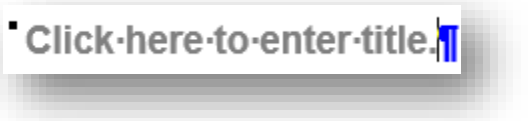
XPS/UPS Template Instructions

Guide to using this Template

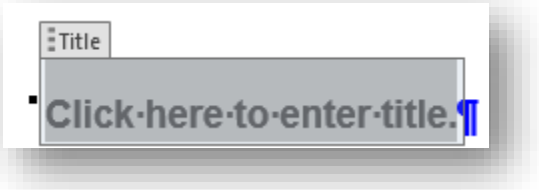
For ease-of-use, this template has been designed as a Microsoft Word form that when filled, will closely resemble a published ***Surface Science Spectra*** article. Authors are encouraged to consult published articles for additional guidance. The form consists of two types of fields: standard and drop down.

Standard Fields

To enter content into a standard field, click on the grey field instructive label.



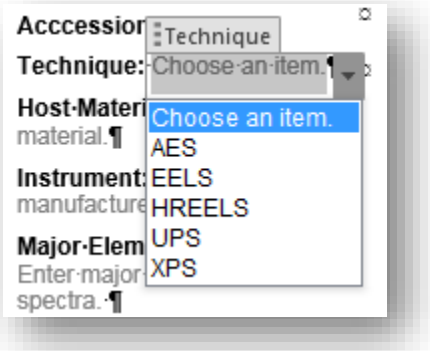
The field will open, and content can be added either by typing directly, or by copy/paste from another document.



Drop-down Fields:

To choose content from a drop-down field, click on the grey field instructive label.

The field will open, and content can be chosen from the menu by clicking on the appropriate item.



Figures:

A key feature of ***Surface Science Spectra*** is the uniformity of its figures. As such, *SSS* adheres to strict figure formatting guidelines (described below). Figure production templates are available for Origin and Excel. For more information of figure formatting, see Appendix A and B of this document.

Initial submission process: Authors may copy/paste (as a picture) spectra into the appropriate spectrum placeholder as indicated. Leave the "Accession #" label shown in the figure template as is during this phase. Unique accession numbers will be assigned to each specimen in the submission once the manuscript has been accepted. The accession number(s) will be sent to the authors to add to the final versions of the figures.

Final submission process: Authors need to send each figure (as a separate file) in one of the following formats: PostScript (.ps), Encapsulated PostScript (.eps), TIFF, JPG, or production-ready PDF. You can name each Figure file with a descriptive title such as Figure1, Figure 2, etc.

Instructions for Origin and Excel:

Font sizes:

1. Accession# label inside plot is **Arial 16 bold**.
2. Axis labels are Arial 14.
3. Tick labels are Arial 11.
4. Peak labels are Arial 11.

Plotting:

Templates are available for producing properly formatted *SSS* figure with Origin or Excel. Workbooks contain worksheets and plots for Survey and High-resolution spectra. Authors need only replace the existing (x, y) data with the data to be plotted. To add additional figures using Origin, create a new worksheet, right-click on the header of the appropriate spectrum type, select duplicate (batch plotting), select the new worksheet, press ok, and then add the data to be plotted to the new worksheet. To add additional figures using Excel, right-click on a bottom worksheet tab, select move or copy, choose the sheet of the appropriate spectrum type, click create a copy, press ok, and then replace the existing data in the new worksheet with the data to be plotted.

Labelling:

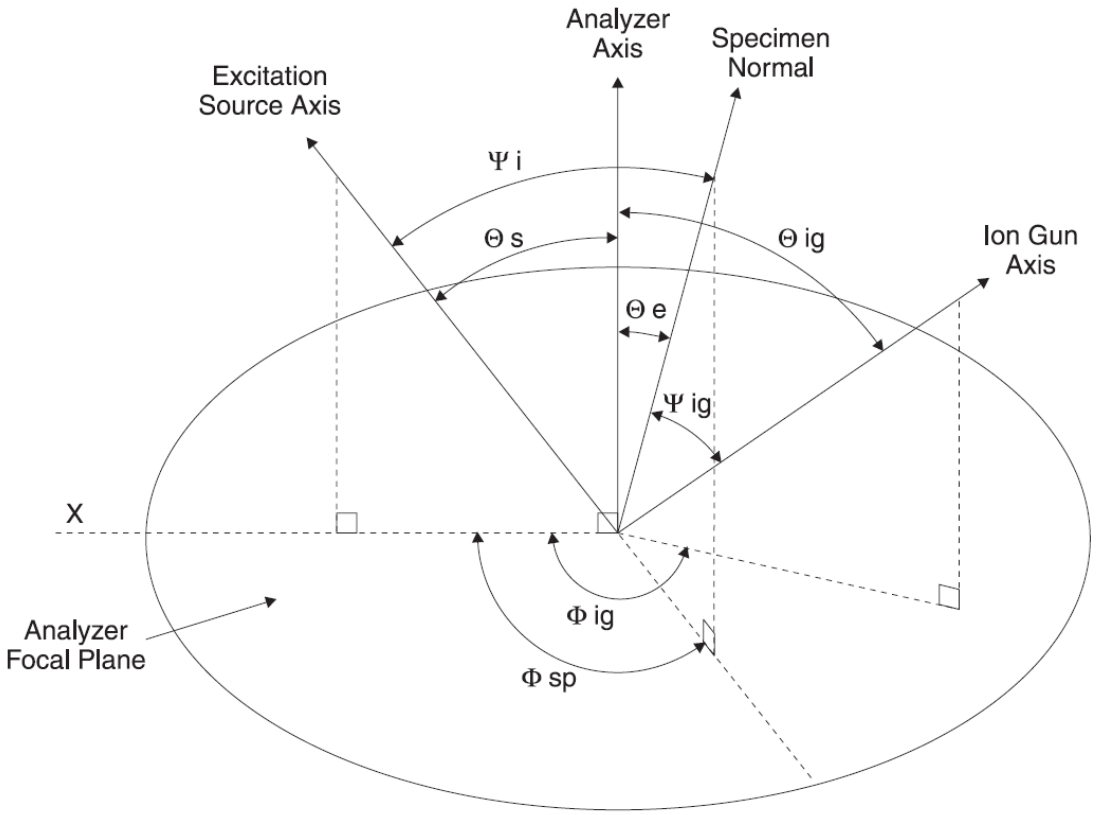
Additional labelling of the figures can be done directly using Origin. Additional labelling of the figures can be done using PowerPoint. To create figures for production, define the slide area as 8.5 x 11 portrait mode and then copy/paste each figure on individual slides.

Datafiles

Please submit your spectral datafiles as tab-delimited raw (not corrected) x, y ASCII datasets (*.asc) with headers indicating the content of the column (*i.e.,* Binding energy or Kinetic energy and counts or counts/s).

Spectrometer Geometry Diagram and Worksheet

The spectrometer geometry is specified with respect to a coordinate system in which the axis of the analyzer defines the polar (Z) axis, and the X-Y axes lie in the analyzer focal plane. The X axis is defined by the normal projection of the excitation source axis onto the analyzer focal plane. If the analyzer and source axes are coincident, the projection of the ion gun onto the focal plane should be used as the azimuthal reference. Another reference may be more convenient. Describe your choice of reference in Section C, Field 20 on the previous page. It is presumed that all component axes intercept at a common point lying on the specimen surface.



Field Name	Label	Value* (in degrees)
Emission Angle	Θ e	
Incident Angle	Ψ i	
Source-to-Analyzer Angle	Θ s	
Specimen Azimuthal Angle	Φ sp	
Sputter Source Incident Angle	Ψ ig	
Sputter Source Polar Angle	Θ ig	
Sputter Source Azimuthal Angle	Φ ig	

Submission Overview

Title: Enter title, beginning with a descriptive reference to the specimen material or other characteristics specific to this data record. Avoid titles which begin with the technique, such as 'AES Study of....'

Authors: Enter authors names as you wish them to appear in *SSS*.

Affiliations: Enter authors affiliations as you wish them to appear in *SSS*.

Abstract: Summarize and include key information about the specimens and spectra, such as specimen material, measurement procedures, and significance of the research. The abstract will be printed verbatim. Because the abstract must stand alone in some databases, **please do not cite references in the abstract**. You may include references beginning with the **Introduction**.

Keywords: Include keywords relevant to your samples.

Technique: (drop down with choices – AES, REELS, UPS, XPS, or XPS, XAES) Choose the spectroscopy technique used.

Specimen: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the specimen is the 'bulk' substance near the surface.

Instrument: Enter the instrument manufacturer's name and model number. If the instrument was custom-built, enter the designer's name, and reference a published article, if applicable.

Major Elements in spectra: Enter major elements.

Minor Elements in spectra: Enter minor elements or 'None' if not applicable.

Published Spectra: Enter the number of specimen spectra for which you are requesting hard-copy publication. An opportunity to identify specific spectra for publication is given within the figure/spectrum caption of the template.

Spectral Category: Choose the suggested category of the data record **drop down with choices: Comparison**, **Reference,** or **Technical** (see overview of instructions for definitions). The editors may suggest an alternate category, based on the recommendations of referees.

Introduction

Enter any descriptive, explanatory, or introductory comments that pertain to your entire submission, *e.g.,* why the work is significant, or what the conclusions show. You may cite references.

Specimen Description

Note: Multiple specimens (or specimen condition) may be included in a single SSS submission. To add additional specimens (or specimen condition), copy/paste the entire 'Specimen Description' section (including the header), placing the new sections in the order you would like to have them appear in the final publication.

Accession number: Replace "00000" with a single letter for initial submission. *i.e.,* "A", "B", "C", … (Select A for the first specimen and continue alphabetically for subsequent specimens). Note that this letter should also be implemented in the figure file, data file, and spectral ID as per the *Information for Contributors* document.

Specimen: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the specimen is the 'bulk' substance near the surface.

Chemical Abstract Service (CAS) Registry #: Enter the CAS registry number of the specimen. Enter 'unknown' if not known.

Specimen Characteristics: Homogeneity: (drop down with choices – Homogeneous, Inhomogeneous, Unknown homogeneity), choose the one that best applies. **Phase:** (drop down with choices – Gas, Liquid, Powder, Solid), **c**hoose the one that best applies. **Crystallinity:** (drop down with choices – Amorphous, Polycrystalline, Single Crystal, Unknown Crystallinity), **c**hoose the one that best applies. **Electrical Characteristics:** (drop down with choices – Conductor, Dielectric, Semiconductor, Superconductor, Unknown Conductivity), choose the one that best applies. **Material Family:** (drop down with choices – Biological Material, Composite, Inorganic Compound, Metal, Organic Compound, Polymer, Semiconductor), choose the one that best applies. **Special Material Classes:** (drop down

with choices – Ceramic, Coating, Fiber, Glass, Other, Powder, Thin Film), choose all appropriate responses. Leave blank if Special Classes do not apply. If 'Other,' describe in 'As Received Condition' (copy/paste this field as necessary).

Chemical Name: Enter the full chemical name of the specimen according to IUPAC conventions, *e.g.*, for Li_3PO_4 you would enter lithium orthophosphate.

Source: Provide the name of the manufacturer and/or supplier of the specimen or give a reference to how the was made, *e.g.,* thermally grown SiO_2 on Si.

Composition: List the principal elements present or the chemical formula, if practical.

Form: Give a physical description of the specimen, *e.g.,* MOSFET, reagent, single-crystal wafer, stub from corroded fender from brand X pickup truck, etc.

Structure: Include information such as a description of the crystal lattice and orientation, *e.g.* [1 0 -1 0] hexagonal close-packed, and/or comments such as fracture surface at grain boundary, etc. You may also submit a hard-copy bonding diagram.

History and Significance: Comment field for background information about the specimen, *e.g.,* moon rock retrieved by Apollo IX mission, or a discussion of why the spectra were taken. Include comments on purity, known contaminants, results of other analytical techniques. Identify the organization that developed any specified alternate standard designator, *e.g.,* AISI in the case of 1003 carbon steel.

As Received Condition: Describe the physical condition of the specimen as it was supplied to the spectroscopist, *e.g.,* as grown, paint delaminating from metal stub, etc. Include the thermal and storage history of the specimen as well as physical condition.

Analyzed Region: Describe the specimen analyzed qualitatively, *e.g.,* shorted FET gate, same as specimen, or weld bead.

Ex Situ Preparation and Mounting: Describe specimen preparation prior to introduction into the spectrometer vacuum system, *e.g.,* as received, washed in ethanol, scraped with a well-pickled file, etc. Also, describe the specimen mounting technique.

In Situ Preparation: Describe specimen preparation or treatment procedures within the spectrometer vacuum system prior to analysis, *e.g.,* ion sputter cleaning and annealing.

Charge Control Conditions and Procedures: Describe the equipment used to control charge of the specimen during measurement. Include flood gun voltages and current, target bias, the use of metal screens, etc. Also describe the procedures used to determine the charge control.

Temperature During Analysis: Enter the specimen temperature during analysis, in Kelvin. Use 300 for 'room temperature' if not otherwise measured.

Pressure During Analysis (in Pa): Enter the maximum pressure chamber pressure during analysis in Pascal (1 Torr = 133 Pascal). Normally expressed using powers of 10, for example 1.33×10^{-6}.

Pre-Analysis Beam Exposure: Describe procedures and include comments on the amount of time the analyzed region was exposed to the x-ray or electron irradiation prior to the measurements for these spectra (especially important for beam-sensitive specimens).

Instrument Description

Manufacturer and Model: Enter the instrument manufacturer name. If the instrument was custom-built, enter the designer's name, and reference a published article, if applicable. Enter the manufacturer's model number.

Analyzer Type: (drop down with choices – CMA, DCMA, Other-describe in next field, SSA) Choose the analyzer type that best applies. If 'Other,' include a description of the 'Non-Standard Analyzer or Lens' by entering this information after the analyzer type drop-down menu.

Detector: Describe the detector used, **(drop down with choices – channeltron, dynode, multichannel resistive plate, other)**.

Number of Detector Elements: Enter the number of detector elements. For a multichannel detector, this would be the number of separate detector data channels that can be output (*e.g.,* 3, 5, 16, 128). For a single-channel detector, the number is '1.'

Instruments Parameters Common to all Spectra

Spectrometer

Analyzer Mode: (drop down with choices – Constant Pass Energy, Constant Retarding Ratio option) Choose **Constant Pass Energy** (fixed analyzer transmission) or **Constant Retard Ratio**, whichever best applies.

Throughput: (drop down with choices – 1, 1/e, 1/√E, e, other) Identify the theoretical energy dependence of the instrument throughput function in the significant spectral range. Choose from 1/E, 1/√E, 1, E, Other. If other, describe any non-standard energy dependence by entering this information after the throughput drop-down menu.

Excitation Source Window or Filter: Describe any electron shield or radiation filter in the source, *e.g.,* 1.5 μm Al window.

Excitation Source: (drop down with choices – Ag L_α monochromatic, Al K_α, Al K_α monochromatic, Cr K_α monochromatic, electron beam, Ga K_α monochromatic, He I, He II, Mg K_α) Choose the Source Label that best applies.

Source Energy (eV): Enter the characteristic energy (in eV) of the excitation source, *e.g.,* 5000 eV for a 5 keV electron beam, 1486.6 eV for Al Kα, 1253.6 eV for Mg Kα, etc.

Source Strength: Enter the strength of the excitation source. Choose the corresponding units in the next field. **Strength Unit: (drop down with choices – nA, nA/mm^2, photons/mm^2, W).**

Source Beam Size, X Value (μm): Enter the X value, in μm, for the excitation source size. Choose X and Y axes to correspond with the manufacturer's definitions. If the beam is cylindrically symmetric, X and Y are equal. In other cases, such as the HP ESCA system, the beam is not cylindrically uniform. In choosing the axes, ensure that X and Y are orthogonal to each other and to the excitation source axis. **Source Beam Size, Y Value (μm):** Enter the Y value, in μm, for the excitation source size.

Signal Mode: (drop down with choices – analog direct, V/F analog, single channel direct, multichannel direct, multichannel indirect), choose the correct data acquisition mode.

Geometry

For all fields, please fill in Angles in degrees. Refer to diagram for details. If the angle varies from one spectrum to another, enter 'v.'

Incident Angle (Ψ i): No instructions

Source-to-Analyzer Angle (Θ s): No instructions

Emission Angle (Θ e): No instructions

Specimen Azimuthal Angle (Φ sp): No instructions

Acceptance Angle from Analyzer Axis (degrees): Enter the acceptance angle. The acceptance angle is usually 42° for CMA and 0° for hemispherical analyzers.

Analyzer Angular Acceptance Width: No instructions

Ion Gun

If an ion gun was used, complete 'Ion Gun Manufacturer' through 'Sputtering Comments'. If no ion gun was used skip this section.

Ion Gun Manufacturer and Model: Enter the ion gun manufacturer or describe as completely as possible if non-standard. Enter the ion gun model, if applicable.

Energy: Enter the ion gun energy in eV.

Current: Current value: Specify the sputtering current in either total current to specimen (units in mA or equivalent) or current density to unit area of the specimen (mA/cm^2). **Current Units: (drop down with choices – mA, mA/cm^2** No instructions

Current Measurement Method: (drop down with choices – Biased Stage, Faraday Cup option) Choose the one that best applies.

Sputtering Species and Charge: Enter the sputter gas species and the sputter charge, *e.g.,* Ar^+ or Ne^+.

Ion Gun Spot Size (μm): Define the full-width-half-maximum (FWHM) diameter of the (unrastered) ion gun beam in micrometers as measured normal to the ion gun axis.

Raster size: X-raster value. Use the x and y deflection electrodes of the ion gun to define the axes. Measure in

μm. Y-raster value. Use the x and y deflection electrodes of the ion gun to define the axes Measure in μm.

Incident Angle (Ψ ig): Enter the ion beam incident angle in degree (°).

Polar Angle (Θ ig): Enter the ion beam polar angle in degree (°).

Azimuthul Angle (Φ ig): Enter the ion beam azimuthal angle in degree (°).

Comment: List any comments to help understand the sputtering procedure, such as equivalent silicon dioxide sputter rate, crater flatness, etc. State whether sputtering was performed with a differentially pumped ion gun or by backfilling the chamber.

Data Analysis Method

Energy Scale Correction: Discuss energy scale calibration and energy shift used to compensate for charging, if any. If no energy scale correction enter "None".

Recommended Energy-Scale Shift: Enter the number(s) which, when added to the original abscissa value(s), will approximately correct the energy scale(s) for the effects of specimen charging or electron flood gun compensation. If there was no shift, enter "0".

Peak Shape and Background Method: Describe background correction technique, *e.g.,* linear subtraction, Shirley function, Tougaard function, Fourier transform cutoff, etc. Describe the procedure used to fit the spectral line shape, *e.g.,* Gaussian, Lorentzian, Voight, etc.

Quantitation Method: Specify the method used to determine the values for the atomic concentrations for the analyzed region. Please cite references for the quantitation method in the References section.

Acknowledgments

Acknowledgments to be published in *Surface Science Spectra.* Acknowledge grants and other people who have contributed to the work (other than authors) here.

Author Declarations

Conflicts of Interest *(required)*

If there are conflicts to report, a statement to that effect must be included. If there are no conflicts to report, the statement "The authors have no conflicts to disclose" must be included.

Ethics Approval *(if applicable)*

Research articles containing experiments on animals and/or human subjects must include a statement that the authors obtained ethics approval. For more information, see author instructions for *SSS*.

Author Contributions *(if applicable)*

Statements about author contributions can be added here if needed.

Data Availability Statement

Manuscripts are required to include a data availability statement. This statement should be placed between Acknowledgements and References. The appropriate statement likely is: "The data that supports the findings of this study are available within the article and its supplementary material."

References

References to be published in *Surface Science Spectra*.

Spectral Features Table

Spectrum ID#: The official ID number will be assigned to you on acceptance. For initial submission, please enter the first part of the data (X,Y) file name (minus the extension), in the rows that relate to that file. Note: There are instructions on the required file naming scheme for initial submission found in *Information for Contributors*.

Element/Transition: Enter the element corresponding to this spectral peak. Enter the transition or electronic level descriptor for this spectral peak. For XPS, typical entries are '*2p*' or '$4f_{7/2}$'. For AES, typical entries are '*KLL*', '$L_3M_{4,5}M_{4,5}$". (Please add the numeric Auger transitions if known.)

Peak Energy: Enter the peak binding energy, in eV, used to fit this spectral peak component. However, Auger peaks should be given in kinetic energy and have an '*' after the Accession # in the 'Spectrum ID #' field with a footnote under the Spectral Features Table denoting "*Peak position is given in kinetic energy."

Peak FWHM: Enter the full width at half maximum (FWHM), in eV, used to fit this spectral peak component.

Peak Area: Enter the peak amplitude for this spectral peak. Units are as specified in the Peak Amplitude Units field. **Peak Amplitude Units: (drop down choices - eV x counts and eV x counts/sec)** No instructions

Sensitivity Factor: Enter the sensitivity factor used in quantitation for this transition.

Concentration: Enter the concentration for this transition.

Peak Assignment: Enter a brief comment on the peak assignment, *e.g.* carboxylate, Mo(IV), C in C-O, etc.

Concentration Units: Give concentration in atomic percent.

Comments to Spectral Features Table: If applicable, enter any comments or additional information pertaining to the entire Spectral Features Table or footnote if comment is specific to a Spectrum ID #.

Analyzer Calibration Table

Spectrum ID#: The official ID number will be assigned to you on acceptance. For initial submission, please enter the first part of the data (X,Y) file name (minus the extension), in the rows that relate to that file. Note: There are instructions on the required file naming scheme for initial submission found in *Information for Contributors*.

Element/Transition: Enter the element corresponding to this spectral peak. Enter the transition or electronic level descriptor for this spectral peak. For XPS, typical entries are '*2p*' or '$4f_{7/2}$'. For AES, typical entries are '*KLL*', '$L_3M_{4,5}M_{4,5}$'.

Peak Energy (eV): Enter the peak energy, in eV, used to fit this spectral peak component.

Peak FWHM: Enter the full width at half maximum (FWHM), in eV, used to fit this spectral peak component.

Peak Area: Enter the peak amplitude for this spectral peak. Units are as specified in the Peak Amplitude Units field. **Peak Amplitude Units: (drop down choices – eV x counts and eV x counts/sec)** No instructions

Sensitivity Factor: Enter the sensitivity factor used in quantitation for this transition.

Concentration: Enter the concentration for this transition.

Peak Assignment: Enter a brief comment on the peak assignment, *e.g.* carboxylate, Mo(IV), C in C-O, etc.

Comments to Analyzer Calibration Table: If applicable, enter any comments or additional information pertaining to the entire Analyzer Calibration Table or footnote if comment is specific to a Spectrum ID #.

Guide to Figures

Spectrum ID#: The official ID number will be assigned to you on acceptance. For initial submission, please enter the first part of the data (X,Y) file name (minus the extension), in the rows that relate to that file. Note: There are instructions on the required file naming scheme for initial submission found in *Information for Contributors*.

Spectral Region: Enter the element(s) corresponding to this spectrum. Enter the transition(s) or electronic level descriptor(s) for this spectrum. For XPS, typical entries are '*2p*' or '$4f_{7/2}$'. For AES, typical entries are '*KLL*', '$L_3M_{4,5}M_{4,5}$'.

Voltage Shift: Enter the number which, when subtracted from the corrected abscissa value, will yield the original abscissa value (*i.e.,* the opposite of the value(s) given in the **Recommended Energy-Scale Shift field**).

Multiplier: Enter the multiplier (scaling factor) applied to the ordinate values of the spectrum. Enter 1 if no multiplier was applied.

Baseline: Enter the baseline offset that was applied to the ordinate values of the spectrum. Enter 0 if no offset was applied.

Comment: Enter any brief comment regarding this spectrum.

Spectra

Paste the spectrum, as you would like it published including all peak labels, into the appropriate place holder (survey or high-resolution). *SSS* will publish plots of corrected data, but please indicate explicitly whether the submitted plotted data represent raw or corrected data. Curve fits will always be plotted on top of the raw (or shifted) data, NOT against background-subtracted data. Authors must provide digital curves representing all components of the fit, including any background subtraction. Preferred file formats for plots are PostScript (.ps), Encapsulated PostScript (.eps), TIFF, JPG, or production-ready PDF.

Survey Spectrum Figure Caption

Specimen: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the specimen is the 'bulk' substance near the surface.

Technique: (drop down with choices – AES, REELS, other, UPS, and XPS) Choose the spectroscopy technique used. If Other, describe below.

Spectral Region: This field is fixed to read survey.

Instrument: Enter the instrument manufacturer name. If the instrument was custom-built, enter the designer's name, and reference a published article, if applicable. Enter the manufacturer's model number.

Excitation Source: (drop down with choices – Ag L_α monochromatic, Al K_α, Al K_α monochromatic, Cr K_α monochromatic, electron beam, Ga K_α monochromatic, He I, He II, Mg K_α) Choose the Source Label that best applies.

Source Energy (eV): Enter the characteristic energy (in eV) of the excitation source, *e.g.,* 5000 eV for a 5 keV electron beam, 1486.6 eV for Al Kα, 1253.6 eV for Mg Kα, etc.

Source Strength: Enter the strength of the excitation source. Choose the corresponding units in the next field. **Strength Unit: (drop down with choices – photons/s, watts)** No instructions with this field since mentioned above

Source Size: Enter the X value, in mm, for the excitation source size. Choose X and Y axes to correspond with the manufacturer's definitions. If the beam is cylindrically symmetric, X and Y are equal. In other cases, such as the HP ESCA system, the beam is not cylindrically uniform. In choosing the axes, ensure that X and Y are orthogonal to each other and to the excitation source axis. Enter the Y value, in mm, for the excitation source size.

Analyzer Type: (drop down with choices – CMA, DCMA, Other-describe in next field, SSA) Choose the analyzer type that best applies. If 'Other,' include a description in 'Non-Standard Analyzer or Lens'.

Incident Angle (Ψ i):

Emission Angle (Θ e):

Analyzer Pass Energy: Enter the analyzer constant value **(drop down with choices - retarding ratio in % or the pass energy in eV)**.

Analyzer Resolution: Enter the analyzer resolution, in **%** if the analyzer is operated with a constant retarding ratio, or in **eV** for constant pass energy analyzers

Total Signal Accumulation Time (sec): Enter the time, in seconds, spent accumulating data into displayed channels.

Total Elapsed Time (sec): Enter the time, in seconds, to complete the acquisition of the spectral data. The total elapsed time includes the Signal Accumulation time (previous field), the settling time, and the over scan time.

Number of Scans: Specify the number of times the signal for a given channel was counted.

Effective Detector Width (eV): Enter the detector width. For a multichannel detector, this would be the width, in eV, of the portion of the spectrum acquired simultaneously by the detector. (In a case where the effective width may vary with energy across the spectrum due to the type of analyzer used, an average detector width may be used, with the behavior described more fully in the 'Detector Description' in Section C.) For a single channel detector, the width can be listed as the eV/step in the spectral data.

Comments: Enter any needed comments or credit line if the figure is reused.

High-Resolution Spectrum Figure Caption

Specimen: Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO_2. For layered structures, the specimen is the 'bulk' substance near the surface.

Technique: (drop down with choices – AES, REELS, UPS, XPS, or XPS, XAES) Choose the spectroscopy technique used. If Other, describe below.

Spectral Region: Enter the element corresponding to this spectral peak. Enter the transition or electronic level descriptor for this spectral peak. For XPS, typical entries are '*2p*' or '$4f_{7/2}$'. For AES, typical entries are '*KLL*', '$L_3M_{4,5}M_{4,5}$'.

Instrument: Enter the instrument manufacturer name. If the instrument was custom-built, enter the designer's name and reference a published article, if applicable. Enter the manufacturer's model number.

Excitation Source: (drop down with choices – Ag L_α monochromatic, Al K_α, Al K_α monochromatic, Cr K_α monochromatic, electron beam, Ga K_α monochromatic, He I, He II, Mg K_α) Choose the Source Label that best applies.

Source Energy (eV): Enter the characteristic energy (in eV) of the excitation source, *e.g.*, 5000 eV for a 5 keV electron beam, 1486.6 eV for Al Kα, 1253.6 eV for Mg Kα, etc.

Source Strength: Enter the strength of the excitation source. Choose the corresponding units in the next field. **Strength Unit: (drop down with choices – photons/s or watts)** No instructions with this field since mentioned above

Source Size: Enter the X value, in mm, for the excitation source size. Choose X and Y axes to correspond with the manufacturer's definitions. If the beam is cylindrically symmetric, X and Y are equal. In other cases, such as the HP ESCA system, the beam is not cylindrically uniform. In choosing the axes, ensure that X and Y are orthogonal to each other and to the excitation source axis. Enter the Y value, in mm, for the excitation source size.

Analyzer Type: (drop down with choices – CMA, DCMA, Other-describe in next field, SSA) Choose the analyzer type that best applies. If 'Other,' include a description in 'Non-Standard Analyzer or Lens'.

Incident Angle (Ψ i):

Emission Angle (Θ e):

Analyzer Constant: drop down with choices - retarding ratio or the pass energy in eV.

Analyzer Resolution: Enter the analyzer resolution, in **%** if the analyzer is operated with a constant retarding ratio, or in **eV** for constant pass energy analyzers

Total Signal Accumulation Time (sec): Enter the time, in seconds, spent accumulating data into displayed channels.

Total Elapsed Time (sec): Enter the time, in seconds, to complete the acquisition of the spectral data. The total elapsed time includes the Signal Accumulation time (previous field), the settling time, and the over-scan time.

Number of Scans: Specify the number of times the signal for a given channel was counted.

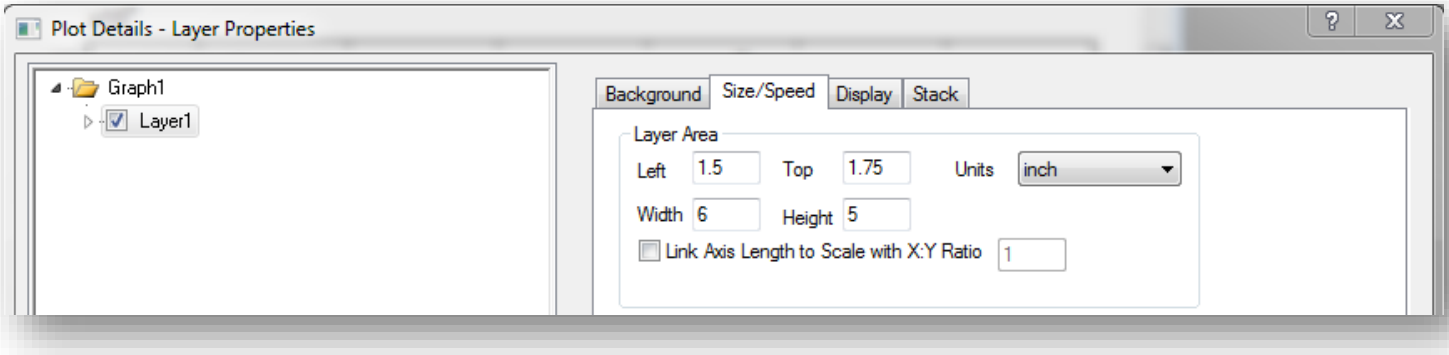
Effective Detector Width (eV): Enter the detector width. For a multichannel detector, this would be the width, in eV, of the portion of the spectrum acquired simultaneously by the detector. (In a case where the effective width may vary with energy across the spectrum due to the type of analyzer used, an average detector width may be used, with the behavior described more fully in the 'Detector Description' in Section C.) For a single channel detector, the width can be listed as the eV/step in the spectral data.

Comments: Enter any needed comments or credit line if the figure is reused.

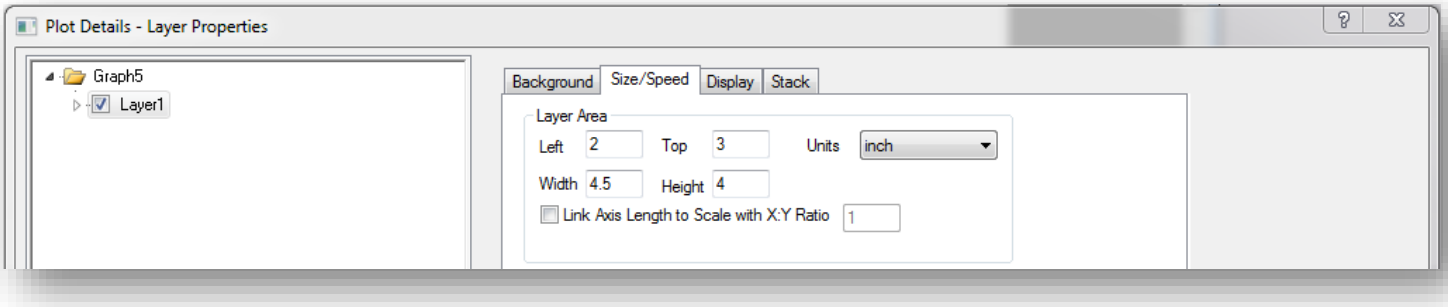
Appendix A- Origin Settings

Plot Details – Layer Properties - Size/Speed:

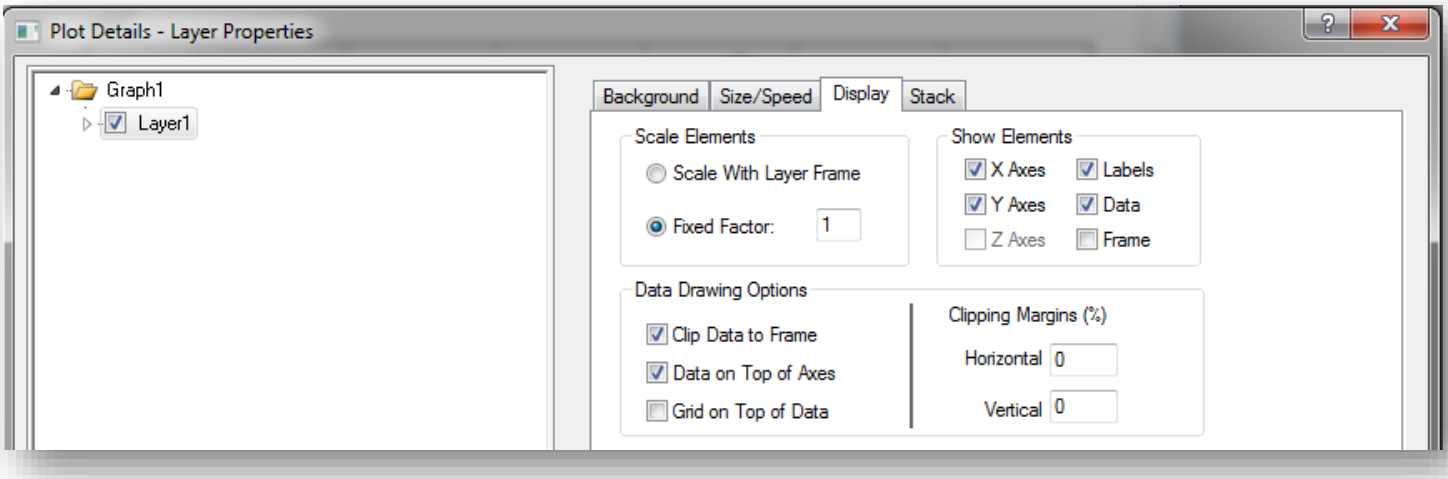
Survey



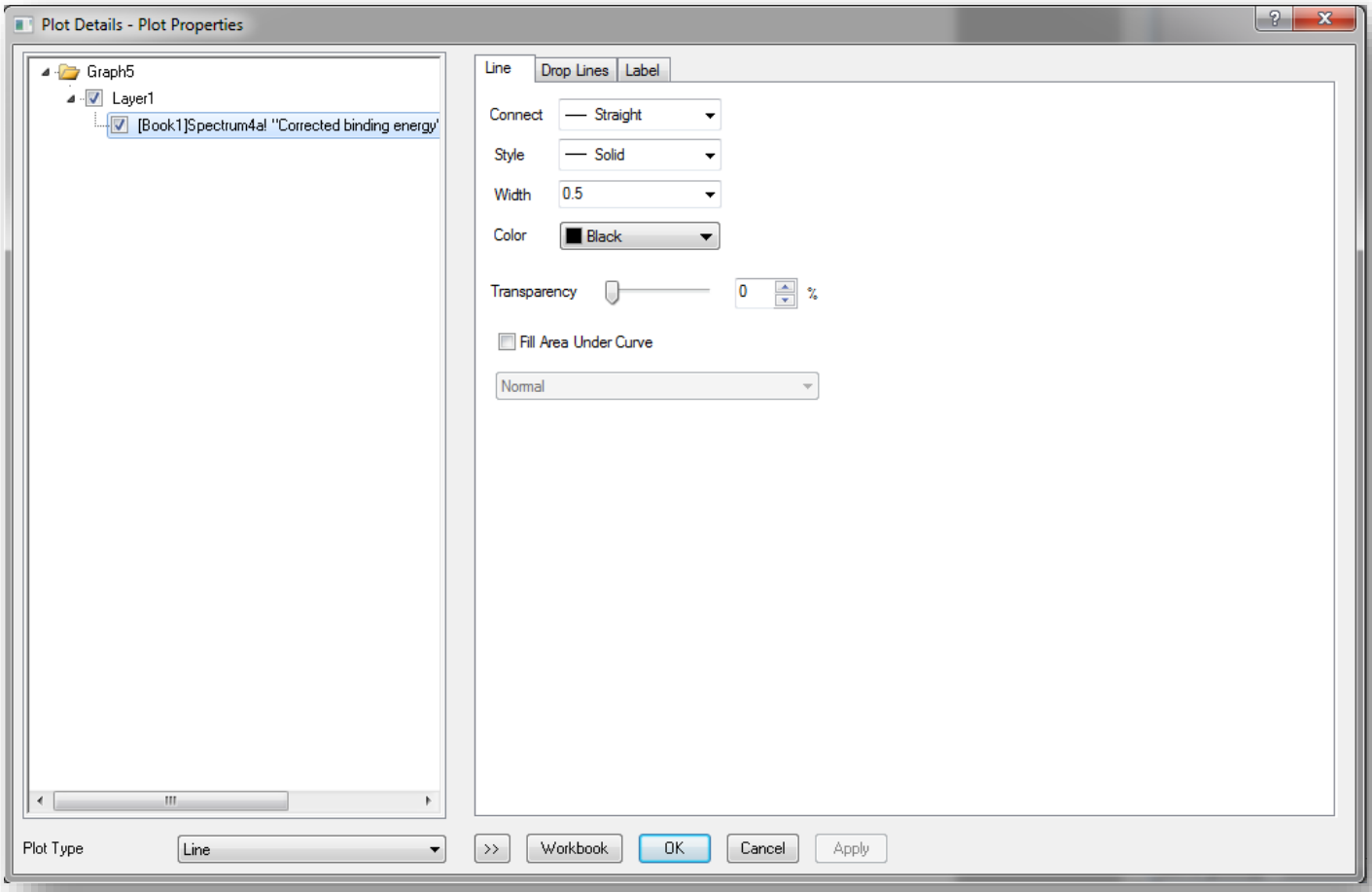
High-resolution



Plot Details – Layer Properties – Display (applies to both Survey and High-resolution)

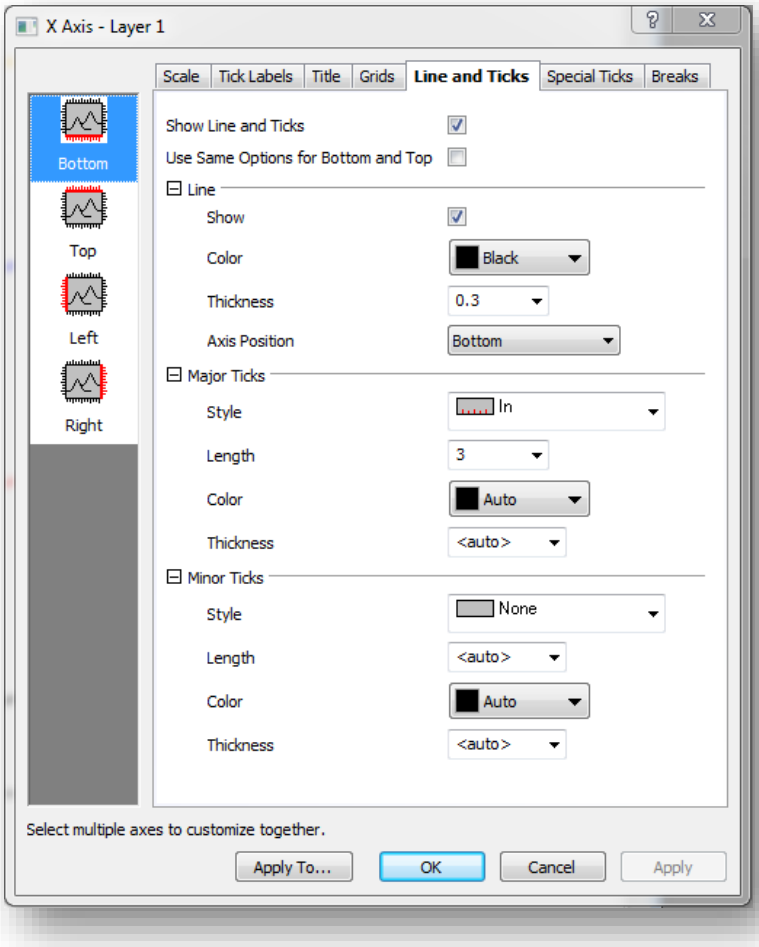


Plot Details – Plot Properties – Line (applies to both Survey and High-resolution)



Note: For stacked spectra, authors may choose different colors for each spectrum.

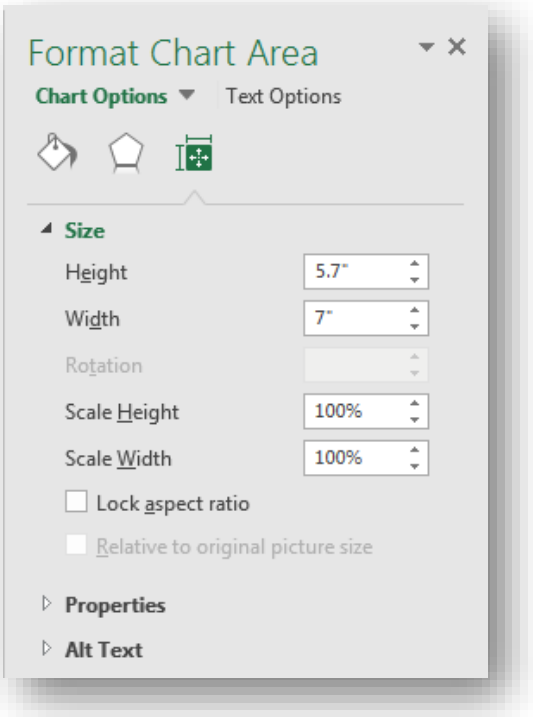
Axes - Line and Ticks (applies to all axes)



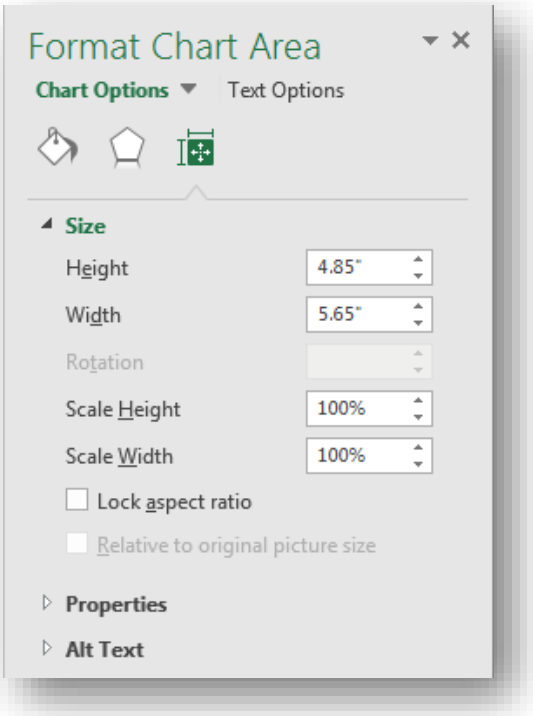
Appendix B- Excel Settings

Format Chart Area:

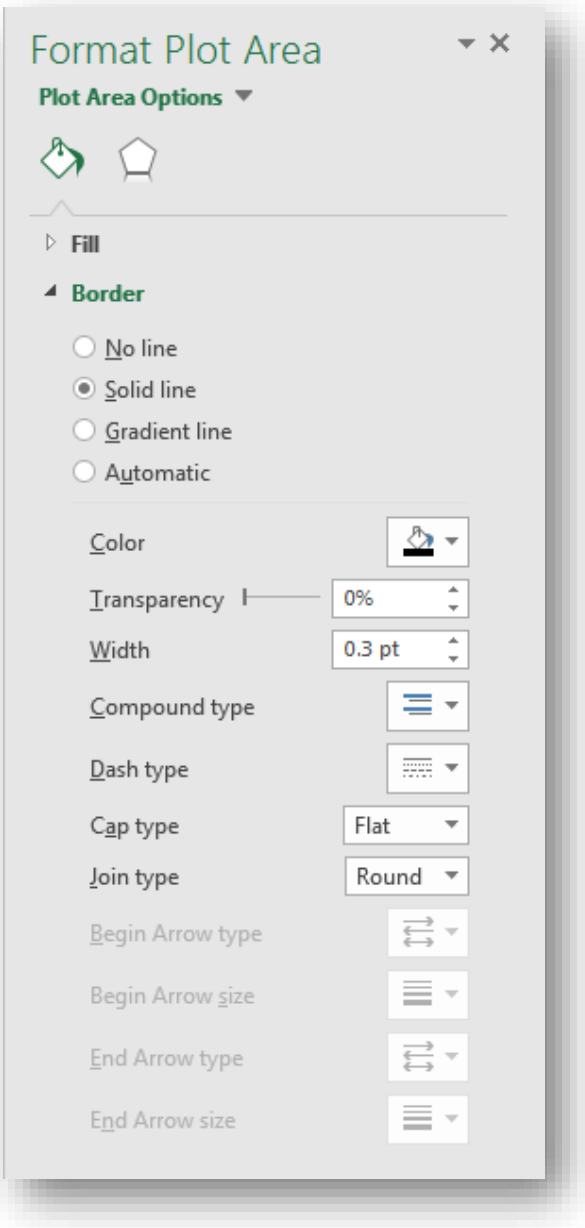
Survey



High Resolution

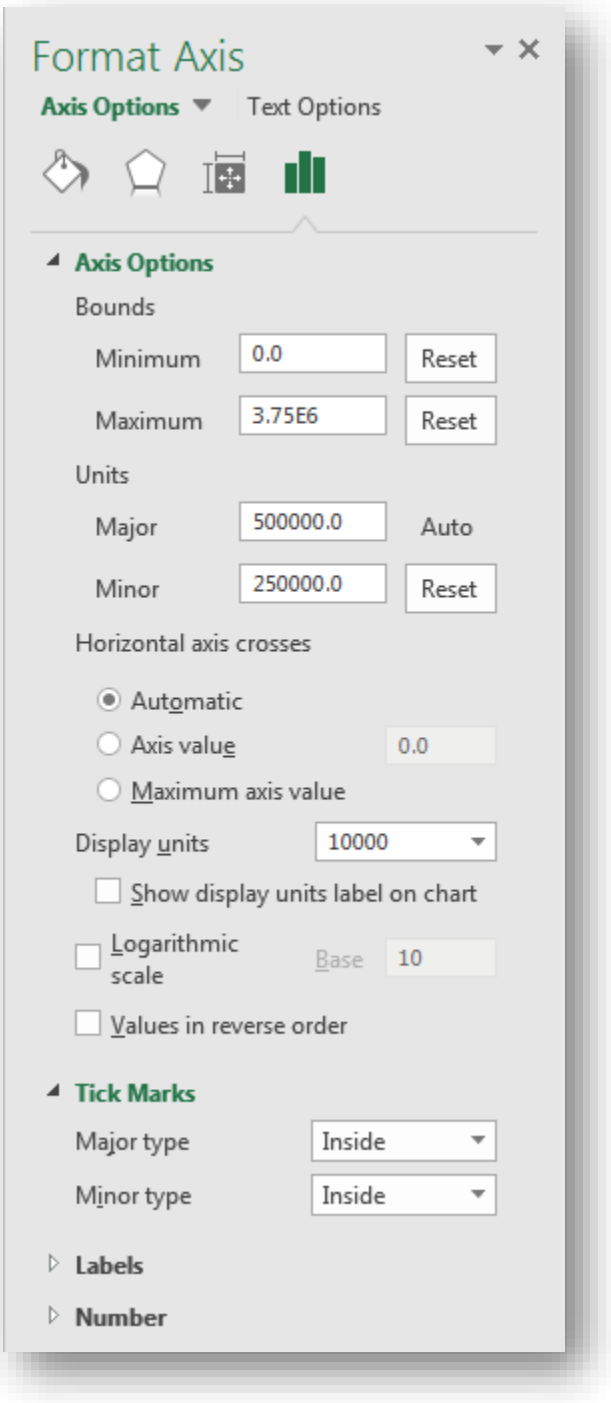


Format Plot Area (applies to both Survey and High-resolution):



Note: plot area border color should be set to black.

Format Axes (applies to both Survey and High-resolution):



Note: For Y-axis, adjust "Display units" so that axis values have no more than 3 significant figures. For both axes, set "Units Minor" value to be half of the "Units Major" value.

Format Data Series (applies to both Survey and High-resolution):