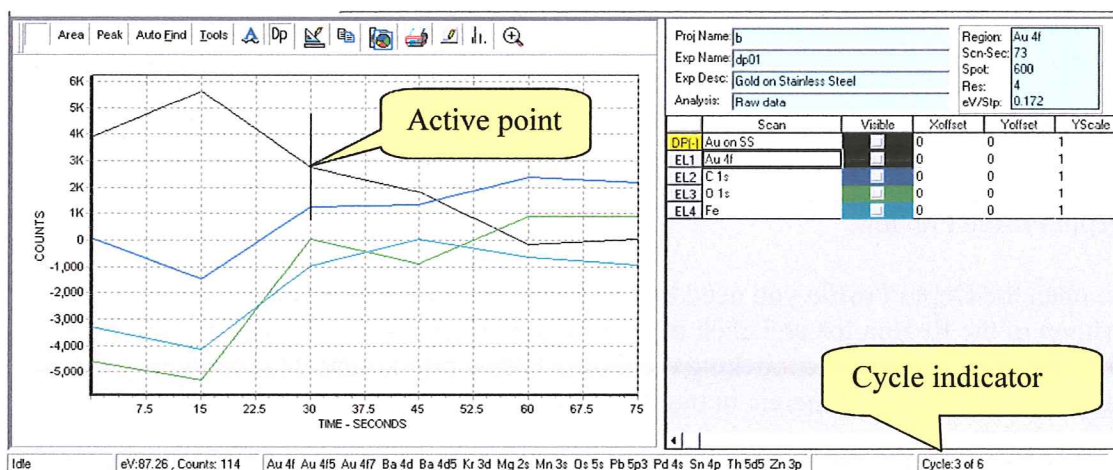


You can move through the cycles for this region by using the shift key and the up or down arrow keys. The current cycle will be displayed in the lower status bar. For the shift-arrow key control to be active the Graphic Window or the Region List must be active. To activate the Graphic Window or the Region list move the cursor to either window then click.

## Depth profiles – cont

To switch to the Depth Profile chart you click the DP icon in the toolbar. The vertical black line indicates the Au 4f graph, cycle 3 at 30 second into the etch. The DP icon provides a toggle that allows you to jump back and forth between the DP chart and a spectral region. You may move the Active Point indicator to any point on any chart line and then click the DP icon to jump to the spectrum for that point.

Hint: The cursor tries to follow your motion when the cursor is in the Graphics Window. When you want to toggle to a new region it is helpful to move the cursor vertical up to the toolbar, keeping the Active Point in place. Then move along the tools to the DP icon to toggle to the Region view.



The Depth Profile shown above has large negative areas for three of the elements. This is a result of poorly selected end points for the area measurements. The default DP sets the end points at the edges of the window to provide an initial presentation. It is important to edit these end points to improve the accuracy of the area measurements.

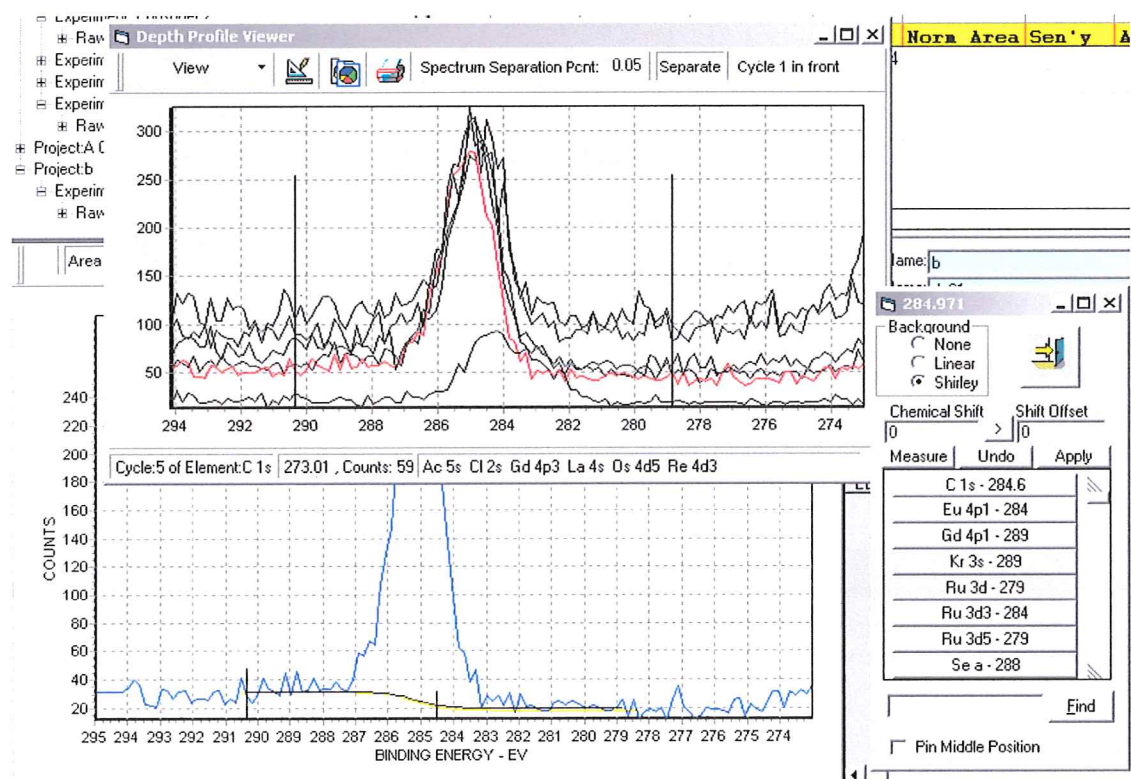
Editing area measurements is very easy. The steps are:

1. Select a representative cycle for one of the regions
2. Click the **(Area)** icon to activate the Area measurement editor.
3. Activate the existing area by clicking the base line near the center between the end points. The baseline will turn black
4. Move the cursor toward one end of the spectrum until the cursor turns into a hand. Left mouse click and drag the endpoint marker to select a new endpoint. Repeat the endpoint edit operation for the other endpoint.
5. Click the **(Measure)** button in the Area Edit Dialog box.
6. Select the XPS emission line form the list.

## Depth profiles – cont

When you click the (**Measure**) button the new endpoints are applied to all cycles for the selected region. You can toggle back to see the effect the edit has made on the DP.

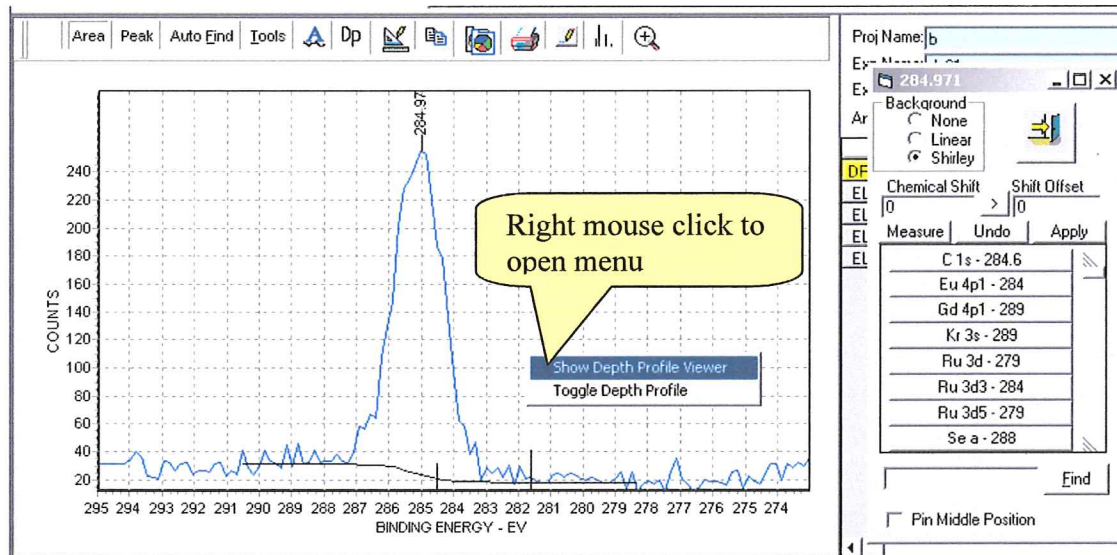
It is often helpful to view all region stacked up. The Depth Profile Viewer is useful for reviewing the endpoint selections.



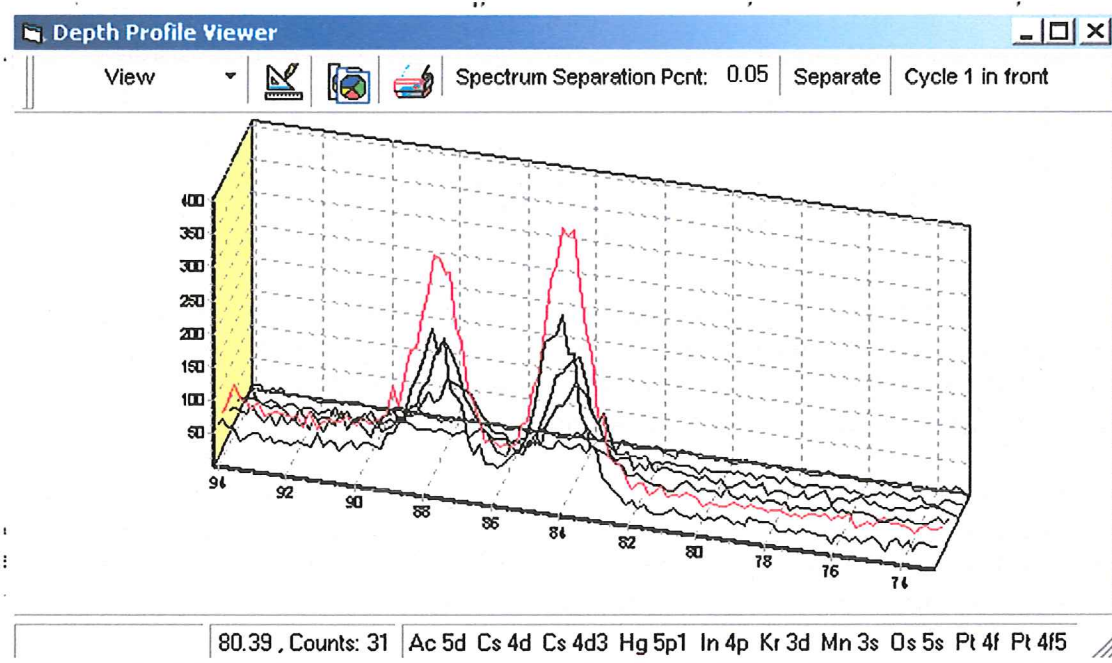
When the Area Edit Tool is displayed and the background line is active for the spectrum in the Graphic Display window then the endpoint markers of the Depth Profile Viewer will track the endpoint marker in the Graphic Viewer. As you drag the endpoint to adjust the background you can also review the endpoints for all cycles for the active region.

To turn on the Depth Profile Viewer be sure the cursor is active in the Graphics Viewer window, then right mouse click. A menu will be displayed that allows you to toggle between Depth Profile and Region View and also to turn on the Depth Profile Viewer. The Toggle control is identical to the (**Dp**) icon in the tool bar.

## Depth profiles – cont



Open the Depth Profile Viewer from the menu displayed after a right mouse click with the cursor on the Graphics Viewer window.



The **(View)** button allows control of which spectra are displayed. The spectrum separation box allows you to separate the spectra in the y direction. The **(Separate)** turns the separation effect on and off. The **(Cycle in Front)** button selects rather the first or last cycle is shown in front. The 3D effect are available through the Graphic Edit icon.

## Depth profiles – Future

A new Depth Profile analysis section is under design. This program structure has reached some technical limits. We have chosen to make fundamental changes instead of patching over the current limitations. Providing a flexible approach to the selection of regions to be included in a Depth Profile that displays atomic concentration is the tip of the iceberg. Labeling the x-axis in terms of depth, given the input of an etch rate, is a second short fall.

## Export - Spectra to Vamas and Excel

The screenshot shows the software interface with the File menu open and 'Export...' selected. A yellow callout box labeled 'Export' points to the menu item. Below the menu is a table of peak data:

1	Inc	XPS Line	Peak ID	Chem Shift	Adj'ed Be	Area	FWHM	% Assy	% Gauss	G
2	N		PK01	0.0	282.588	6989	2.309	.000	80.000	
3	N		PK02	0.0	280.964	5796	2.589	.000	80.000	
4			PK03	0.0	284.747	1831	3.606	.000	80.000	
5										
6										
7										
8										
9										

Below the table is a spectrum plot showing counts versus binding energy (eV) with peaks labeled PK01, PK02, and PK03. To the right is a table of regions:

Scan	Visible	Xoffset	Yoffset
Regn1	0	0	1
Regn2	1	0	1

A yellow callout box labeled 'Marked Visible' points to the 'Visible' column for Regn2.

1. Select an Experiment. If only some regions are to be exported mark them visible.
2. Select Export in the File menu.

The screenshot shows the 'Review Source Information - EXPORTER' dialog box. It contains the following information:

Active Experiment in Capture Viewer

- Source Project: a
- Source Experiment: survey for test
- Experiment Description: short scan

Region Control for Active Experiment

- All regions
- Only visible regions

Export Format

Buttons: Cancel, VAMAS, EXCEL, Fakedata

3. Choose All regions or Only Visible Peaks. Select type of export.



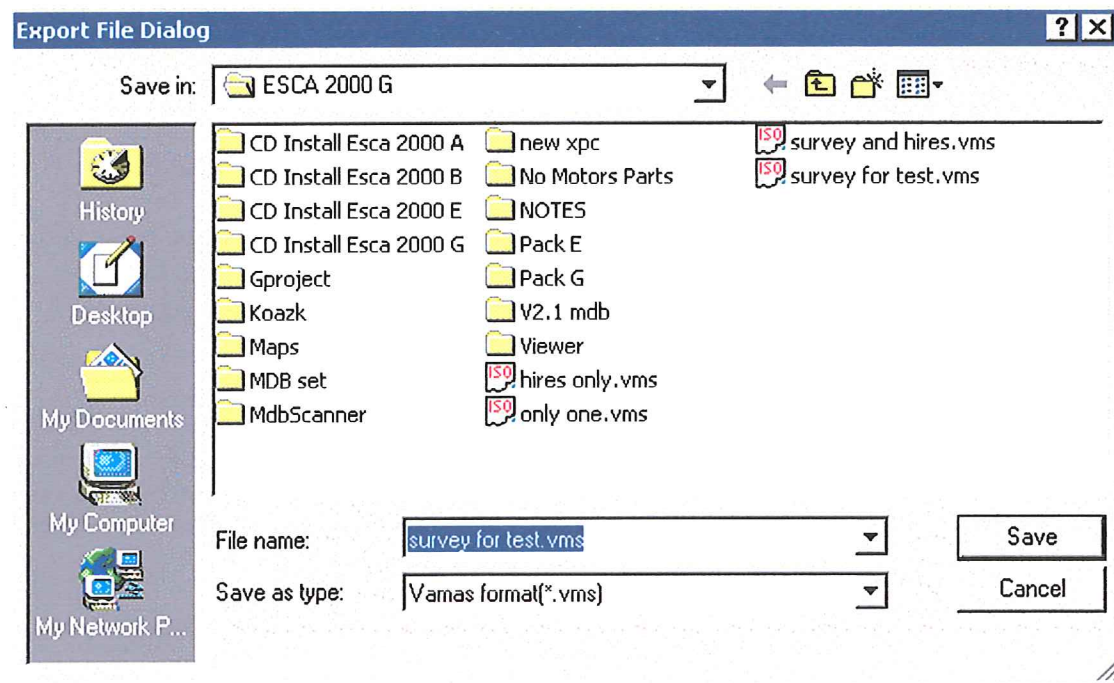
## Export To VAMAS and EXCEL – Cont.

The VAMAS export is an ASCII file readable by any text editor. The arrangement of information follows the international standard for Surface Science Data. All region of the MRS can be included in one VAMAS file. The VAMAS file can hold a complete depth profile. This is a very flexible and well-defined export file.

To use the Excel export, Excel must be available on the computer running the ESCA application. It does not need to be running. The export will open an Excel notebook, fill header cells with instrument parameters and provide a column of numbers representing the spectrum data. A crude graph is also created for quick review. There will be one page per spectrum. All spectra for a MRS table or just the regions marked visible can be included. A depth profile can be exported.

In the Analysis Application, if the EXCEL export is chosen, the data that describes the backgrounds for surveys and peak fits will be exported. For peak fits the peak envelopes will also be exported. This provides all information necessary to general purpose graphing programs.

Fakedata.txt is an internal text file used for demonstration purposes. Any spectra can be converted to a fakedata.txt file and then used by the Demo program to simulate the collection of data. This can be convenient for training and remote investigation of the program operation.



The Export File Dialog is used with the VAMAS export. This is a standard Windows dialog. File storage for the Excel is handled out of the Excel program.

## Export - Spreadsheet to Excel

Operator: Administrator		Date: 3/20/2001		Cycle: 1			
File		Shift: 2.25					
Print Preview							
Print Setup...							
Save All							
RS Line	Adj'ed Be	Area	Norm Area	Sen'y	Aton %	Scans	Exp
2	N	25.020	635				.70
3	Y	Zn 3p	90.647	563	16.32	3.14	.819

**Esca Save As Dialog** [?] [X]

Save in: Esca 2000

- Manual
- ServicePhysics
- Viewer
- \_S.xls

File name:

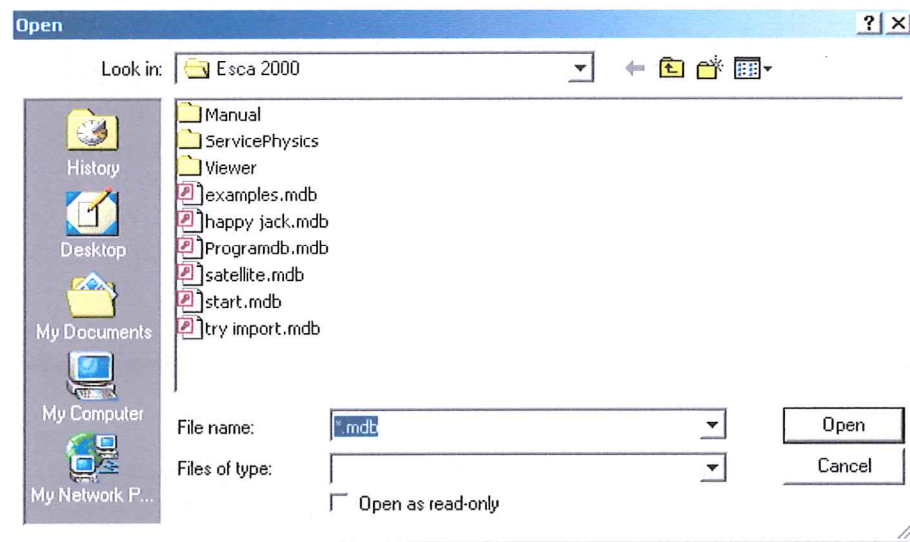
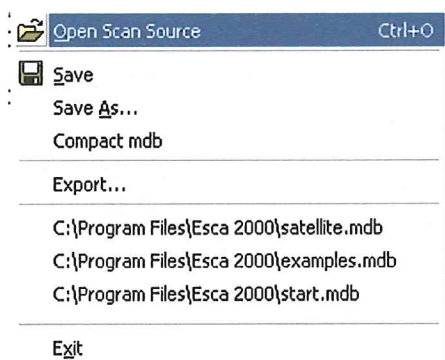
Save as type:

Enter the file name for the Excel spreadsheet you want to create and click Save.

Open Excel and open the file. The full spreadsheet for all three tables will be presented. Field for all parameters of the collected and reduced data are presented. The formulas that are used to compute field of derived data are imbedded so the spreadsheet is functional.

1	CFI	Inc	XPS	BE	Sb	Chen	Adj'ed	Area	Norm	AFVHH	Sen	Group	Aton %	Src	Ex	Ev	Dwell	Det	Sca	Exp	Accum	Cross
2	8	N		2.25	0.0	25.020	635		3.2967		1.653			1486.6	400	200.000	21.975	1	70	10.9877	-	999
3	7	Y	Zn 3p	2.25	3.647	90.647	563	16.32	1.4157	3.14	1.465		.819	1486.6	400	200.000	21.975	1	70	10.9877	2.828	
4	6	Y	Si 2p	2.25	4.531	103.531	2240	226.18	2.7043	.90	5.830		11.359	1486.6	400	200.000	21.975	1	70	10.9877	0.817	
5	5	N		2.25	0.0	154.609	2399		3.3709		6.243			1486.6	400	200.000	21.975	1	70	10.9877	-	999
6	4	Y	C 1s	2.25	-0.003	284.597	10699	991.92	3.5037	1.00	28.364		49.813	1486.6	400	200.000	21.975	1	70	10.9877	-	1
7	3	Y	Ca 2p	2.25	1.187	348.187	1959	36.53	2.7567	4.88	5.098		1.834	1486.6	400	200.000	21.975	1	70	10.9877	-	5.07
8	2	Y	O 1s	2.25	0.407	532.407	19730	720.34	3.4449	2.49	51.347		36.175	1486.6	400	200.000	21.975	1	70	10.9877	-	2.93

## File menu - Open Source



The (**Open Scan Source**) menu brings up a very general dialog that let you find a database any where on the host computer or network. Select an ESCA 2000 data base and click the (**Open**) button.

## File menu – Save and Save As

The (**Save**) and (**Save As**) operations store the Spectra, Composition Tables, Peak Fits and Annotations into the Database as documents. The named documents have links back to the raw data. A list of raw spectra and Analysis documents are displayed in the tree view in the upper left corner of the program display.

An Analysis document can be re-loaded and edited. The edited document can be saved back to the database or saved as a new document using (**Save As**).

## File menu – Back up

If backup is used a copy of the database is stored in a location of your choice. The default name is “original name.mdb.bak”. To use the backup database remove the .bak suffix. Then open the database with the Open Scan Source menu item.

When attempting to remove the .bak suffix be sure the original database is not in the same folder. Windows will not let you have two files with the same name in one folder. Rename the original file by adding a suffix .bad or some other name before you restore the backup file.

## File menu – Compact Database

As the database is used space is reserved to accommodate many possible inputs. Most of this space is never used. The compact operation is a house cleaning operation performed by the Access database engine. This does not change the form of the data stored in the database. The database does not need to be unpacked to use. The only downside of compacting the database is it must not be in use by any application.

The Analysis and Capture Applications attempt to compact the database when it is selected but before it is loaded. If the selected database is already open by any other program, including Import from Dos, then it just goes ahead and loads. If the database is never closed and reopened then it will not be compacted. Either of these cases can lead to bloating of the database.

**It is important to compact the database on a routine basis or it will get very large. Depth profiles can cause the database to get very large fast. If the database exceeds about 2 G bytes then Access fails. Some users have suffered crashed program operation.**

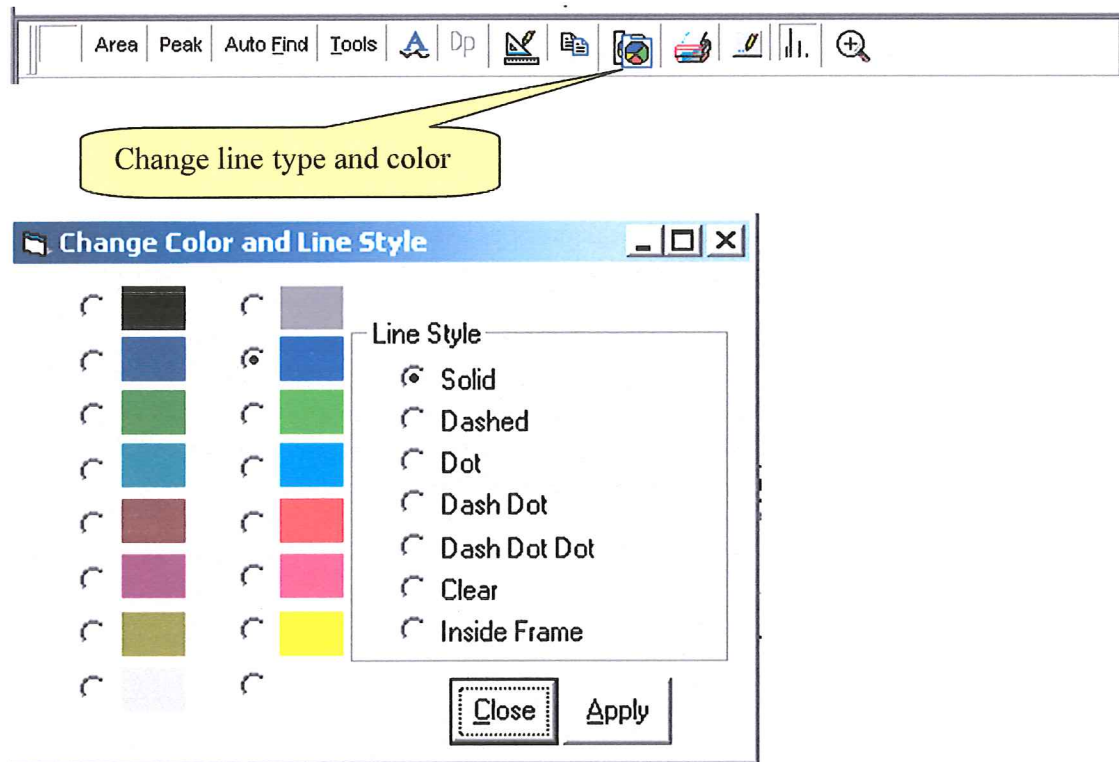
Choose one of two procedures. Have all users who have access to the same copy of one database close down all their ESCA 2000 programs. While all programs are closed start up one copy of either the Analysis or Capture program and load the database to be compacted.

If only one computer has access to a database then close all but one application. For example if the computer is running the ESCA then close down the Analysis Application and the Import Application. Then select the (**Compact database**) item in the File menu. The same idea can be used with a stand alone data reduction computer.

## File menu - Export

See previous section on Export to Vamas and Excel.

## Manipulating Spectra - Change line type and color



To change color of the line use to plot the spectrum:

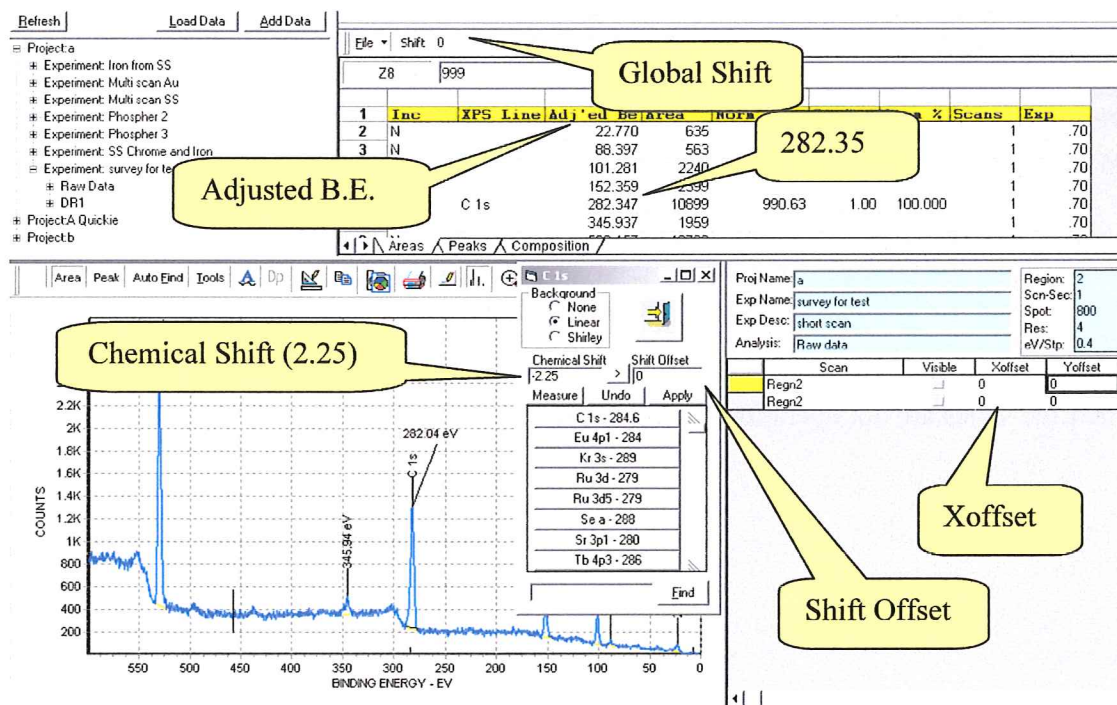
1. Select the region from the Region List. This will establish the active spectrum.
3. Open the Change Color and Line Style dialog.
4. Click the button to the left of the desired color.
5. Click Apply

The Line styles are not operational in this release.

## Manipulating Spectra - Charging Spectra - Shift

There are three controls that effect the position of the spectra on the graph.

1. The Composition Table Toolbar has a **(Shift)** window that provides a Global Shift for all regions listed in the Region List.
2. The Area Edit and Peak Edit dialog has a set of controls that show the chemical shift for a selected peak compared to the typical value listed in the Scofield table. The displayed chemical shift can be set to zero by shifting the spectrum. This allows the selected peak to become the reference peak for the entire spectrum. By clicking the (>) button to zero out the chemical shift a shift offset is applied to the spectrum and entered in to the Global Shift for the composition table. This Peak referencing then applies to all regions in the Region List. All entries in the adjusted Binding Energies column, of the composition table, are adjusted by this shift offset.
3. The Region List has a column named Xoffset. This column shifts the display of the spectrum but has no effect on the Binding Energy values recorded in the table. This control is useful for offsetting overlays and restoring the displayed spectrum to it captured position with out disturbing the composition table.



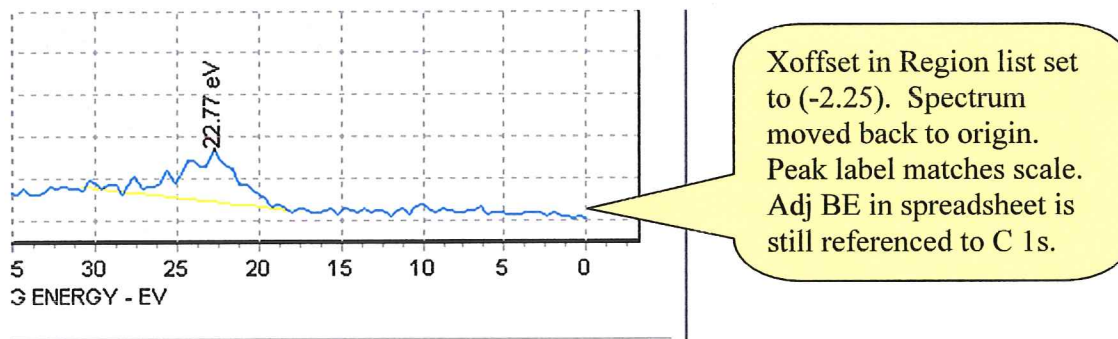
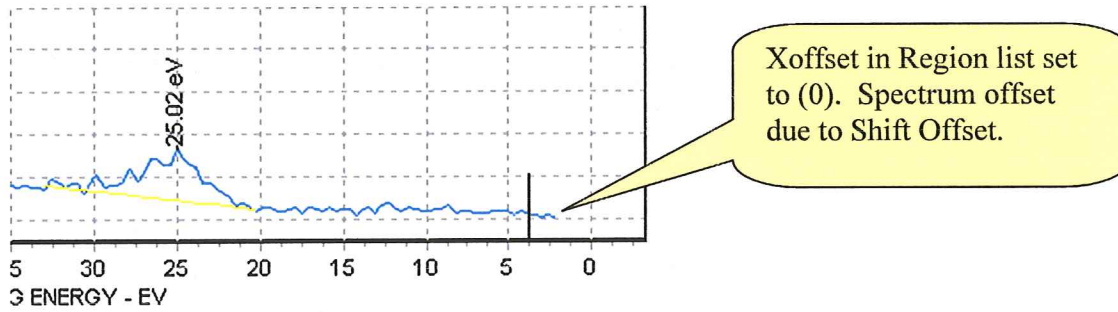
# Manipulating Spectra - Charging Spectra – Shift - cont

The screenshot shows the software interface with a spreadsheet at the top and a plot below. The spreadsheet has columns: Line, Adj'd Be, Area, Norm Area, Sen'y, Atom %, Scans, Exp. A callout bubble points to the value 284.6 in the 'Adj'd Be' column for Line 6.

Line	Adj'd Be	Area	Norm Area	Sen'y	Atom %	Scans	Exp
25	020	635				1	.70
90	647	563				1	.70
103	531	2240				1	.70
154	609	2399				1	.70
284	597	10899	991.92	1.00	100.000	1	.70
348	187	1959				1	.70

The plot shows 'COUNTS' vs 'BINDING ENERGY - EV'. A peak is labeled '284.6 eV'. A 'Reference Btn.' is highlighted in the 'Chemical Shift' menu. A callout bubble indicates 'Xoffset = 0' in the 'Region' list. Another callout bubble indicates 'Shift offset (2.25)' in the 'Shift Offset' field.

After clicking the Reference button the Global Shift is 2.25, the adjusted B.E. is 284.597 and the Shift Offset is 2.25. The Xoffset for the region is not affected.



## Manipulating Spectra - Tools Menu for manipulating spectra



The [Tools] button on the toolbar opens a tool kit for manipulation of spectra. The icons from left to right provide the following operations.

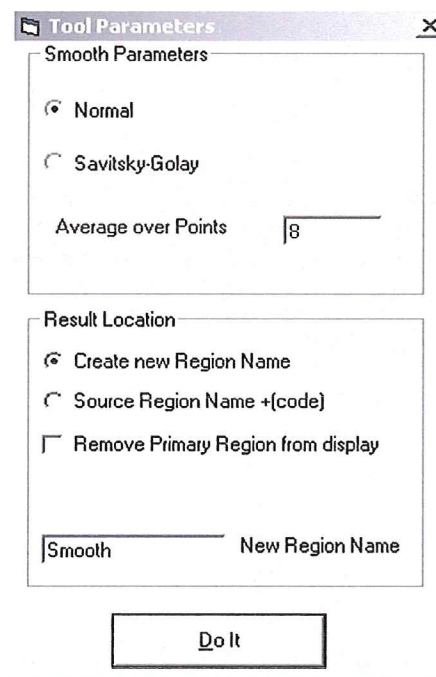
1. Add two spectra
2. Subtract one spectra from another
3. Smooth
4. Integrate
5. Differentiate
6. Subtract satellites

The [>DoIt] button puts the tool bar into an immediate action mode. With this button selected the conditions set for each of the tool icons will be used without review when the icon is clicked. This mode is useful when the tool will be applied to many spectra using exactly the same setup conditions.

The [w/Setup] button puts the tool bar into a mode that shows the setup dialog before the tool is applied to a spectrum. The setup dialogs have a lower section that is very similar for all tools. This section, called the Results Location, defines how the display of the Primary or Source spectrum and the resultant spectrum will be handled. It also defines the region naming protocol.

If the [Create new Region Name] button is selected then the [New Region Name] box will be open and you can enter a name of your choice.

If [Source Region Name + {code}] button is selected then the [New Region Name] box will be disabled and the program will append a code to the existing Region Name. Clicking the [Remove Primary Region from display] check box will cause the source spectrum to be replaced by the modified spectrum.





## Manipulating Spectra - Tools Menu for manipulating spectra –cont.

The [Do It] button at the bottom causes operation to be performed on the target spectrum.

The dialog is slightly different for the [Add] and [Subtract] tools.

The Primary Region is established by checking the [Visible] box for the region you want to subtract another spectrum from. The Secondary Region is established by activating the Region. Click on the region name in the Scan column of the Region List to activate. This spectrum will be subtracted from the Primary Region.

The option to Remove either or both the Primary or Secondary Regions is added to the Result Location operations.

	Scan	Visible
	Regn1	<input checked="" type="checkbox"/>
	Regn2	<input type="checkbox"/>

**Tool Parameters** [X]

Spectrum Alignment for Subtract Mode

The primary (red) spectrum is not changed. The secondary (green) spectrum will be shifted and/or scaled. The points marked with arrows will match after shift/scale. Before scale operation move vertical line to mark a second B.E. Adjusted spectra will match at pointer and line.

Shift Scale

Result Location

Create new Region Name

Source Region Name +(code)

Remove Primary Region from display

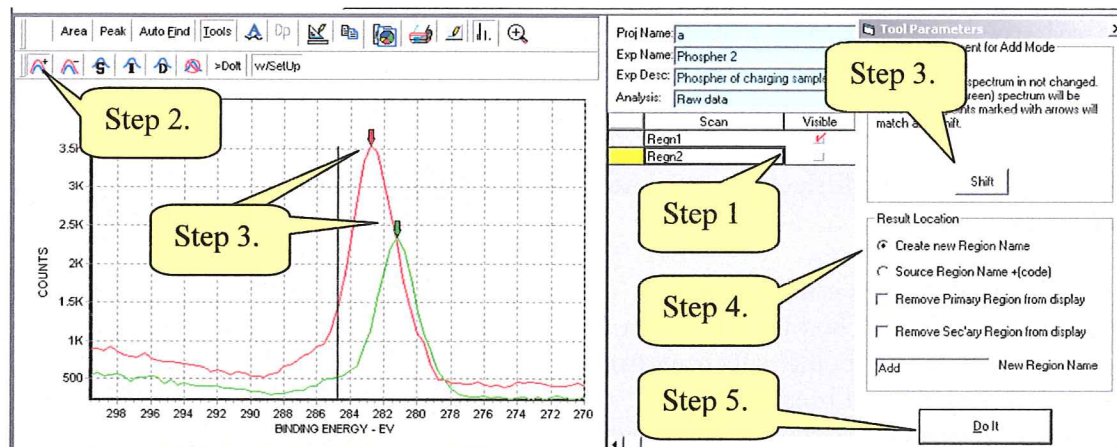
Remove Sec'ary Region from display

Sub \_\_\_\_\_ New Region Name

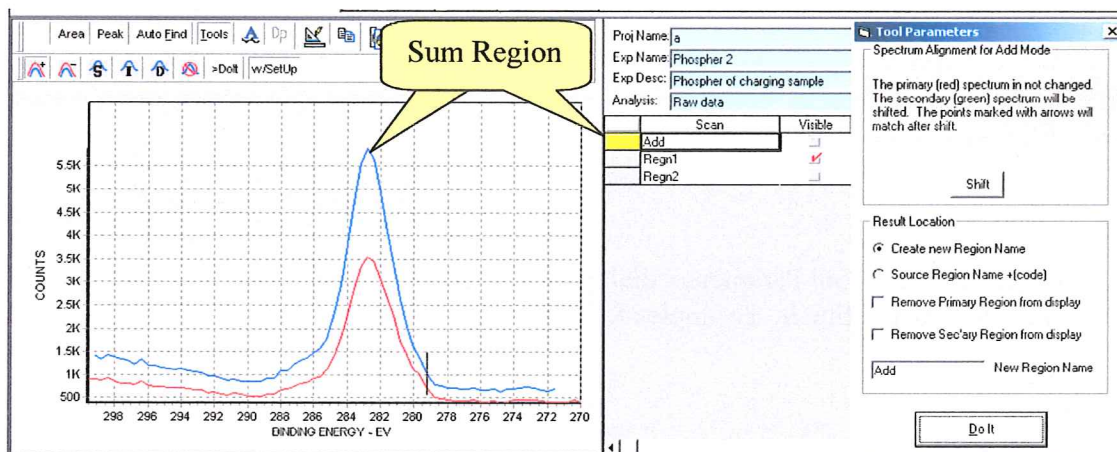
Do It

The top part of each Tool Parameters dialog describes the operation to be performed and the parameters that define it. Examples follow.

## Manipulating Spectra – Add two spectra

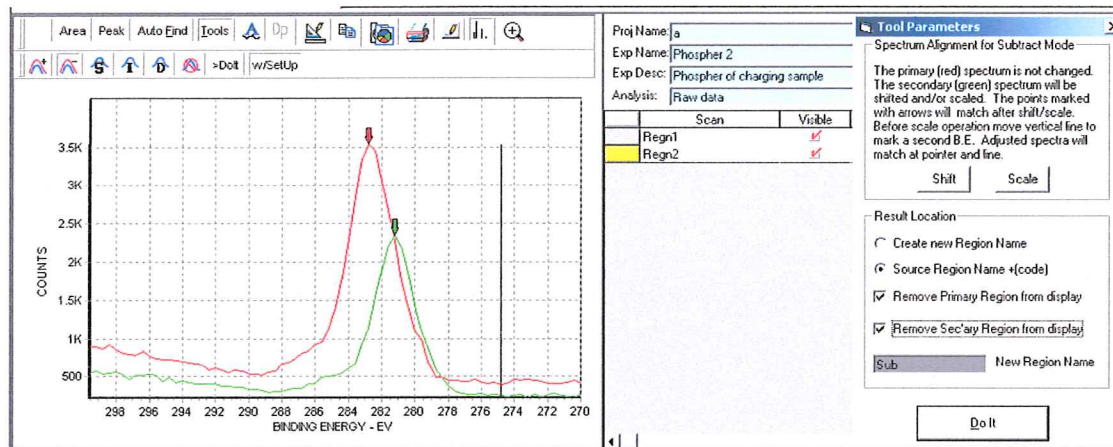


- Step 1. Check visible for Primary region and select Secondary region.
- Step 2. Click [Add] Icon
- Step 3. Shift spectra (Optional). Move arrows to mark alignment points. Click Shift.
- Step 4. Configure Result Location dialog.
- Step 5. Click [Do It]



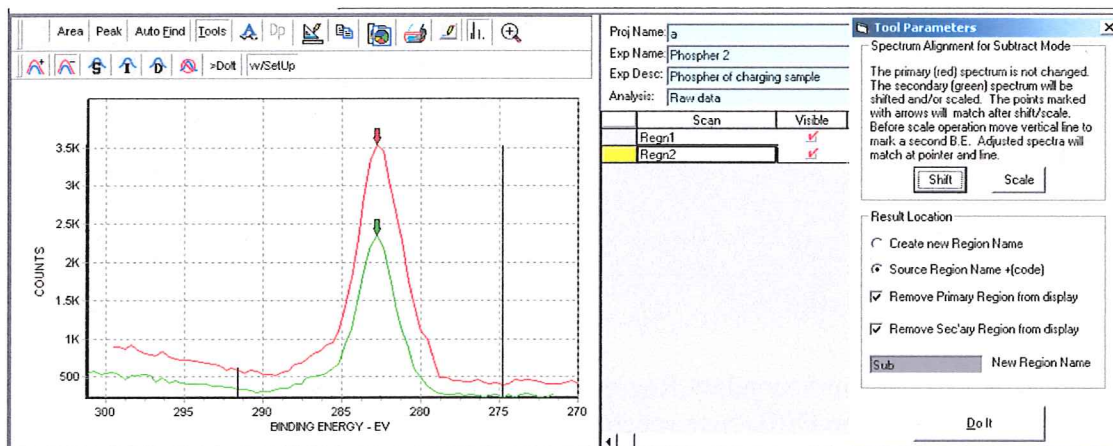
The Primary Spectrum is showing because the Visible box is checked. Both the Primary and Secondary spectra are still listed in the Region list.

## Manipulating Spectra – Subtract two spectra



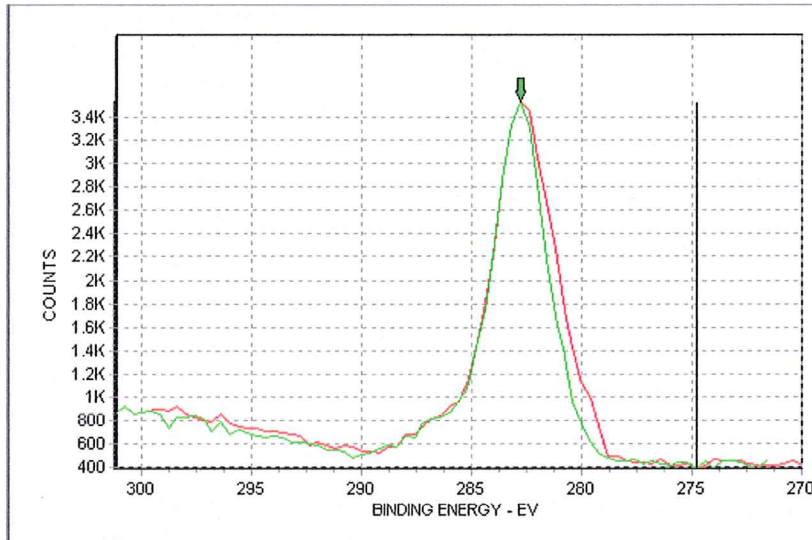
The steps are the same to set up the Subtract and Add spectra tools. The Subtract tool has the additional ability to scale the Secondary spectra to the Primary spectra. The above figure shows the display after moving the pointers to the alignment points on the two spectra. The long vertical line is used to establish a third point, along the background, where the two spectra will be matched.

To match the two spectra first [Shift] the spectra to align the points marked by the green and red arrows. This step is optional.

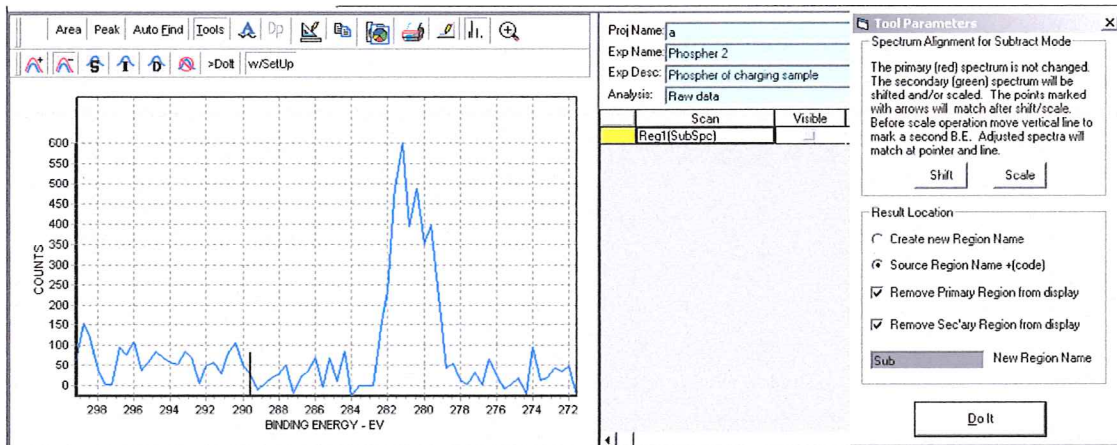


Next the scaling operation will match the spectra at the points marked by the arrows and at the point marked by the vertical line. This involves both a scale and Y offset operation. If the Vertical line is moved to the same location as the arrows then the Secondary peak will simply be scaled up. The background will not offset to match.

## Manipulating Spectra – Subtract two spectra -cont



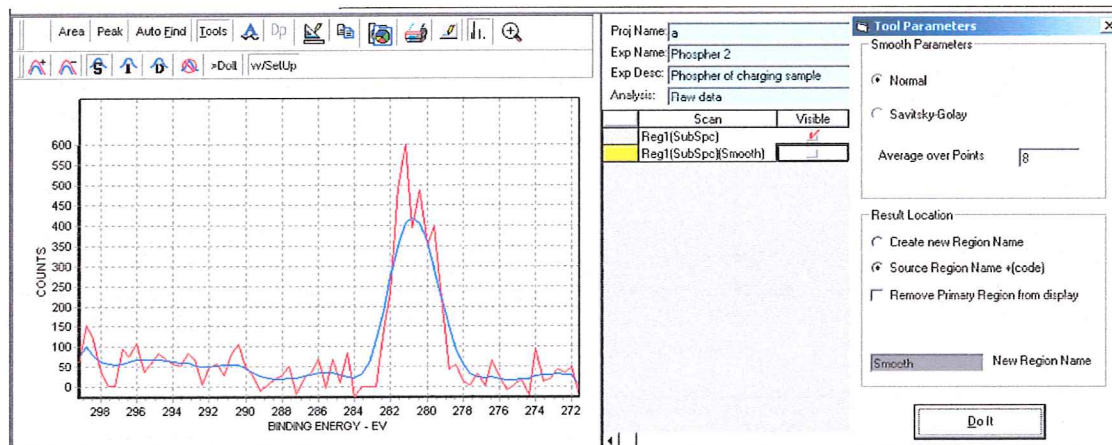
After the [Scale] button is clicked the difference between is noticeable at the right side of the spectra.



The Primary Region and Secondary Region are removed both removed from the region list and the display. The Difference spectrum is displayed and is listed as `Reg1{SubSpc}`.

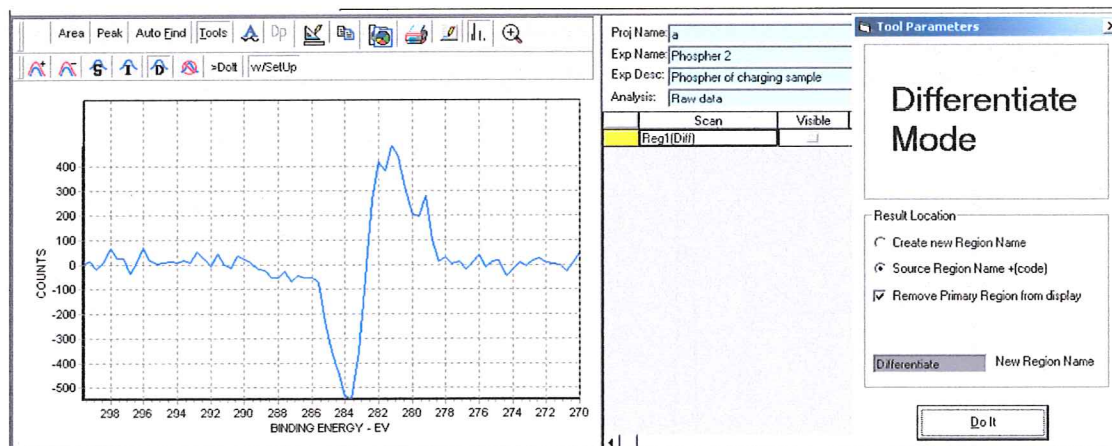
The difference spectrum can now be operated on by any of the tools including peak fitting and area measurement. In the next section we will smooth the peak.

## Manipulating Spectra – Smooth, Integrate and Differentiate



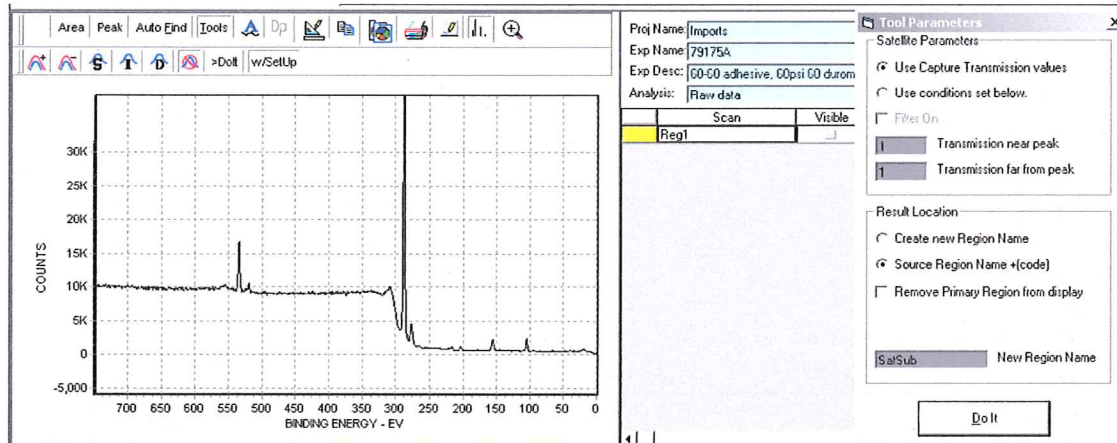
In this example we used an 8 point, Normal smooth. The result was saved by appending the code {smooth} so the Region name is now Regn1 {SubSpc}{Smooth}. Source was left in the Region List. The Source was made visible after the smooth operation so we could compare it with the smoothed spectrum.

This approach of appending the code to the current Region name provides the history of operations to be encoded onto the region name.



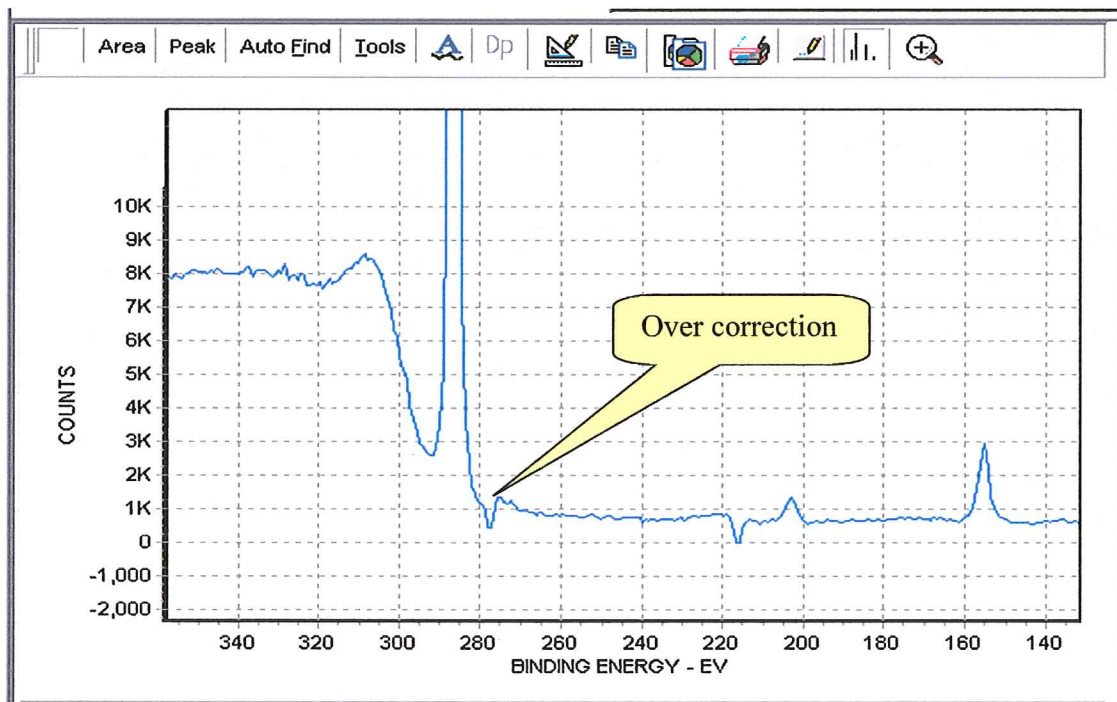
The integrate and differentiate modes work the same way. Neither operation has additional parameters.

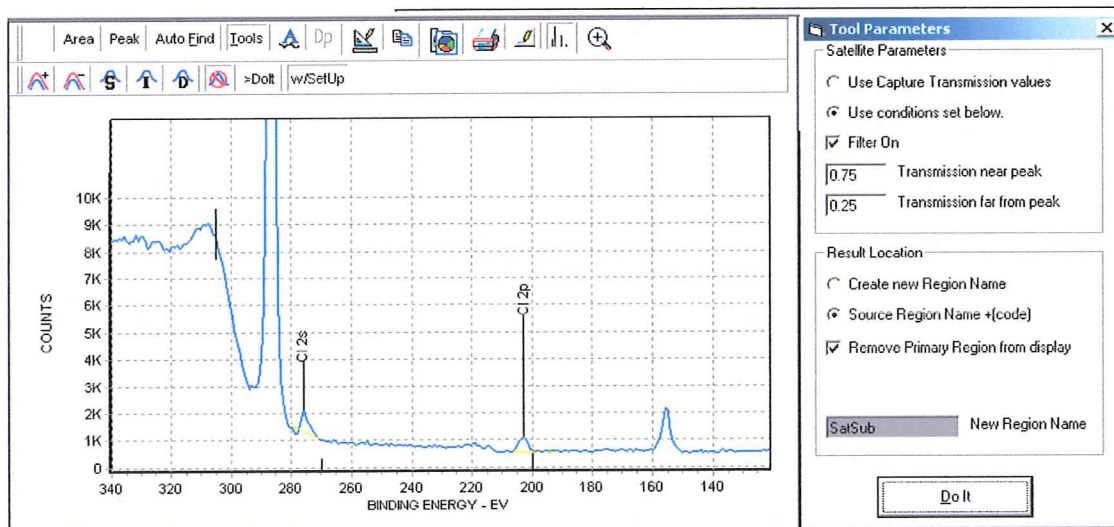
## Manipulating Spectra – Satellite Subtract



The parameter section of the Satellite Subtract allows for use of the satellite parameters stored with the spectra or if non are stored the full strength of the satellite peaks will be used. If adjustment of the Satellite peak strength is desired then the filter can be turned on a new values can be established. These values are stored until new numbers are entered in the dialog box.

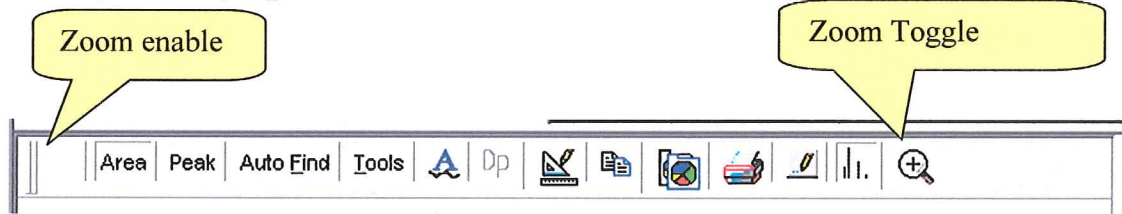
The first example is to use the existing parameters. In this case the parameters described full strength satellite peaks.





The over correction has been minimized and the Cl 2s peak remains.

## Manipulating Spectra - Zoom and Pan



The (**Zoom Toggle**) icon provides a toggle between displaying the full spectrum and the expanded spectrum. To zoom in on a region of the spectrum follow the directions that follow.

### ZOOM

A zoom box can be defined using the mouse.

Click and hold the left mouse button at the upper left corner of the area to be expanded.

Drag the mouse to the lower right direction until the area of interest is enclosed.

Releasing the left mouse button now displays the expanded area.

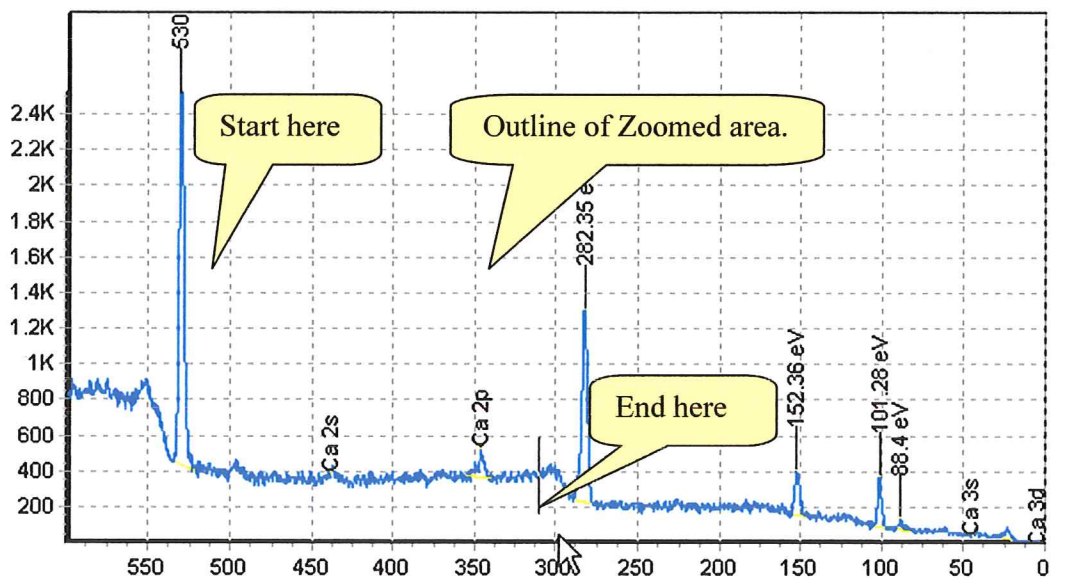
The Zoom action can be repeated.

To reverse the Zoom left click and hold. Draw any size box from lower right to upper left. When the mouse button is released the display will return to the initial state.

The Zoom window can be moved along the spectrum in the X and Y directions.

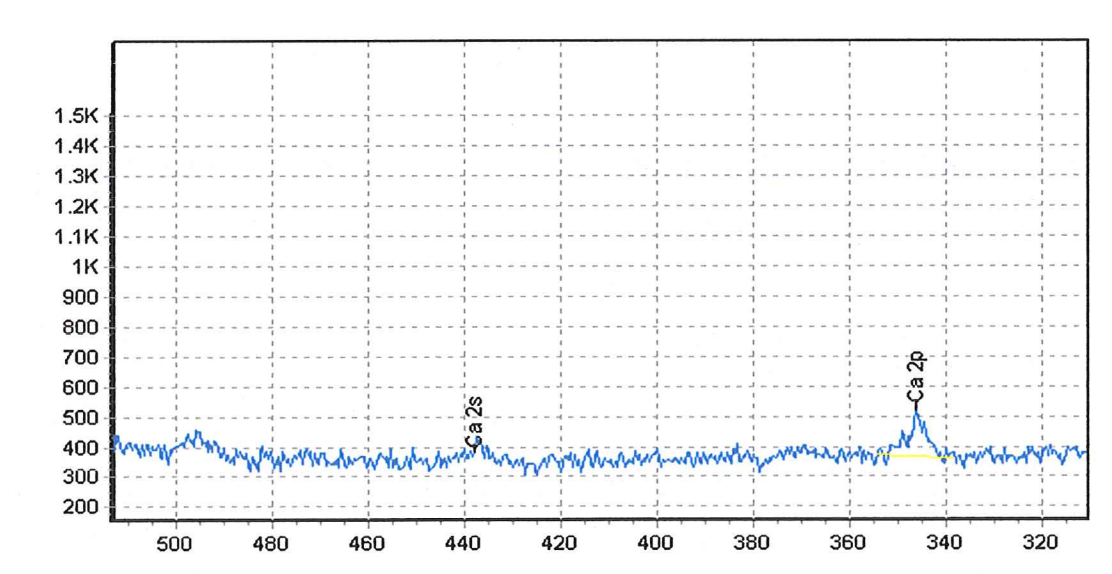
Depress the right mouse button and drag the window to the new location.

This provides a convenient way to scan along a spectrum looking for small features.





After zoom



The (**Zoom enable**) icon can be used to restore the zoom function if it becomes disabled.

If you are using a mouse with a “page up/page down” wheel between the right and left mouse buttons this function will step the spectrum up and down within the graph. This is useful to set the minimum point of the spectrum on the X-axis. This produces the equivalent of a background-subtracted spectrum.

# PEAK FITTING

Click on Peak.

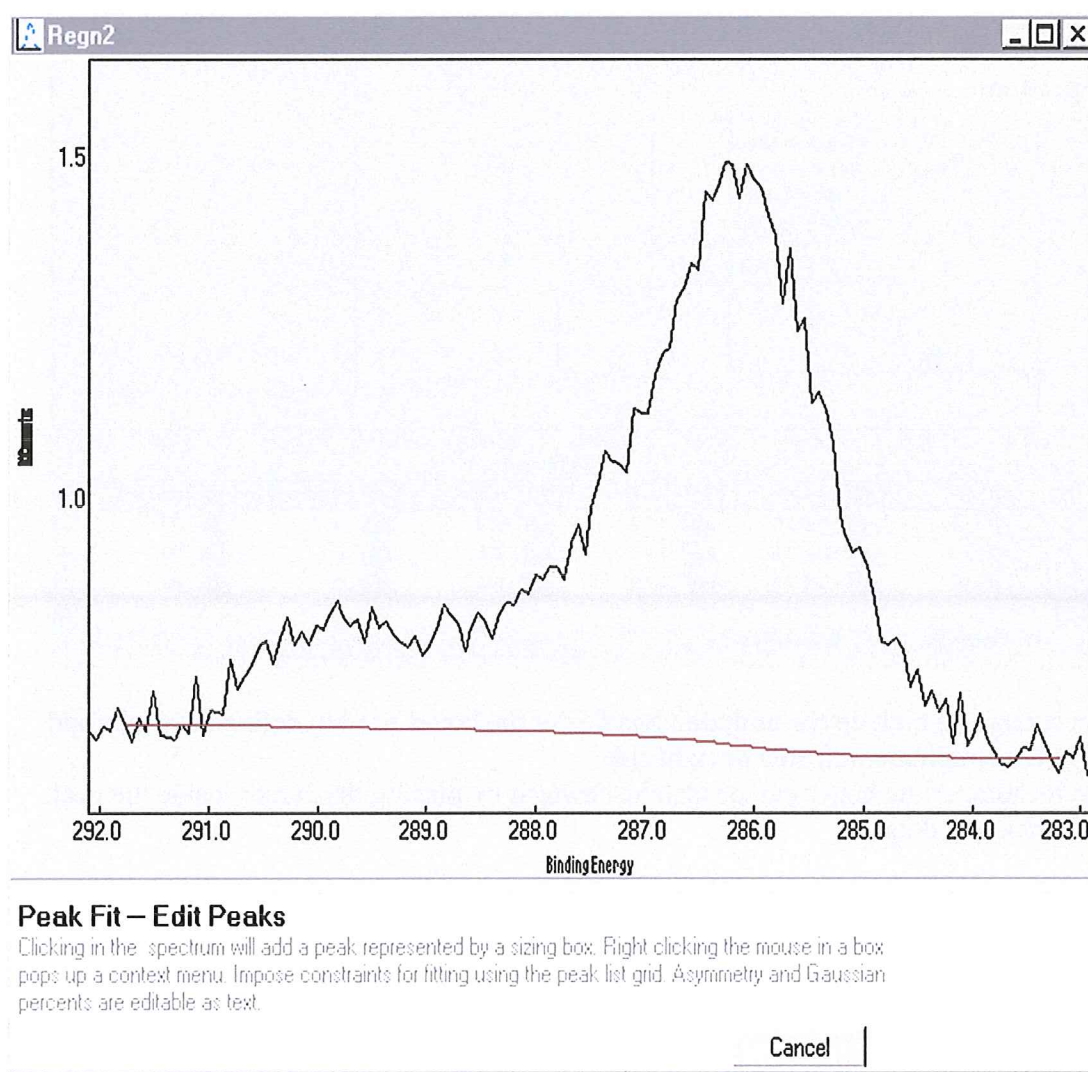
In the Measure Peak dialog box choose the appropriate background type, establish the background end points and then click on Measure.

The screenshot displays the 'Graphics Viewer' window with the following components:

- File Menu:** File, Print...
- Current Source File:** C:\Program Files\ESCAVB\data
- Project Information:** Proj: DAK, Regn: 2; Exper: Au on Fe + ??, CBE/LBE: 286/276; Recipe: Au, Width: 20; Func: HiRes, Ti/Scn: 10; Op: Administrator, Spot: 200
- Tree View:** A Quickie, DAK, Au Experiment Comment 01/18/2002, Au on Fe + ?? Experiment 01/18/2002
- Table:**

	Inc	XPS Line	Peak ID
1			
2			
- Background List:** Background, None, Linear, Shirley
- Measure Peak Dialog Box:** Measure, Undo, Apply, Chemical Shift, Shift Offset, Proj Name: DAK, Exp Name: Au or, Exp Desc: Exper, Regn1, Regn2, Regn3, Regn3, Pin Middle Position, End
- Spectrum Plot:** Y-axis: 600 to 1400; X-axis: 295.9 to 277.9
- Status Bar:** Idle, eV: 285.94, Counts: 1451, C 1s, Eu 4p1, Gd 4p1, Kr 3s, Ru 3d3, Se a, Tb 4p3, Th 5s

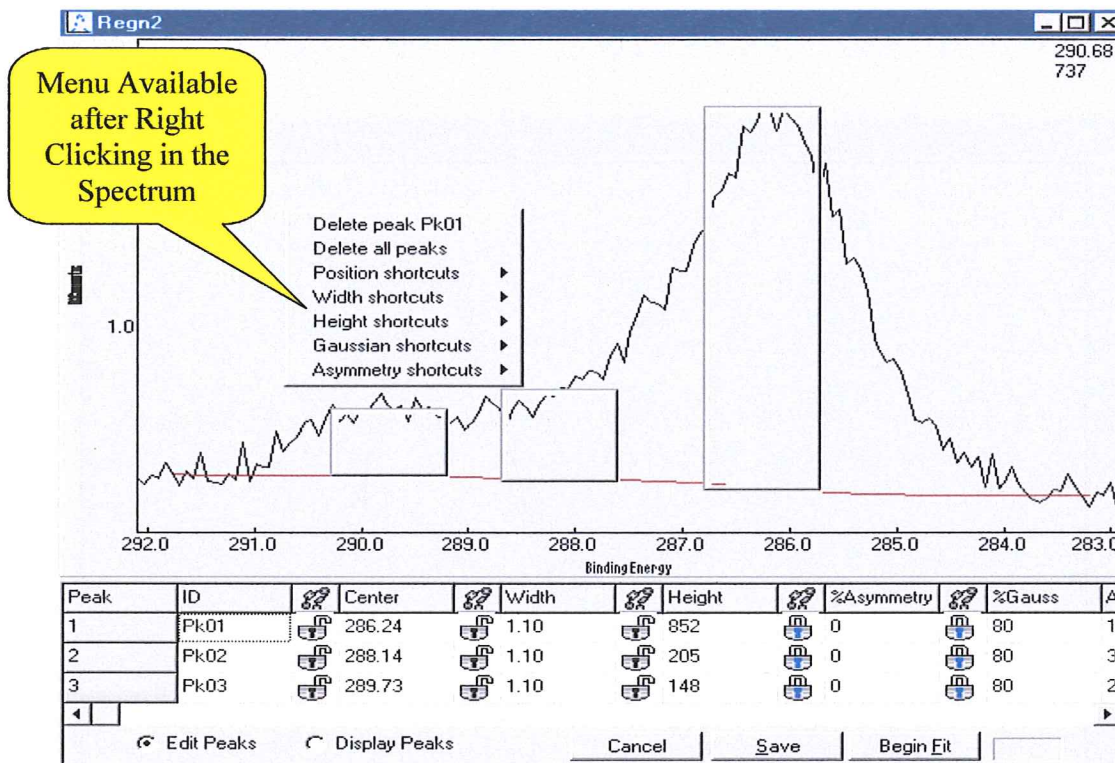
The **MEASURE** button will transfer that portion of the spectrum defined by the baseline endpoints to the Peak Fit Window.



Click near the center of each component peak. This will draw boxes that show the peak amplitude, center and a FWHM estimate.

A menu of the peak parameters appears below the spectrum window.

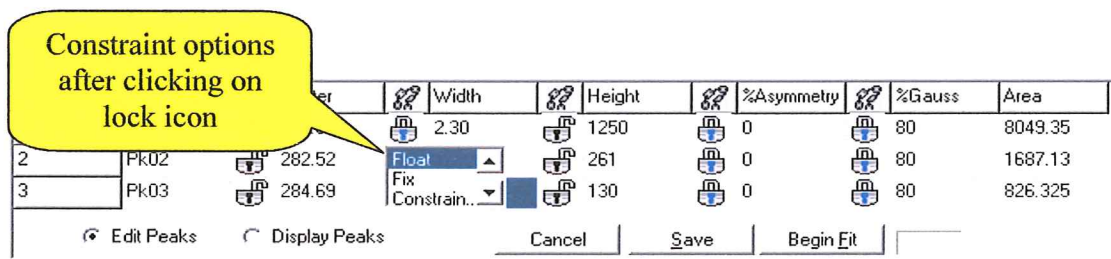
Right click the mouse for a menu of peak fitting controls and shortcuts.



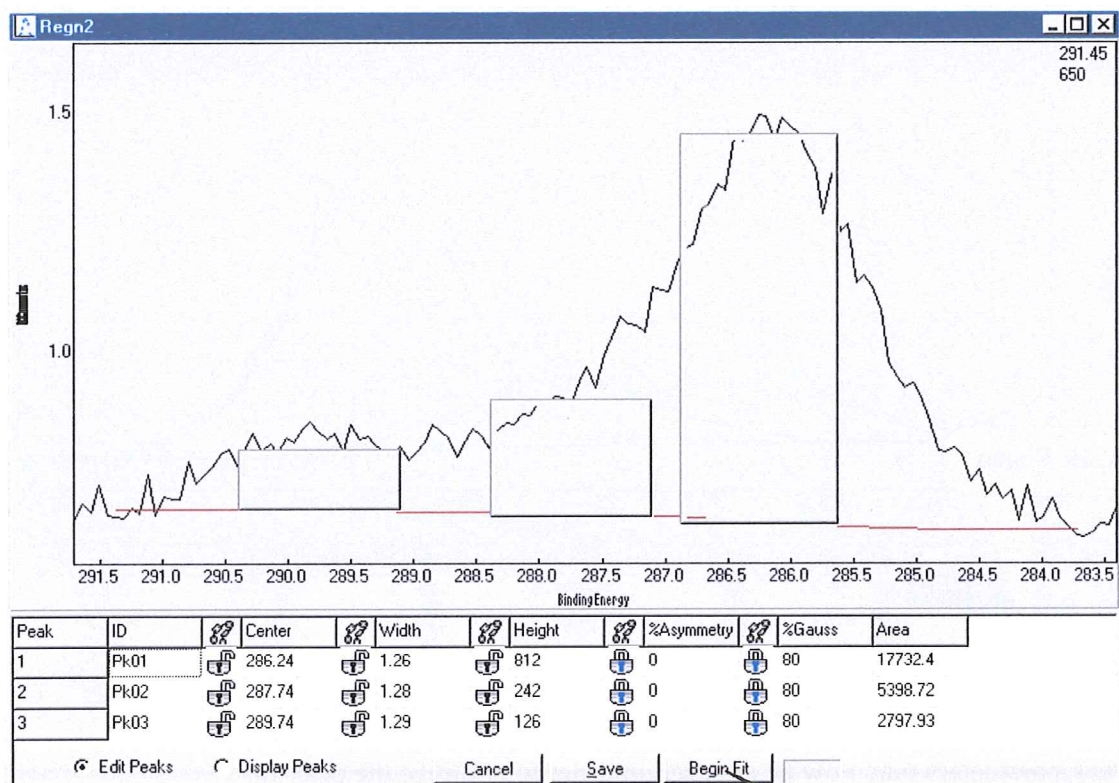
The cursor can pick up the midpoint handles of the boxes used to define the peaks and move the amplitude, left side or right side.

The location of the boxes can be also be changed by placing the cursor inside the peak then click and drag.

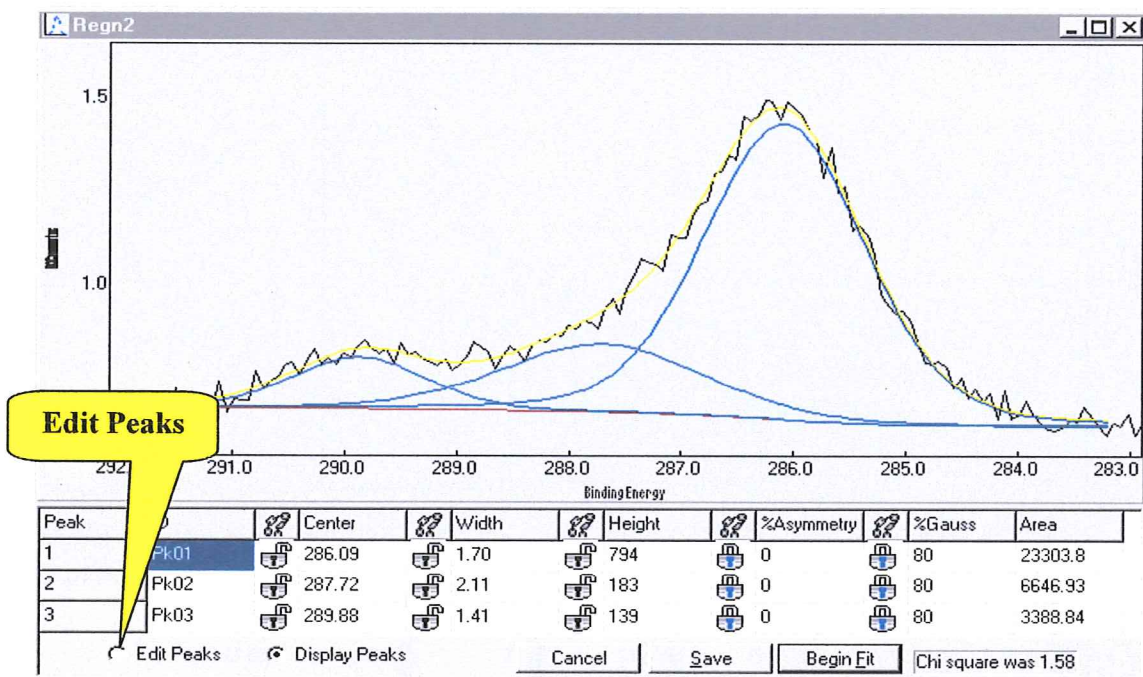
Peak parameters may be individually constrained and unconstrained by clicking on the “lock” icons left of the parameter value. This will also display a menu of constraint options.



Click on Begin Fit.



Begin Fit.

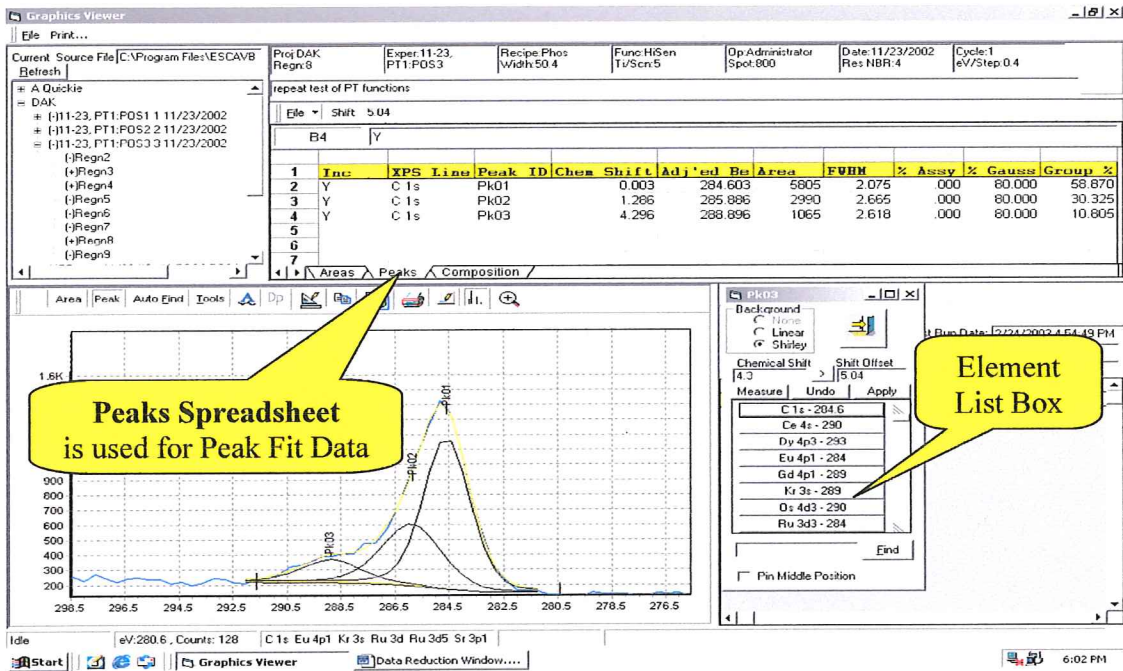


Peak parameters may now be adjusted in order to optimize the peak fit. Click on **Edit Peaks**, make necessary parameter changes, and again click on **Begin Fit**.

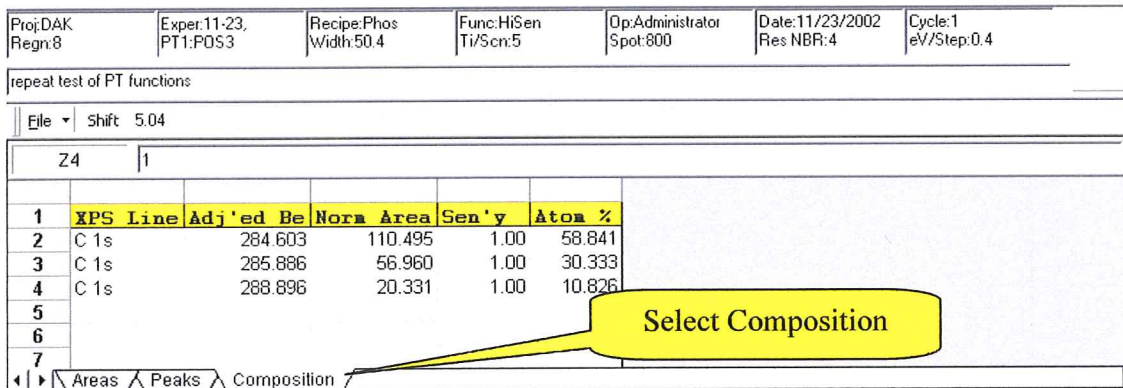
Upon completion of an acceptable peak fit click on the “Save” button. This will save the spectrum and show the component peaks in the **Spectrum Viewer**. “Save” also saves the peak parameters and displays them in the Peaks spreadsheet of the **Data Notebook**.

In order to make the peak fit area values available to the Composition spreadsheet in the **Data Notebook** use the **Element List** to label the peaks and Enter “Y” for each component peak in the Inc column.

**In order to make survey and/or peak areas available to the Composition spreadsheet assign the peaks in the XPS line column (use the element list box for assignment) and place “Y” into the “Inc” column of the appropriate rows of the “Areas” or Peaks” spreadsheets. Hit the “Enter” key.**



With Y entered for each C (1s) peak the peak compositions are now available in the Composition Table.



The REGION LIST in the **DOCUMENT CONTROL** window can be used to review the peak fit results. As various **REGIONS** are made active the spectrum will be shown in the **SPECTRUM VIEWER**, the peak fit curves will be overlaid on the raw data and the peak fit data will be displayed in the **PEAKS** sheet of the **DATA NOTEBOOK**.

Move the cursor near the bottom of the peak identifier until a hand icon appears.  
The **Change Annotation Properties** window will appear.

**Change Annotation Properties**

Caption:

Text Alignment:

Color:

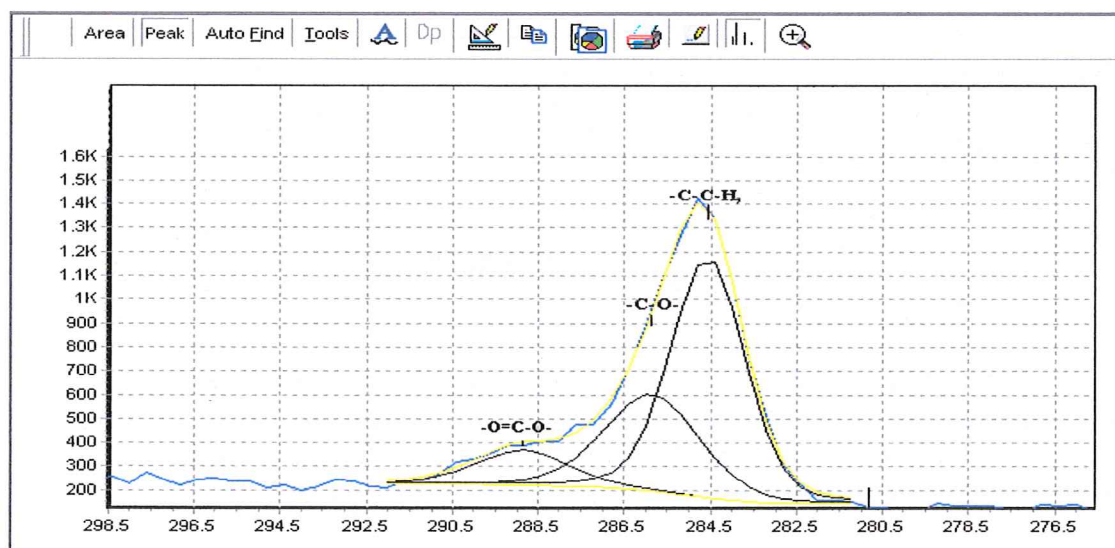
Angle:

Font:

Pitch:

Effects:

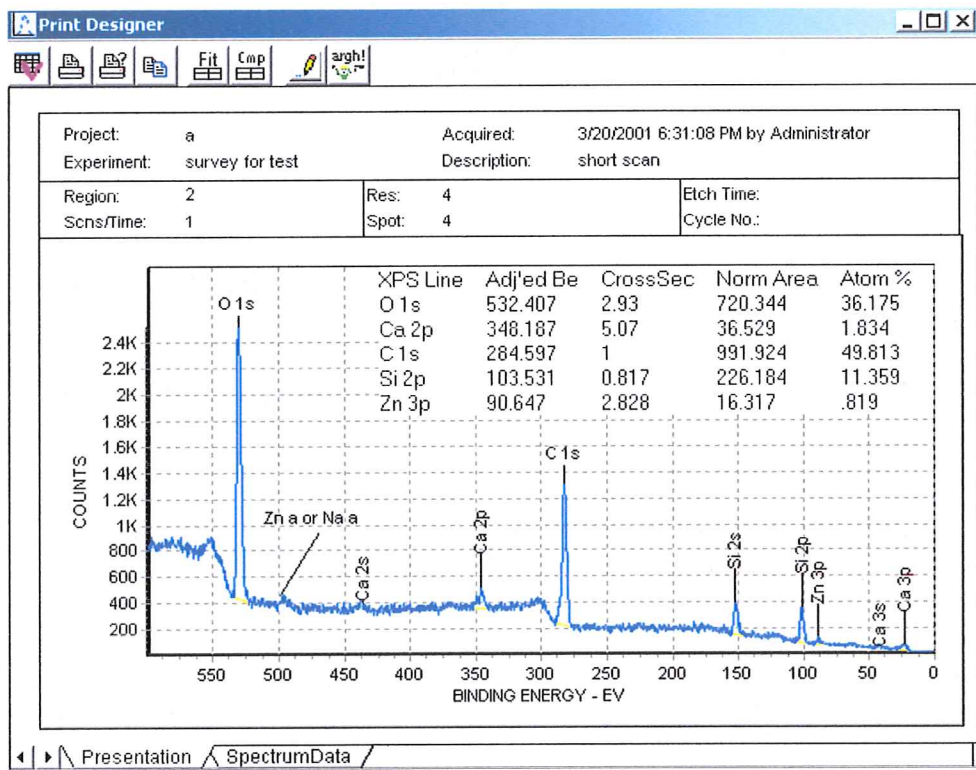
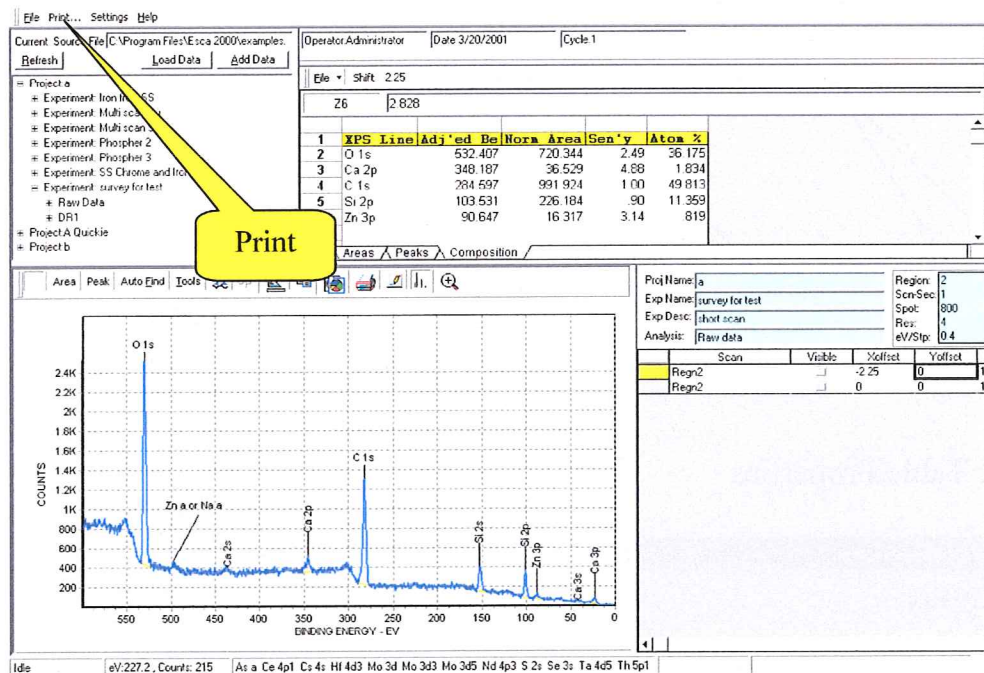
Use these tools to place captions or other labels onto the spectra.





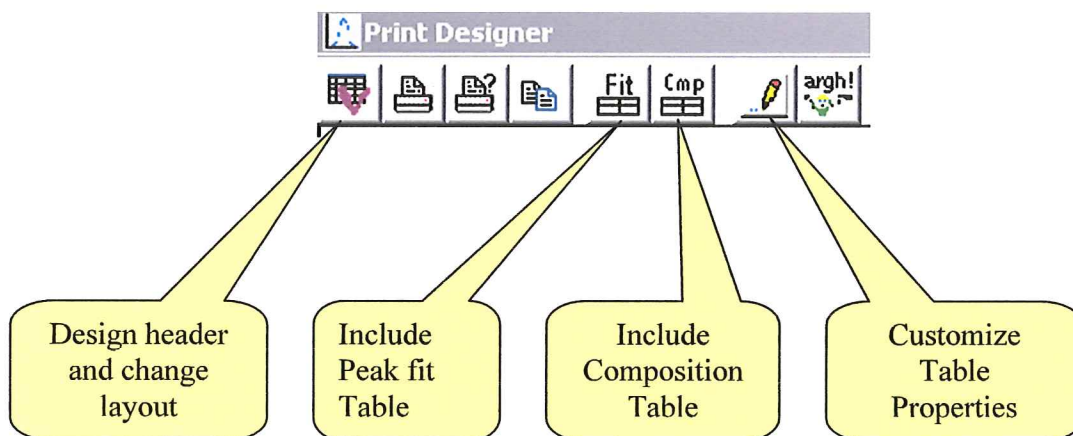
## Print and Paste operations

The **Print** command opens **Print Designer**, which offers a set of tools to enhance data presentation.

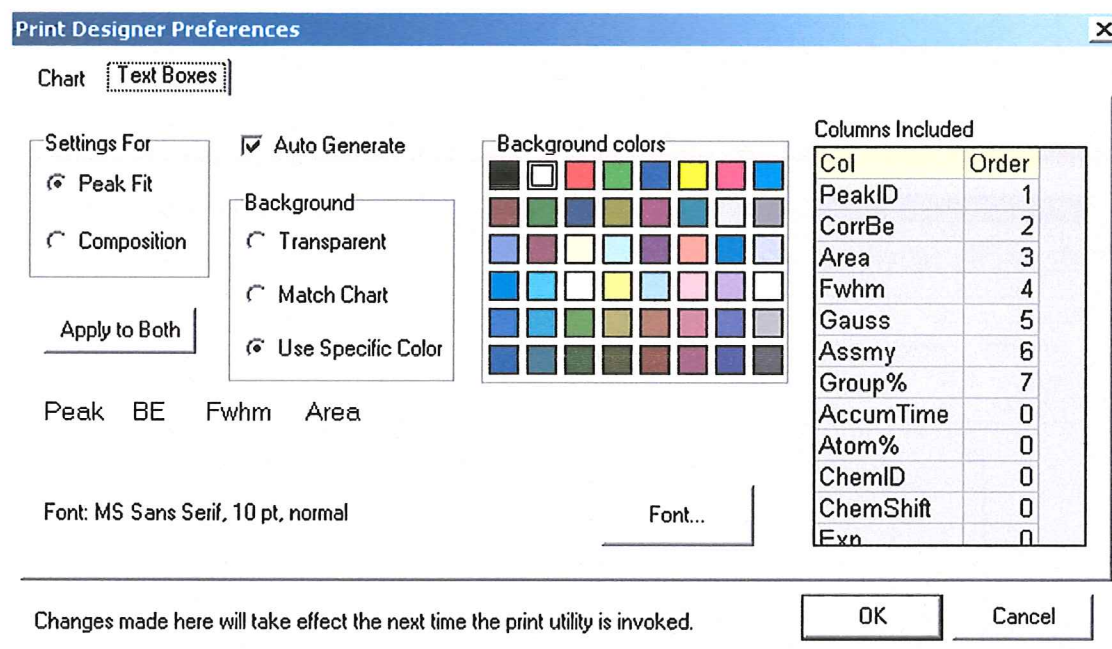


## Print and Paste operations – Print Designer

The **Print Designer** tool set.



## Customize Table Properties



**Settings For.** At the beginning of a session with the Print Designer Preferences you must select the Table that is being configured. Select either the Peak Fit or the Composition Table.

**Auto Generate.** Check the box to include a table when the Print Designer is opened. The table selected depends on the table showing in the Analysis window when the Print

## Print and Paste operations – Customize Table Properties -cont

Designer is opened. If the Peak fit table is showing then it will be copied to the Print Designer. If either the Composition tables is showing then the it will be copied.

If the box is not checked the **(Include Peak fit)** or **(Include Comp)** icons can be used to copy one of the tables to the Print Designer. Again the table to be copied must be showing in the Analysis window.

**Background.** The background for the Comp Table or the Peak fit Table can be chosen from the color chart or set to match the spectrum background. The spectrum background is inherited from the Graphics Editor in the Analysis Window.

The transparent mode is not operational.

**Columns included.** This tool allows the selection of the parameters displayed in the Table and their order of display. Enter a <0> in the (Order) column to not display a parameter. If you set a parameter position to <0> it will remove the parameter and move all remaining parameters to the left. For the parameters you want to display enter an integer that represents the column display position for that parameter. If you enter a number that exist it will insert the parameter in that position and move all the remaining parameters to the right.

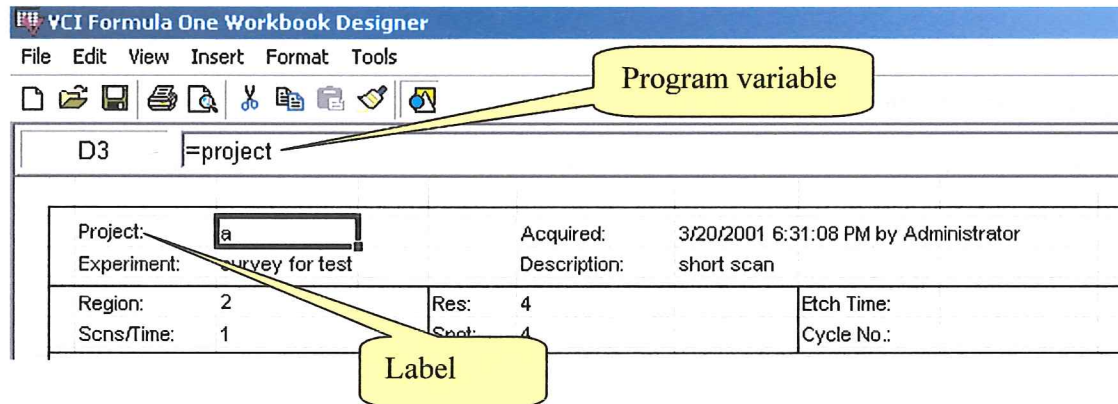
**Font.** The font tool provides the standard Windows font controls.

**Note:** After changes are made using the Customize Tables Properties dialog the Print Designer must be closed and then the Print button on the Toolbar of the Analysis Window must be clicked to show the Print Designer changes.

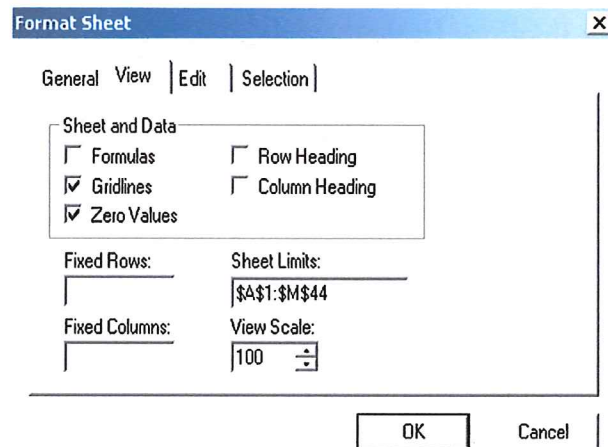
## Print and Paste operations - Design header and change layout

The Print Designer is built on a spreadsheet model. The full spreadsheet designer is available to compose the layout of the imported metafiles for the Spectrum and the Table. Cell programming is used to construct the header. Enter labels in cells and then imbed the corresponding program variables in the adjacent cell. Standard cell formatting is used to create the header cell borders and other enhancements.

Select the (Design header and change layout) icon to open the VCI Designer.

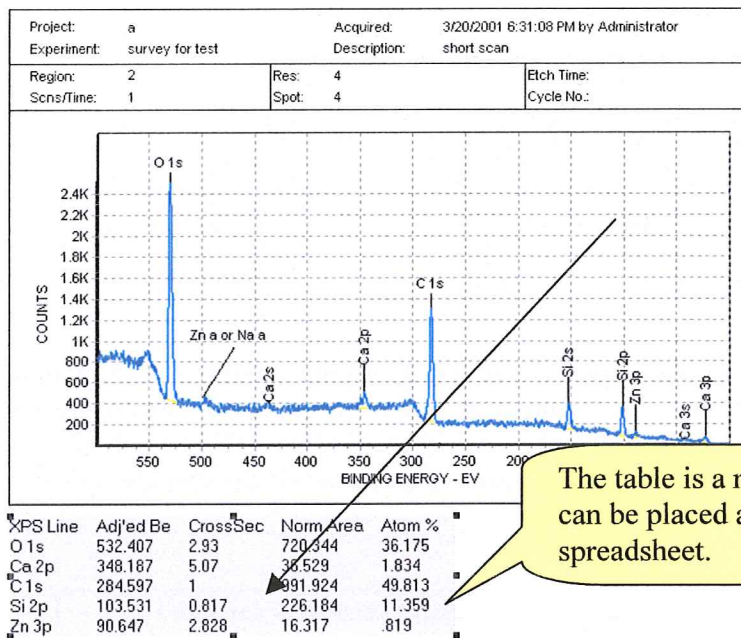


The grids are shown by opening the sheet formatting dialog and checking the Gridlines check box. After editing the header turn the gridlines off and exit the VCI Designer. To open the Format Sheet dialog select the Format menu > Sheet > Properties.



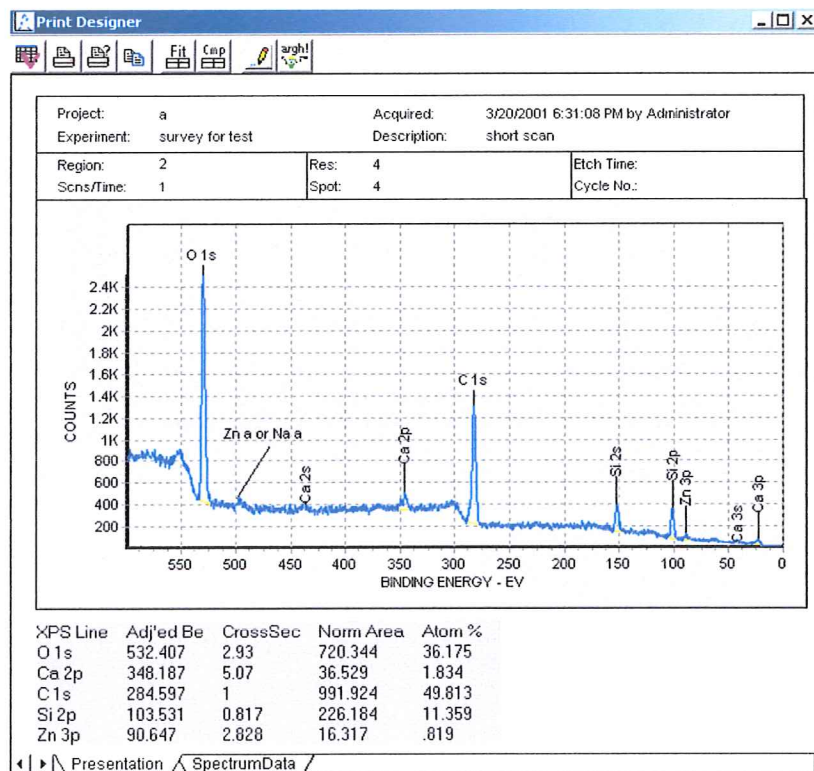
To print long tables the sheet limits need to be extended from \$44 to \$88.

## Print and Paste operations - Design header and change layout – cont.

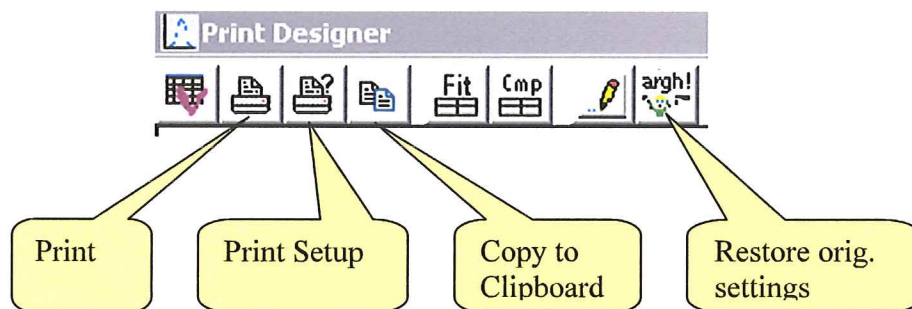


The table is a metafile object that can be placed any where on the spreadsheet.

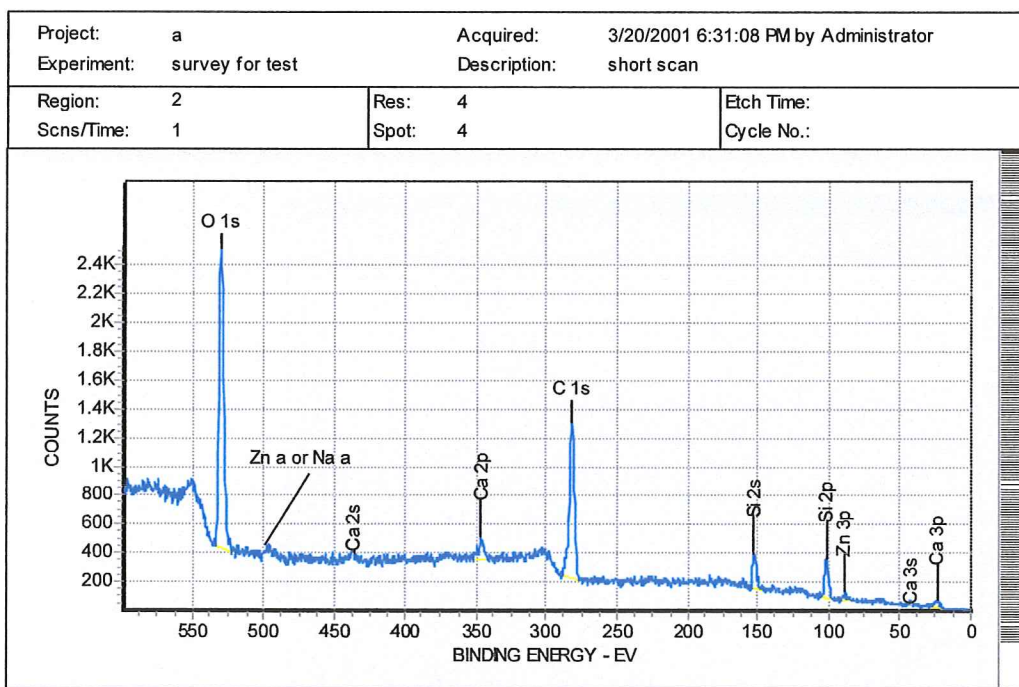
Close the VCI Designer and move the lower boarder of the Print designer window.



## Print and Paste operations – From Print Designer

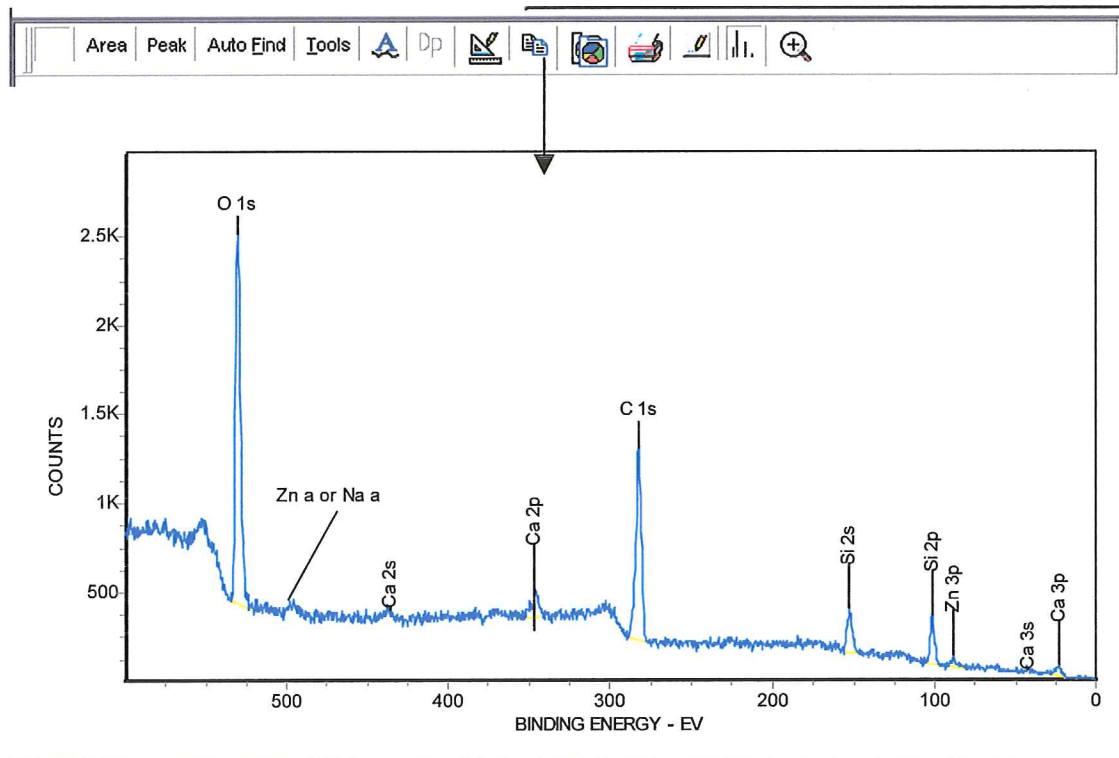


Before printing bring the bottom of the window up and the right side of the window in to leave a small white space around the part of the form you want to print or copy to the clipboard. The print object that is transferred is the size of the window. This object will be centered on and scaled to the page. Strange distortions take place if the window is left too large.



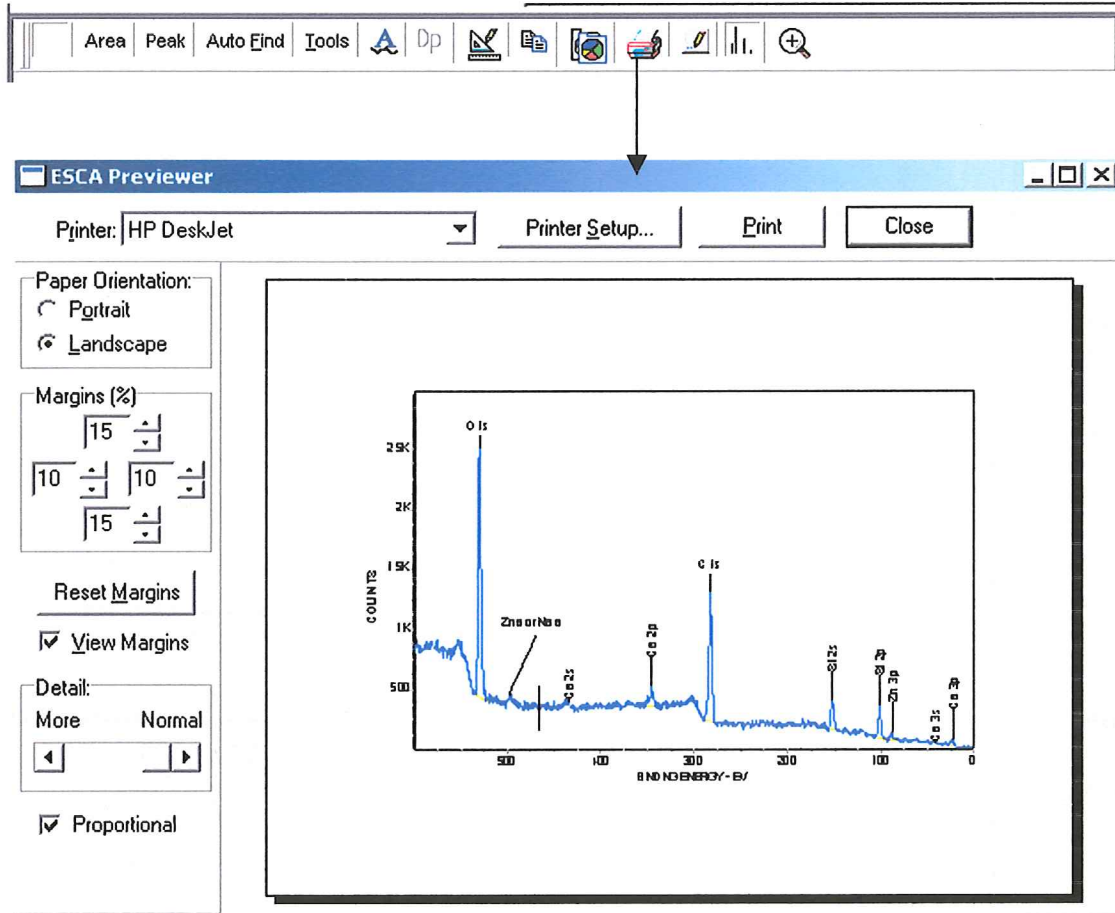
XPS Line	Adj'ed Be	CrossSec	Norm Area	Atom %
O 1s	532.407	2.93	720.344	36.175
Ca 2p	348.187	5.07	36.529	1.834
C 1s	284.597	1	991.924	49.813
Si 2p	103.531	0.817	226.184	11.359
Zn 3p	90.647	2.828	16.317	.819

## Print and Paste operations – Spectrum View Window - Clipboard



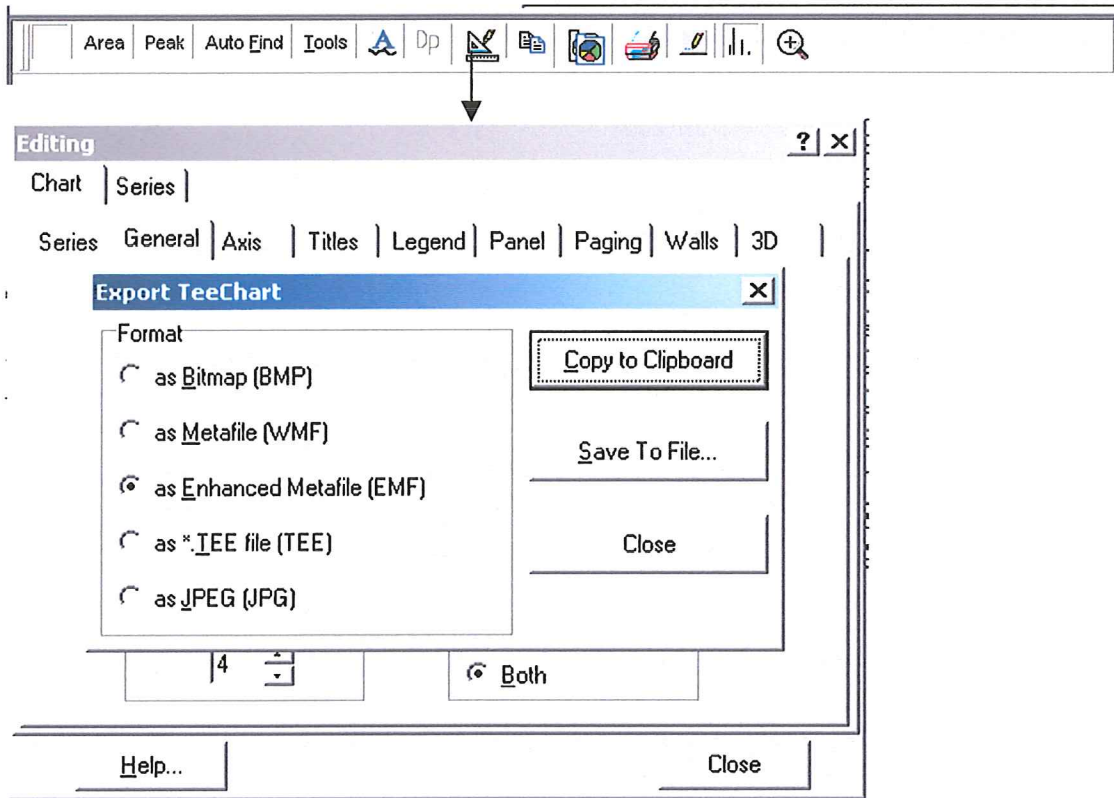
The above graph was copied to the clipboard and pasted into this word document. No scaling or readjustments were necessary.

# Print and Paste operations – Spectrum View Window – Print

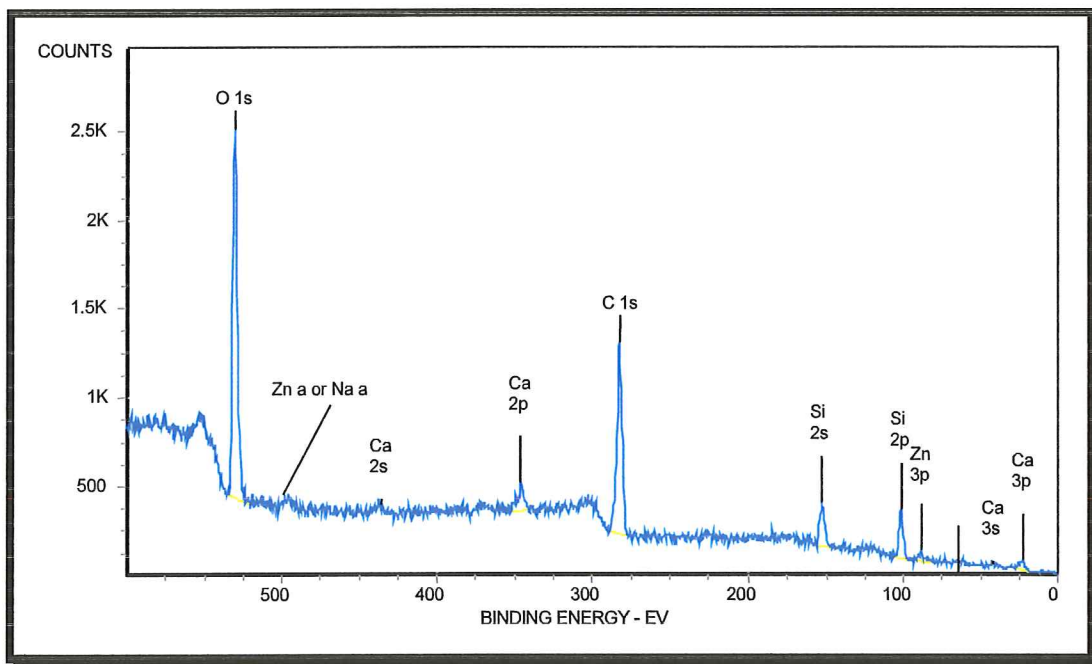


This print setup provides Portrait and Landscape print, margin control, printer selection and Printer setup for the selected printer.





The TeeChart Export tool in the Graphics Editor provides a wide range of export formats for the spectrum. The Enhanced Metafile provides a format that can be edited in Word, Power Point and Paint. The frame was added and the line labels formats changed.



## Print and Paste operations – Comp and Peak Tables

Operator: Administrator    Date: 3/20/2001    Cycle: 1

File    Shift 2.25

- Print Preview
- Print Setup...
- Save All

		Adj'ed Be	Norm Area	Sen'y	Aton %
2	O 1s	532.407	720.344	2.49	36.175
3	Ca 2p	348.187	36.529	4.88	1.834
4	C 1s	284.597	991.924	1.00	49.813
5	Si 2p	103.531	226.184	.90	11.359
6	Zn 3p	90.647	16.317	3.14	.819
7					

Areas    Peaks    Composition

Print Preview

Print...    Next Page    Prev Page    Close

YPS T	Adj'ed	Norm A	Sen'y	Aton
O 1s	532.407	720.344	2.49	36.175
Ca 2p	348.187	36.529	4.88	1.834
C 1s	284.597	991.924	1.00	49.813
Si 2p	103.531	226.184	.90	11.359
Zn 3p	90.647	16.317	3.14	.819

The print preview button, in the File menu of the Spreadsheet window, provides a print out of the table. The Area, Peaks and Composition Table will be previewed depending on which one is displayed.