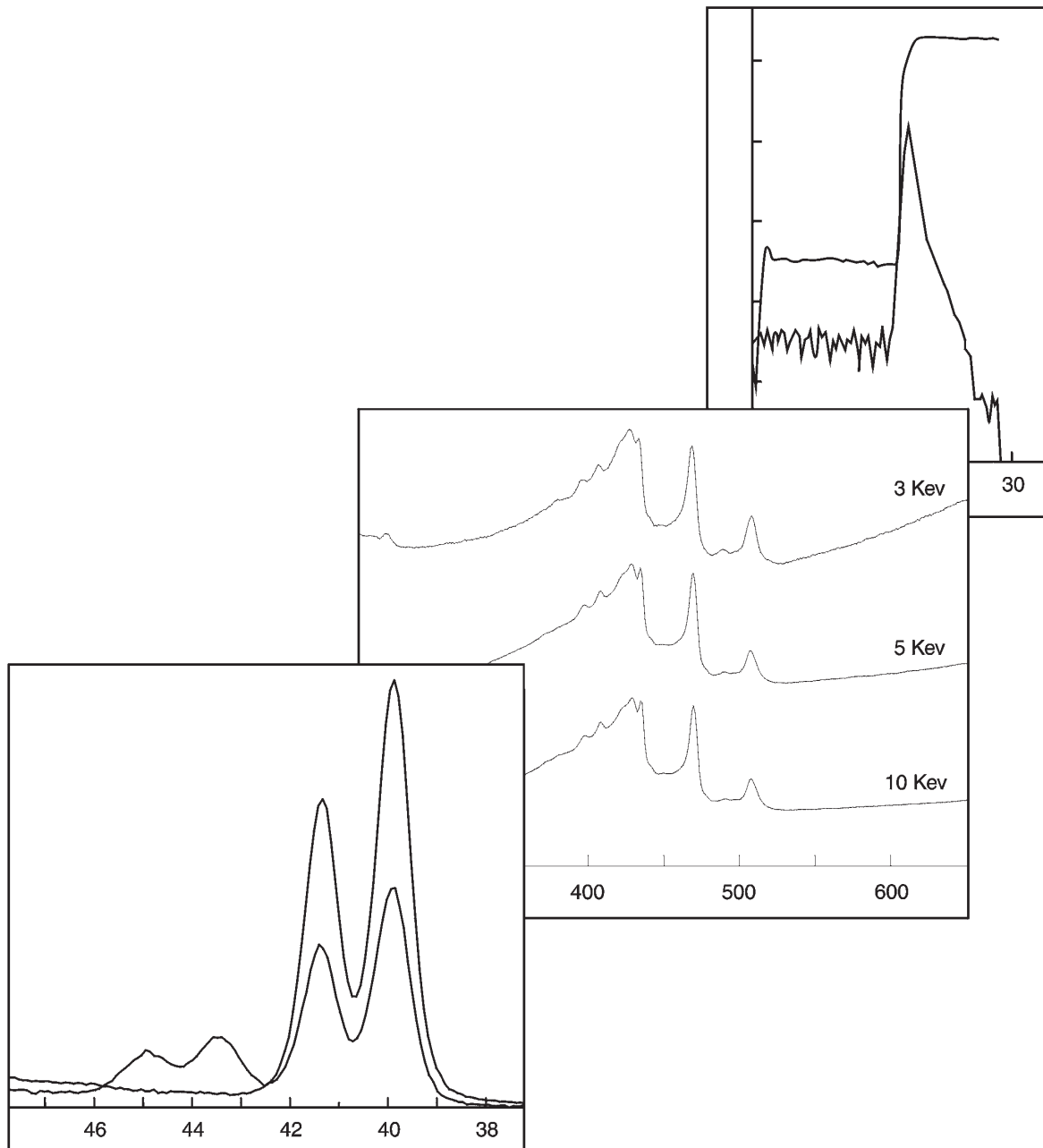


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# ***SURFACE SCIENCE SPECTRA***

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## ***AES/XPS Contributors Form***



## AES/XPS Contributors Form

### About Surface Science Spectra

*Surface Science Spectra* (SSS) is a journal and electronic database devoted to the distribution of surface spectroscopy data files. Spectra of any material of scientific and technological interest will be considered for inclusion. This form is for use primarily with XPS, UPS, and AES spectra. Closely related techniques, such as BIS, XAS, and XPD, have also utilized this form. SIMS measurements require a different contributor's form, which may be obtained from the SSS Web site at <http://www.vacuum.org/sss/sss.html>, or by contacting the SSS Editorial Office at [sss@jvst.org](mailto:sss@jvst.org). Additional techniques will be added later.

### What Data to Submit

The SSS database is designed to serve a wide range of needs. The objectives of the database include, but are not limited to, the following:

1. It provides examples of spectra from a wide range of materials that enable researchers and analysts to estimate, or predict, the type and quality of information that may be available from surface analytical techniques for problems they are encountering.
2. It provides a spectral library to allow comparisons of data from one laboratory and instrument to what others have found on different instruments or under different conditions.
3. It provides a spectral library that assists users of surface science data in extracting the most information possible by providing spectra from known materials and systems for comparison.
4. It provides a forum to present complete data sets for information published elsewhere where full presentation of the data was not possible due to space limitations.

To best accomplish the first three objectives, the database needs as many data sets as practical from as wide a range of materials as possible. To serve the last objective, submitted data need to satisfy the first three objectives as well as allow a full examination of the data supporting the ideas presented in the original publication.

It should be noted that even though spectra from a particular material have already appeared in SSS, we encourage the submission of data on the same or similar materials obtained from other instruments in order to meet the stated objectives. Remember—not everyone has the latest or highest performance machine. A tremendous amount of good work is being done on older machines and should be featured in the SSS database.

### Categories of Data Records

Three categories of data records are published in SSS:

- **Technical:** Data records characterizing complex surfaces that are of technological interest.
- **Comparison:** Data records characterizing chemically well-defined surfaces that can be used in identifying surface chemistry.
- **Reference:** Data records that can be used in calibrating energy scales and identifying chemical states of compounds of surfaces.

### The Submission Cycle

Submissions to SSS are distributed to recognized experts for peer review before acceptance into the database. Submissions determined to be of sufficient quality or interest to the applied surface science community will be accepted for publication, entered into the AVS database, and prepared for publication in SSS. They will be placed in the earliest issue in which there is space.

### Submitting a Data Record

To submit a data record to SSS, you must:

1. Prepare three copies of the AES/XPS Contributors Form.
2. Prepare three hard copies of each spectrum in the data record.
3. Send electronic records of all spectra, including calibration spectra, on magnetic disk.

At least one survey spectrum must be included with each data record to characterize the elements present. Survey scans cannot be obtained with certain experimental techniques (e.g. UPS); in those cases the criteria for determining surface quality must be described. Authors may submit, for inclusion in the electronic database, the full set of spectra necessary to completely characterize the surface, even if the number of spectra is too large to print in SSS. Fields are provided in the AES/XPS Contributors Form to designate which spectra are only for entry into the electronic database. For example, calibration spectra will be entered into the electronic archives as part of the data record but will not necessarily be printed in SSS.

### The Data Center

Data are sent from the editors to the AVS Data Center located in Pasadena, CA. The Data Center manages the flow of documents among the publishers, the editors, and, on occasion, the contributors.

The Data Center manages the SSS database, handles data entry from the Contributors Form, and converts spectra data and chemical structure diagrams into a common digital format, which is then made accessible to subscribers online.

The Data Center will attempt to convert data files from all commercial spectrometer systems. As there are many combinations of physical and logical media formats, the following guidelines are suggested to streamline the translation process:

1. When possible, send files on disk, zip disks, CD, or as ASCII e-mail attachments.
2. MS-DOS format disks are preferred. Hewlett-Packard LIF format, Apple ProDOS, or Macintosh formats can easily be converted.
3. ASCII formats, when available, are preferred over binary formats.

PHI: The .DIF or .ASC logical formats are standard, whereas native formats may be system-dependent. On Apollo or Perkin-Elmer computers, MS-DOS compatible readable disk format is generally available and is preferred.

SSI: Most SSI products are based on HP-9000 computers that write in LIF format to standard 3.5" floppy disks. The binary format is acceptable, but disks should be formatted using the DEFAULT option of the X-Probe software in order to produce MS-DOS compatible sectoring.

Magnetic disks should be labeled with the corresponding author's name and telephone number, the title of the submission, the spectrum numbers of the spectra on the disk, and the data format (e.g., PHI .DIF).

All submissions should be mailed to the SSS Editorial Office, Caller Box 13994, 100 Park Drive, Suite 105, Research Triangle Park, NC 27709.

### Preparing the AES/XPS Contributors Form

The information required to complete the Contributors Form falls in three categories:

#### 1. Information pertaining to the entire submission:

Section A: Authors, Institutions, Overview  
Section C: Overall Instrument Description  
Section D: Calibration Information  
Section H: Analysis Methods  
Section I: Spectral Features Descriptions

#### 2. Information pertaining to each sample, instrument configuration, or experimental variable in the submission:

Section B: Specimen Description  
Section E: Variable Instrument Parameters  
Section G: Experimental Variables

#### 3. Information pertaining to each spectrum submitted:

Section F: Spectrum Parameters

Test cases show that the typical amount of time needed to complete this form is 2-4 hours—a relatively short period in which to produce a refereed, archival publication. Future submissions should take even less time if the contributor photocopies partially completed sections of the AES/XPS Contributors Form at appropriate stages in the preparation of the first submission.

For example, a number of data items, such as those in Section C that describe the basic characteristics of the spectrometer, will tend to be the same for all submissions of data from a given instrument. Such entries should be identified and filled in. Then, the entire form can be photocop-

ied for future use before making additional entries. Also, the Variable Instrument Parameters section constitutes a profile of how an instrument is set up to take a series of spectra. For most laboratories, only a few entries in this section will change from one data record to another, and a small set of partially completed forms can be assembled. It is well worth the effort to examine the form before filling it out and to design a set of partially completed forms tailored to your typical measurement procedures. It might also be noted that the Contributors Form is a useful way to document data records, even if they are not submitted to SSS.

One copy of the Spectrum Parameters section is required for each spectrum, including calibration spectra, in the data record. Different copies of the Variable Instrument Parameters section are required, depending on how many instrument configurations were used to take the spectra. As an example, in a typical XPS submission, there would be one Variable Instrument Parameters section (VIPS) for the survey spectrum, one VIPS for the high-resolution spectra, and one VIPS for the valence band spectra.

The section on Experimental Variables is for use in documenting data records showing the effects of parameters (e.g., gas exposure or temperature), that are varied from one spectrum to another. This section needs to be included with the submission only for data records featuring variable parameter studies. The data entries for the remaining sections should be the same for all spectra.

### Submission Illustration

For example, for a submission with six submitted spectra, two sample treatments, and two instrument configurations, you should complete the forms as shown in the diagram on the following page.

### Calibration Spectra

Because the condition of the instrument used to take the data submitted to SSS directly affects the data, we require that calibration spectra be submitted with all "comparison" and "reference" data sets and strongly recommend submission of calibration spectra for "technical" data sets. With access to the actual calibration data, SSS users can assess the condition of the instrument used to collect the data. Today, only the peak energies that appear in the calibration summary table are used most often from calibration data details. In the future, as more understanding of the techniques is available, the intensity data will be used to allow better quantification. Having the calibration data, such as a survey scan of Cu, Ag, or Au, as part of the SSS data record will facilitate this quantification in the future.

One copy of Section B, Specimen Description, must be completed for the calibration sample, and one copy of Section F, Spectrum Parameters, should be completed for each calibration spectrum included in the submission.

## Peak Labeling

For XPS spectra, label all transitions on the hard copy spectra. Identify the element and transition—optionally including the spin-orbit coupling if the spin-orbit coupling peaks are resolved. Assignment of spectral features due to different oxidation states, shake-up, shake-off, or other satellites should be reserved for the *Table of Spectral Features*. The valence band and Auger transitions may be identified as a region unless the author wishes to identify specific peaks.

For AES spectra, Auger transitions may be identified individually or as a region. Peak energies in the N (E) or derivative spectra should be identified in the *Table of Spectral Features*.

## Completing Entries

The information you provide should be complete enough so that the experiment can be reconstructed by SSS readers. Each data field is coded 1, 2, 3, 4, or 5 to assist you in assessing the consequences of omitting an entry.

- ① Level 1: Mandatory entry—An entry must be made, even if the only valid entry is N/A (not applicable). The absence of an entry is not equivalent to entering zero, none, or N/A.
- ② Level 2: Mandatory entry—An entry must be made unless there are special considerations. Failure to make an entry would be acceptable only if the data record were of such unusual technical importance that it should be archived, even in the absence of some data entries at this level.
- ③ Level 3: Recommended entry—An entry, though not required, is important to readers who wish to have a complete interpretation of the data record.
- ④ Level 4: Recommended entry—An entry allows the most critical uses of the data record.

- ⑤ Level 5: Optional entry—An entry should be made at the author's discretion (e.g., see Field 11, Section A).

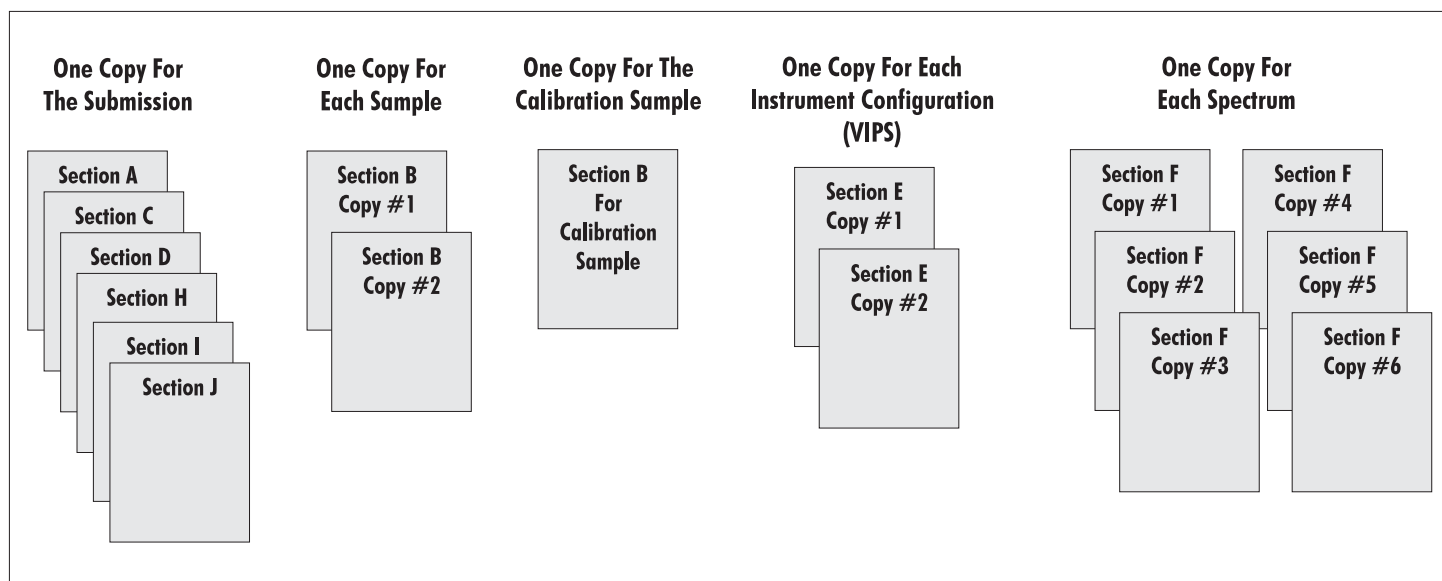
The completeness level code is listed to the left of every field number. If you cannot determine how to complete an entry and need assistance, please contact the SSS editor:

### Stephen W. Gaarenstroom

General Motors R&D Center  
Chemical and Environmental Sciences Laboratory  
30500 Mound Road, 480-106-320  
Warren, MI 48090-9055  
Phone: (586) 986-0835, Fax: (586) 986-0817  
E-Mail: Stephen.W.Gaarenstroom@gm.com

If you need additional room, attach pages and note the question number to which the information refers.

*Thank you for contributing to Surface Science Spectra, "an international journal devoted to archiving surface science spectra of technological and scientific interest." The editors are interested in constructive criticism of the AES/XPS Contributors Form and its data fields and would appreciate your comments on page 21.*



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## A. Authors, Institutions, Overview

- ① | **1. Title**—Enter a title, beginning with a descriptive reference to the specimen materials or other characteristics specific to this data record, e.g., “Polyvinyl Acetate Degradation During XPS Measurements.” Please refrain from using titles beginning with the name of the spectroscopy, e.g., avoid titles like “AES Study of ...”

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

- ① | **2. Authors, Institutions, and Locations (city, state, province, or country)**—List authors and affiliations in order of appearance in SSS. List addresses and names as you wish them to appear in SSS.

\_\_\_\_\_

Author

\_\_\_\_\_

Institution

\_\_\_\_\_

Department or M/S

\_\_\_\_\_

Address

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Country

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Author

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Country



① | **5. Technique**—Check the technique used:  XPS  AES  UPS  Other (specify) \_\_\_\_\_

① | **6.**

<p><b># of digitally submitted specimen spectra for SSS publication</b>—Enter the number of specimen spectra for which you are requesting hard-copy publication. All submitted spectra for accepted data records will be entered into the AVS electronic database, but, in cases where large numbers of spectra are submitted, it may be feasible to publish only a representative number in Surface Science Spectra. An opportunity to identify specific spectra for publication is given in Field 2, Section F.</p>	
<p><b># of digitally submitted specimen spectra for electronic database only.</b></p>	
<p><b># of digitally submitted calibration spectra</b>—(A survey-scan spectrum of an accepted reference material—such as Au, Ag, or Cu—is mandatory for reference and comparison spectra and recommended for technical spectra. Calibration spectra are not normally published in the hard-copy journal.)</p>	
<p><b>Total # of digitally submitted spectra</b>—Enter the number of spectra being submitted, including all calibration spectra. Complete a copy of Section F for each submitted spectrum.</p>	

Note: the number you enter *here* should equal the sum of the top three boxes.

⑤ | **7. Publish Auger Derivative Spectra**—Auger survey spectra submitted may be displayed in Surface Science Spectra as N(E) data alone or as superimposed N(E) and derivative forms. The default display mode will include both forms. Check your preference:  
 Display Both Forms  Display N(E) Only

① | **8. Key Words**—List selected phrases and words to help readers search for information in the database, e.g., oxidation, corrosion, and surface segregation. Be selective, but thorough.

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① | **9. Spectra Category**—Check the suggested category of the data record: Technical, Comparison, or Reference (see the overview of instructions for definitions). The editors may suggest an alternate category, based on the recommendations of referees.  
 Technical  Comparison  Reference

③ | **10. References**—List citations to articles related to the data record using the style of J. Vac. Sci. Technol. The references must be cited in other data fields in this record.

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⑤ | **11. Acknowledgments**

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Specimen # \_\_\_\_\_

For **each** specimen or specimen treatment submitted, complete one copy of Section B.

Incomplete items for this copy should be (check one):  left blank or  replaced by answers from Section B, specimen # \_\_\_\_\_.

## B. Specimen Description

- ② | 1. **Host Material**—Provide a generic description of the specimen, such as nylon, 6061 Al, or SiO<sub>2</sub>. For layered structures, the host material is the “bulk” substance near the surface. For instance, XPS of an ultra-thin metal film on a thick SiO<sub>2</sub> layer on an Si substrate would be SiO<sub>2</sub> because the depth of analysis by XPS without sputtering would not probe the Si.
- \_\_\_\_\_
- \_\_\_\_\_
- \_\_\_\_\_
- ③ | 2. **Chemical Abstract Service (CAS) Registry #**—Enter the CAS registry number of the host material.
- \_\_\_\_\_
- ③ | 3. **Material Designation Code and Organization**—Provide any alternate standard designator code specifying the host material, e.g., 1033 for carbon steel, and identify the organization that developed the designated code, e.g., AISI.
- Code \_\_\_\_\_
- Organization \_\_\_\_\_
- ② | 4. **Host Composition**—Enter the chemical formula, if practical, e.g., Li<sub>3</sub>PO<sub>4</sub>, or list the principal elements present, e.g., Li, P, O.
- \_\_\_\_\_
- \_\_\_\_\_
- ③ | 5. **Chemical Name**—Enter the full chemical name of the host material according to IUPAC conventions, e.g., for Li<sub>3</sub>PO<sub>4</sub>, lithium orthophosphate.
- \_\_\_\_\_
- \_\_\_\_\_
- ③ | 6. **Specimen Manufacturer/Supplier**—Provide the name of the manufacturer and/or supplier of the host material or give a reference to how the host was made, e.g., thermally grown SiO<sub>2</sub> on Si.
- \_\_\_\_\_
- \_\_\_\_\_
- ② | 7. **Specimen Form**—Give a physical description of the host, e.g., MOSFET, reagent, single-crystal wafer, etc.
- \_\_\_\_\_
- \_\_\_\_\_
- ④ | 8. **Lot Number**—Provide the code that identifies the production run, etc.
- \_\_\_\_\_
- \_\_\_\_\_
- ③ | 9. **Structural Formula**—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 the grain boundary, etc. At a later date, this field will use a formula encoding scheme.
- \_\_\_\_\_
- \_\_\_\_\_
- \_\_\_\_\_
- \_\_\_\_\_
- Fields 10-13 refer to the *host material*. They are included to facilitate database searches.
- ② | 10. **Homogeneity**—Check one that best applies.
- Homogeneous     Inhomogeneous     Unknown

Specimen # \_\_\_\_\_

- ① | **11. Phase**—Check one that best applies.  
 Solid     Powder     Liquid     Gas
  
- ① | **12. Crystallinity**—Check one that best applies.  
 Single Crystal     Polycrystalline     Amorphous  
 Unknown Crystallinity
  
- ③ | **13. Electrical Characteristics**—Check one that best applies.  
 Conductor     Superconductor  
 Semiconductor     Dielectric     Unknown
  
- ① | **14. Material Family**—Check one that best applies.  
 Semiconductor     Polymer  
 Organic Compound     Inorganic Compound  
 Biological Material     Composite     Metal
  
- ③ | **15. Special Material Classes**—Check all appropriate boxes. No entry is needed if these special classes do not apply. If “Other,” describe in “as received condition” in Field 17 below.  
 Ceramic     Glass     Thin Film  
 Powder     Fiber     Coating     Other  
 Suggested New Class Types \_\_\_\_\_
  
- ⑤ | **16. History and Significance**—This is an important comment field for background information about the specimen and the investigation, e.g., moon rock retrieved by Apollo IX mission, or a discussion of why the spectra were taken. Also, include comments on purity or known contaminants and results of other analytical techniques and references to publications in which analysis and interpretation of the data is presented.  
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- ② | **17. As Received Condition**—Describe the physical condition of the specimen as it was supplied to the spectroscopist, e.g., as grown, cold rolled steel, etc. Include the thermal and storage history of the specimen as well as physical condition.  
 \_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_  
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- ② | **18. Analyzed Region**—Describe the specimen analyzed qualitatively, e.g., FET gate oxide, same as host material, or weld bead.  
 \_\_\_\_\_  
 \_\_\_\_\_
  
- ② | **19. 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.  
 \_\_\_\_\_  
 \_\_\_\_\_  
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- ② | **20. In Situ Preparation**—Describe specimen preparation or treatment procedures within the spectrometer vacuum system prior to analysis, e.g., ion sputter cleaning and annealing.  
 \_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_
  
- ③ | **21. Specimen Temperature During Analysis**—Enter the temperature in Kelvin.  
 \_\_\_\_\_ K

Specimen # \_\_\_\_\_

② | **22. Maximum Chamber Pressure During Analysis**—*Enter the pressure in Pascal (1 Torr = 133 Pascal).*

\_\_\_\_\_ Pa

③ | **23. Pre-Analysis Beam Exposures**—*Describe procedures and include comments on the amount of time the analyzed region was exposed to the x-ray or electron radiation prior to the measurements for these spectra (especially important for beam-sensitive materials).*

\_\_\_\_\_  
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\_\_\_\_\_  
\_\_\_\_\_

② | **24. Charge Control Conditions and Procedures**—*Describe the equipment used to control charge at 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.*

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## C. Overall Instrument Description

The fields in this section describe the system excitation source, the analyzer, and the ion gun used in the experiment. The equipment description is divided into parameters universal to all of the spectra in the record, such as electron spectrometer. Parameters that could vary, depending on the experimental conditions, such as energy range and increment, are in Section E. The universal parameters need to be described only once. If one of these parameters varies, list it as "V" in this section and fill out Section G.

- ① | **1. Spectrometer Manufacturer**—Enter the designer's name, if the instrument was custom-built, and reference a published article, if applicable.

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- ① | **2. Manufacturer Model #**

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- ① | **3. Analyzer Type**—Check one that best applies. If "Other," include a description in Field 4 below.

Cylindrical Mirror Analyzer (CMA)     Double Pass CMA  
 Spherical Section Analyzer     Other

- ① | **4. Non-Standard Analyzer or Lens**—Describe any non-standard analyzer or lens used and/or any modification or enhancement made in house. If this information is not applicable to this data record, enter "N/A."

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- ② | **5. Acceptance Angle from Analyzer Axis**—Enter the acceptance angle. The acceptance angle is usually 42° for CMA and 0° for hemispherical analyzers.

\_\_\_\_\_ degrees

- ① | **6. Analyzer Mode**—Check one that best applies.

Constant Pass Energy (fixed analyzer transmission)  
 Constant Retard Ratio

- ② | **7. Instrument Throughput Function**—Identify the theoretical energy dependence of the instrument throughput function in the most significant spectral range. If "Other," the description in Field 8 below is mandatory.

1/E     1/√E     1     E     Other

- ④ | **8. Instrument Throughput Function Comment**—Elaborate on any non-standard energy dependence.

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- ① | **9. Excitation Source Label**—Check one that best applies.

Al Kα (non-monochromated)  
 Al Kα (monochromated)     MgKα  
 Other X-Ray \_\_\_\_\_     Electron Beam  
 Other: describe the source \_\_\_\_\_

- ② | **10. Excitation Source Window or Filter**—Describe any electron shield or radiation filter in the source, e.g., 1.5-μm Al window.

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- ③ | **11. Detector Description**—Describe the detector used, e.g., spiraltron, dynode, multichannel resistive plate, etc.

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- ① | **12. 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 (for example, 3, 5, 16, or 128). For a single-channel detector, this number is "1."

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⑤ | 13. **Ion Gun Manufacturer and Model #**—Describe the ion gun as completely as possible if it is non-standard.

\_\_\_\_\_

③ | 14. **Sputtering Current Measurement Method**—Check one that best applies.

Biased Stage     Faraday Cup

③ | 15. **Ion Gun Operating Parameters**—Specify the current used to sputter the specimen in either total current to specimen (units in mA) or current density to unit area of the specimen [mA/cm<sup>2</sup>].

\_\_\_\_\_ Energy (in eV)

\_\_\_\_\_ Current Value (in mA) or \_\_\_\_\_ Current Density Value (in mA/cm<sup>2</sup>)

\_\_\_\_\_ Sputtering Species and charge, e.g., Ne<sup>+1</sup>

③ | 16. **Ion Gun Spot Size (normal to source)**—Define the full-width-at-half-maximum (FWHM) diameter of the unrastered ion gun beam in micrometers as measured normal to the ion gun axis.

\_\_\_\_\_

③ | 17. **Ion Gun Raster Parameters (normal to source)**

Rastered?     Yes     No

Use the X and Y deflection electrodes of the ion gun to define the axes. Measure in micrometers.

\_\_\_\_\_ X-Raster (μm)

\_\_\_\_\_ Y-Raster (μm)

⑤ | 18. **Sputtering Comments**—List any additional comments you believe will help to understand the sputtering procedure used in this record, such as the equivalent silicon dioxide sputter rate, crater flatness, etc. State whether sputtering was performed with a differentially pumped ion gun or by backfilling the chamber.

\_\_\_\_\_

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19. Please fill in the angles (in degrees) for the submission. Refer to the diagram on page 9 for details.

	Field Name	Label	Value* (in degrees)
①	Emission Angle	Θ e	
②	Incident Angle	Ψ i	
①	Source-to-Analyzer Angle	Θ s	
②	Specimen Azimuthal Angle	Φ sp	
③	Sputter Source Incident Angle	Ψ ig	
③	Sputter Source Polar Angle	Θ ig	
③	Sputter Source Azimuthal Angle	Φ ig	

\*If the angle varies from one spectrum to another, enter "v."

③ | 20. **Angular Geometry Comments**—Present any additional comments on the scattering geometry that are important to understand the measurements; e.g., the take-off angle may be important relative to the specimen structure. In other fields, several geometric factors are requested, such as raster area of ion sputter, dimensions of excitation area, etc. If the X and Y axes of the sputtered region, excited region, etc. do not coincide, describe the orientation of the various regions.

\_\_\_\_\_

\_\_\_\_\_

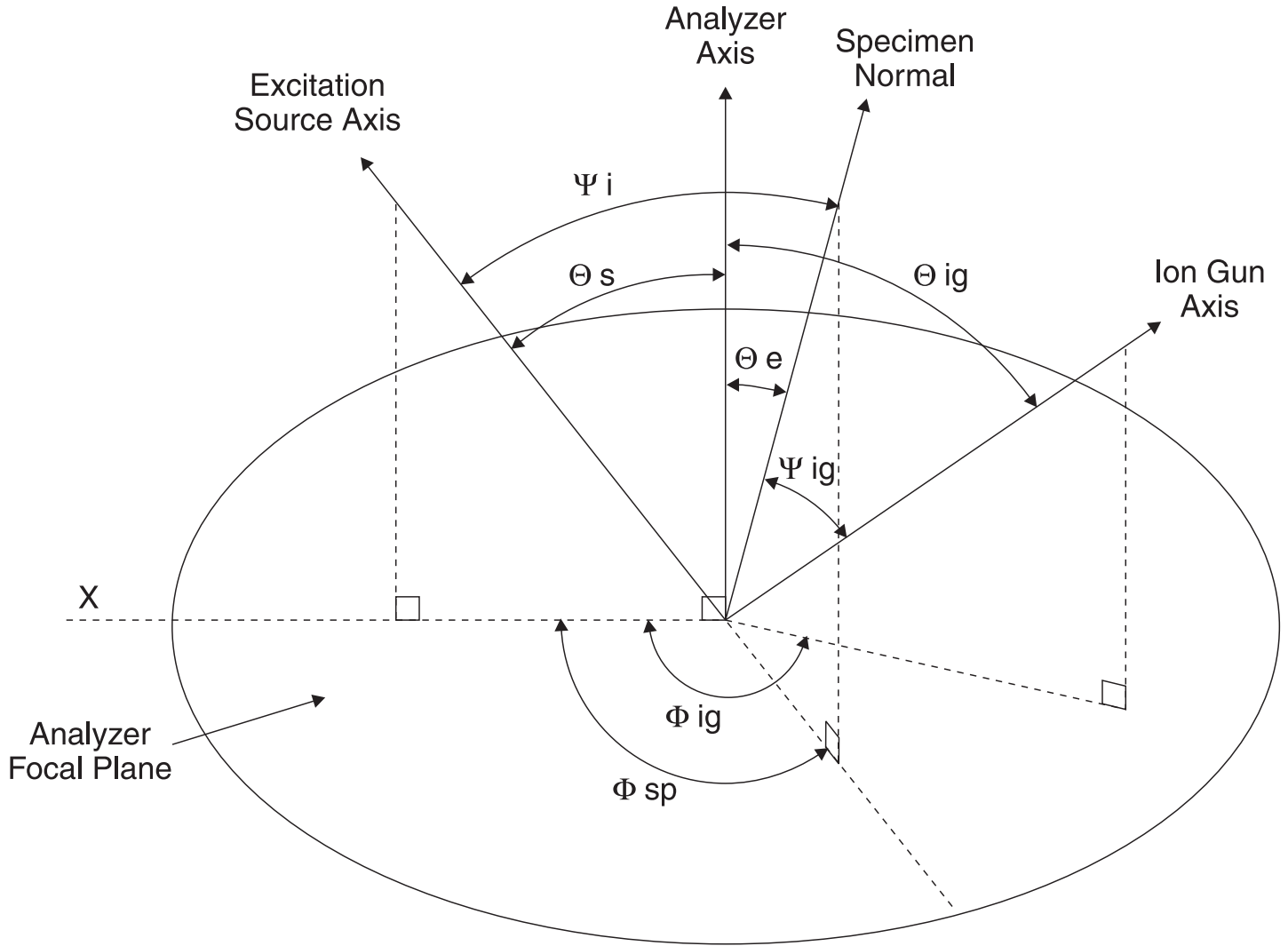
\_\_\_\_\_

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\_\_\_\_\_

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 coinci-

dent, 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.



### D. Calibration Information

- ② | 1. **Calibration Summary**—Describe the calibration of your spectrometer by completing the table below. For each calibration point, enter the element and transition of the calibration peak, the energy (in eV) measured for that peak after calibration, the measured peak width (in eV), and the amplitude. The peak amplitude method and units for amplitude must be the same as those specified in Section I. Care should be used to ensure that the correct number of significant figures is entered since the precision is a substantive aspect of calibration. If the calibration spectra are included in the data record, each calibration point should be identified with the spectrum used to obtain the data for that transition by entering the corresponding spectrum ID number (Field 1, Section F).

Spectrum ID #	Element, Transition	Peak Energy, eV	Peak Width (FWHM), eV	Peak Amplitude	Sensitivity Factor	Concentration	Peak Assignment	Peak Comment

Parameter Set # \_\_\_\_\_

For **each** instrument configuration submitted, complete one copy of Section E.

Incomplete items for this copy should be (check one):  left blank or  replaced by answers from Section E, parameter set # \_\_\_\_\_.

## E. Variable Instrument Parameters

Complete a copy of this section for each set of instrument settings. For example, you might be contributing two survey scans and four high-resolution scans that have different energy resolutions, scan rates, etc. You would then fill out one Section E for the survey scan and one Section E for the high-resolution scans.

- ① | **1. Parameter Set #**—Enter an identifying serial number, starting with "1" for each set of variable instrument parameters. These numbers will be used in the individual data records to reference the appropriate parameter set for each spectrum described in Section I.

\_\_\_\_\_  
\_\_\_\_\_

### Source Operating Parameters

- ① | **2. Source Energy**—Enter the characteristic energy (in eV) of the excitation source, e.g., 5,000 eV for 5 keV electron beam, 1486.6 eV for AlK $\alpha$ , 1253.6 eV for MgK $\alpha$ , etc.

\_\_\_\_\_  
(eV)

- ③ | **3. Source Strength Value and Units**—Enter the strength of the excitation source and the correct corresponding units. For XPS, this could be anode power in Watts or radiation flux density on the specimen in photons/mm<sup>2</sup> sec or, for electron beams, nanoamps or nanoamps/mm<sup>2</sup> sec.

\_\_\_\_\_  
Strength Value

\_\_\_\_\_  
Units

- ③ | **4. Source Beam Size**—List the X and Y values for the un-scanned excitation source size. Choose the X and Y axes to coincide with the manufacturer 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, insure that X and Y are orthogonal to each other and to the excitation source axis.

\_\_\_\_\_  
X Value ( $\mu\text{m}$ )

\_\_\_\_\_  
Y Value ( $\mu\text{m}$ )

- ③ | **5. Source Raster**

Yes  No

- ③ | **6. Source Beam Size at Specimen Surface**—Enter the X and Y dimensions, in m, of the excitation beam at the specimen surface. Note that this can differ from the source beam size entered previously by virtue of beam rastering or a non-normal angle of incidence on the specimen, or both.

\_\_\_\_\_  
X Value ( $\mu\text{m}$ )

\_\_\_\_\_  
Y Value ( $\mu\text{m}$ )

- ③ | **7. Raster Frame Rate**—Give the time required to return the beam to a given spot on the sample (in Hertz) if the source is scanned over the sample.

\_\_\_\_\_

- ② | **8. Analyzer Resolution**—Enter the percent resolution used in the measurement on the left line below if the analyzer is operated with a constant retarding ratio. If the analyzer is operated at a constant pass energy, specify the analyzer energy resolution (not the system resolution) used on the right line below.

\_\_\_\_\_  
in % (constant retarding ratio) or in eV (constant pass)

- ① | **9. Analyzer Constants**—Enter either the retarding ratio used in the measurement or the pass energy in eV.

\_\_\_\_\_  
Retard Ratio

or

\_\_\_\_\_  
Pass Energy (eV)

---

 Parameter Set # \_\_\_\_\_
 

---

For fields 10-11 below, the X and Y axes are the axes defined on the scattering geometry figure from Section C. If an analytical expression is available for the energy dependence of either the analyzer width or acceptance angle, enter it in the comment field 20, Section C.

The throughput, or entendue, of an instrument analyzer can be described by the system analyzer lateral width, called Analyzer Width here, and the Analyzer Angular Acceptance Width solid angle at the sample plane. Normally, electron optics require that one or both of these parameters vary with the energy of the electrons being analyzed.

Some instrument designs could have neither the analyzer width nor the analyzer acceptance width vary, but they do so at the expense of efficiency; therefore, they are not common. As a result, the answer "Energy Dependent" should be indicated for either or both 10 or 11 below.

- ③ | **10. Analyzer Widths**—Enter the size, in  $\mu\text{m}$ , of the analyzer entrance slit image projected onto the specimen surface. This is the analyzer "field of view" expressed in terms of the dimensions of the region on the specimen being analyzed, which may be energy dependent.

Was the analyzer width constant with energy?

Constant       Energy Dependent

If energy dependent, enter the electron energy at which the widths were measured.

\_\_\_\_\_

X Value ( $\mu\text{m}$ )      Y Value ( $\mu\text{m}$ )      at Energy (eV)

- ③ | **11. Analyzer Angular Acceptance Width**—Enter, in degrees, the angle (FWHM) for the signal to reach the analyzer in the X direction. The acceptance angle is centered about the acceptance angle from the analyzer axis (which is  $0^\circ$  for a spherical sector analyzer and  $42.3^\circ$  for a CMA).

Was the analyzer angular acceptance angle constant with energy?

Constant       Energy Dependent

If energy dependent, enter the electron energy at which the angles were measured.

\_\_\_\_\_

X Angle (degrees)      Y Angle (degrees)      at Energy (eV)

Spectrum # \_\_\_\_\_

For *each* spectrum—including calibration spectra—submitted, complete one copy of Section F.

Incomplete items for this copy should be (check one):  left blank or  replaced by answers from Section F, spectrum # \_\_\_\_\_.

## F. Spectrum Parameters

- ① | **1. Spectrum #**—Number the spectra in the data record serially from 1. Begin numbering with the required survey spectrum, followed by the spectra to be published in SSS in the order in which they should appear in the journal, followed by other spectra not to be published, and, finally, followed by calibration spectra not to be published.

\_\_\_\_\_

- ① | **2. Suggested Publication Status of This Spectrum**

- Print in *Surface Science Spectra*  
 Enter in AVS electronic database only

- ① | **3. Spectrum File Name**—Enter the file name of this spectrum as designated on the magnetic media submitted.

\_\_\_\_\_

- ① | **4. Is This a Calibration Spectrum?**

- Yes       No

- ① | **5. Parameter Set # to Use**—Provide the number identifier (Field 1, Section E) for the set of instrument parameters used to measure this spectrum.

\_\_\_\_\_

- ③ | **6. Date**—Enter the date that the spectrum for this region was measured. The format is YYYYMMDD.

\_\_\_\_\_

- ② | **7. Species Label**—Provide the symbol for the element being measured in this spectral region, e.g., Cl, N, etc. More than one element may be represented. If this is a survey spectrum, enter “survey;” if a valence band spectrum, enter “valence band.”

\_\_\_\_\_

- ② | **8. Transition Label**—Record the core-level transition that is producing this spectrum, e.g., “KLL” for AES, “2p” for XPS, etc. List the corresponding transitions in the same order as you listed the elements in Field 7 previously. If the spectrum is a survey, enter “survey;” if a valence band spectrum, enter “valence band.” The transition label(s) must agree with those indicated on the figure (see page 9)

\_\_\_\_\_

\_\_\_\_\_

- ⑤ | **9. Spectral Region Comment**—Enter comments describing the spectrum more fully when the element and transition do not adequately characterize the spectrum. For example, provide information about critical experimental variables (temperature, etc.) that should be emphasized or provide comments on the identification of peaks arising from multiple chemical states, satellites, interference between peaks, etc. in the spectrum.

\_\_\_\_\_

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\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

- ① | **10. Abscissa Label**—Check the appropriate box for the energy axis.

- Kinetic Energy       Binding Energy

Spectrum # \_\_\_\_\_

- ① | **11. Abscissa Values**—Enter the energy, in eV, of the first datum point displayed on the left in the spectrum plot and the energy increment, in eV/channel, used in the energy scan of this spectrum. For display purposes, Auger kinetic energies will increase from left to right (positive increment value), and XPS binding energies will decrease going from left to right (negative increment value).

\_\_\_\_\_  
Starting Value\_\_\_\_\_  
Increment Value

- ① | **12. Ordinate Label**—Specify the Y axis label, such as intensity, etc.

\_\_\_\_\_

- ① | **13. Ordinate Units**—Specify the units of signal in each channel, such as “counts,” “counts/sec,” etc. For AES spectra measured with a V/F conversion, or normalized spectra (e.g. synchrotron measurements), enter “arbitrary units” and explain in field F-21.

\_\_\_\_\_

- ① | **14. Number of Data Channels**—Specify the total number of data points in the measured spectrum.

\_\_\_\_\_

- ② | **15. Number of Scans**—Specify the number of times the signal for a given channel was counted.

\_\_\_\_\_

- ② | **16. Signal Mode**—Check the appropriate box to identify the data acquisition mode: direct for an analog measurement that is then digitized; V/F for an analog signal digitized using an analog-to-digit converter; pulse single for single-channel pulse counting; multichannel pulse for counting a position-sensitive detector; and multichannel indirect for a multichannel detector with photon conversion.

 Direct Analog     V/F Analog     Pulse Single Channel

 Multichannel Pulse     Multichannel Indirect (photon)

- ① | **17. Detector Width**—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, Field 11, Section C.) For a single-channel detector, the width can be listed as the eV/step in the spectral data.

\_\_\_\_\_

\_\_\_\_\_

- ② | **18. Total Signal Accumulation Time**—Enter the time, in seconds, spent accumulating data into displayed channels.

\_\_\_\_\_ seconds

- ① | **19. Total Elapsed Time**—Enter the time, in seconds, it took to complete the acquisition of the spectral data. The total elapsed time includes the “Signal Accumulation Time,” the settling time, and the overscan time.

\_\_\_\_\_ seconds

- ④ | **20. Signal Intensity Correction**—Does the spectral data in the “raw data” file include any corrections for detector saturation, counter response, noise spikes, source intensity variations, etc.?

 Yes     No

- ④ | **21. Signal Intensity Correction Comment**—If corrections were made to the data, please describe how they were made.

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

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Spectrum # \_\_\_\_\_

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- ① | **22. Signal Modulation Method**—Check the appropriate field for the signal modulation. Describe any tailored modulation function in Field 2, section H. Note that only “raw” data, not computer-differentiated data, should be submitted.

- None
- Sinusoidal (sinusoidal modulation/demodulation)
- Tailored (using special modulation function)
- Beam Blanking (chopped beam modulation)
- Beam Amplitude (modulated beam strength)

- ② | **23. Lock-in Parameters**—Complete only if appropriate.

\_\_\_\_\_  
Peak-to-peak amplitude of the modulation in eV or nA

\_\_\_\_\_  
Modulation frequency of the reference signal in Hz

\_\_\_\_\_  
Time constant of the lock-in amplifier used in seconds

Copy # \_\_\_\_\_

For **each** experimental variable in the submission, complete one copy of Section G.

### G. Experimental Variables

Some data records document spectral changes resulting from controlled variations in an independent variable, e.g., take-off angle for angle-resolved measurements, temperature for thermal studies, gas exposure for adsorption studies, etc. Typically, such data records will include a survey spectrum characterizing the initial specimen conditions, one or more sets of spectra for each value of the independent variable, and, possibly, a final set of spectra characterizing the specimen condition at the end of the study. This section provides the means for documenting the independent variable in such studies. If more than one parameter is varied, make a copy of this section for each variable. This section need not be submitted if there was no experimental variable.

In some cases (e.g., angle-resolved measurements), the experimental variable will correspond to an entry in another section of this form. In such cases, enter "v" or "variable" as the entry in the section. In the example of angle-resolved studies, "variable" would be entered for both the Emission Angle and Incident Angle Fields in the geometry table in Section C. In this case, the incident angle can be derived from the emission angle value, and it is only necessary to record the variation of one of the two angles (preferably the emission angle) in this section.

- ⑤ | **1. Experimental Variable Label**—Enter a concise label, suitable for annotation of the published spectra, describing the experimental parameter that is being varied, for example, "sputter time," "emission angle," "temperature," or "gas dose."

\_\_\_\_\_

- ⑤ | **2. Experimental Variable Units**—Enter the unit of measurement for the experimental parameter that is being varied. The use of SI units is preferred. Examples of appropriate units are: "seconds," "degrees," "Kelvin," and "Langmuirs."

\_\_\_\_\_

- ⑤ | **3. Experimental Variable Values**—Enter the numerical value (in the units declared in the Experimental Variable Units field) for the experimental variable. The value array is keyed to the Spectrum Number (Field 1, Section F). For each value, enter the number of the spectrum or spectra taken when the experimental variable had this value.

Value				
Spectrum #				

Value				
Spectrum #				

Value				
Spectrum #				

Value				
Spectrum #				

Value				
Spectrum #				

Value				
Spectrum #				

- ⑤ | **4. Experimental Variable Comment**—Enter information concerning this variable parameter experiment and its significance.

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_

\_\_\_\_\_



## I. Spectral Features Descriptions

- ② | **1. Major Elements**—List the principal elements identified in the spectra submitted in this record.

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- ② | **2. Minor Elements**—List the trace elements identified that appear in the spectra submitted in this record.

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The following three fields define the quantitative portions of the feature table on the next page. Completing the following fields is mandatory if any data are present in the Features Table (Field 6, next page).

- ③ | **3. Peak Amplitude Method**

Peak Height       Peak Area

- ③ | **4. Peak Amplitude Units**

Total Counts       Counts/sec  
 Normalized to a selected peak intensity  
 eV x counts       eV x counts/sec

- ③ | **5. Concentration Units**

Atomic %       Weight %       Monolayers  
 mg/m<sup>2</sup>       Other





### Appendix: Contributor's Comments

**Comments for the Editors**—Please add any comments or suggestions you might have concerning this form or Surface Science Spectra. We value your feedback.

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**Checklist**—A complete submission must include the following:

- Completed AES/XPS Contributors Form (3 copies).
- Hard copies of all spectra (3 copies).
- Digitized RAW spectra on magnetic disk.

**Reviewer Recommendations**—Please list three names and contact information for potential reviewers of your submission:

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Record the disk characteristics below:

Medium (e.g., high-density 3.5" floppy).

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Data Format (e.g., PHI: .DIF files).

---

Data Files Source (e.g., MS-DOS, HP BASIC).

---

Mail completed Contributor Form to:

**SSS Editorial Office**  
**Caller Box 13994**  
**100 Park Drive, Suite 105**  
**Research Triangle Park, NC 27709**  
**Phone: (919) 361-2498**  
**Fax: (919) 361-1378**  
**E-Mail: sss@jvst.org**

**End of the AES/XPS Contributors Form.**

## Manufacturer Information: PHI XPS Systems

Dr. Kenneth D. Bomben  
Physical Electronics, Inc.

The following information was supplied for PHI Models 5100, 5200, 5300, 5400, 5500, 5600, and 5700 XPS Systems including the 5000LS, 5500LS, 5600LS, and 5700LS.

The items appearing in bold italic capital letters are the required answers for the *Surface Science Spectra* Contributors Form. Items marked with an asterisk (\*) are user-supplied or user-selected. Other information is provided to help users determine which answer best describes their system parameters.

### Section C. Overall Instrument Description

#### Line 1. Spectrometer Manufacturer

**PHYSICAL ELECTRONICS. INCORPORATED**

#### Line 2. Manufacturer Model #

**5100** . . . . . single channel detector (SCD), four-element lens  
**5200** . . . . . SCD, Omni Focus lens  
**5300** . . . . . position sensitive detector (PSD), four-element lens  
**5400** . . . . . PSD, Omni Focus lens  
**5500. 5600 or 5700** . . . . . multi-channel detector (MCD), Omni Focus lens  
**5000LS** . . . . . SCD or PSD and either lens  
**5500LS. 5600LS or 5700LS** . . . . . MCD, Omni Focus lens

#### Line 3. Analyzer Type

**SPHERICAL SECTION ANALYZER**

#### Line 4. Non-standard Analyzer or Lens

\*

#### Line 5. Acceptance Angle from Analyzer Axis

**0°**

#### Line 6. Constant Pass Energy

**CONSTANT PASS ENERGY** . . . . . 5100, 5200, 5300, 5400 and 5000LS, 5500, 5500LS  
**\*(choice of FAT or FRR)** . . . . . 5600, 5600LS, 5700, and 5700LS

#### Line 7. Instrument Throughput Function

**1/E** . . . . . Four-element lens  
**1/E** . . . . . Omni Focus I and IA . . . . . (Large Area Mode)  
**1** . . . . . (Small Area Mode)  
**1** . . . . . Omni Focus II, III, IV and V: . . . . . (FAT Mode, all area modes)  
**E** . . . . . (FRR Mode)

#### Line 8. Instrument Throughput Function Comment

\*

#### Line 9. Excitation Source Label

\*

#### Line 10. Excitation Source Window or Filter

**2 μm AL** . . . . . for conventional X-ray sources  
**NO WINDOW** . . . . . for any model monochromator

**Section C. Overall Instrument Description (continued)****Line 11. Detector Description**

*SINGLE CHANNELTRON* . . . . . 5100 and 5200  
*POSITION SENSITIVE* . . . . . 5300 and 5400  
 \* (has either SCD or PSD) . . . . . 5000LS  
*MULTICHANNEL RESISTIVE PLATE* . . . . . 5500, 5600, 5700, 5500LS, 5600LS, and 5700LS

**Line 12. Number of Detector Elements**

*1* . . . . . 5100 and 5200  
*64* . . . . . 5300 and 5400  
 \* (has either SCD or PSD) . . . . . 5000LS  
*16* . . . . . 5500, 5600, 5700, 5500LS, 5600LS, and 5700LS

**Line 13. Ion Gun Manufacturer and Model #**

*PHI MODEL 04-303 OR MODEL 04-303A* . . . . . 5 kV Ion Gun  
*PHI MODEL 04-300* . . . . . 4 kV Ion Gun

**Line 14. Sputtering Current Measurement Method**

\*

**Line 15. Ion Gun Operating Parameters**

\*

**Line 16. Ion Gun Spot Size**

Note: These are minimum spot sizes. Beam conditions required to achieve minimum size vary from component to component.

*200 μm*: 04-303 or 04-303A on 5100, 5200, 5300, 5400, or 5000LS  
*250 μm*: 04-303 or 04-303A on 5500, 5600, 5700, 5500LS, 5600LS, or 5700LS  
*800 μm*: 04-300

**Line 17. Ion Gun Raster Parameters**

\*

**Line 18. Sputtering Comments**

\*

**Table 19. Angles**

Note: Emission angle varies from 0° to 90°. These values assume 45° (sample is horizontal). The angles that change with different tilt are noted with a dagger (†).

Conventional X-Ray Source		Monochromator X-Ray Source	
Emission Angle	45°	Emission Angle	45°
Incident Angle †	9°	Incident Angle †	45°
Source-to-Analyzer Angle	53.8°	Source-to-Analyzer Angle	90°
Specimen Azimuthal Angle	0°		
Sputter Source Incident Angle	40°		
Sputter Source Polar Angle	45°		
Sputter Source Azimuthal Angle	111°		

**Line 20. Angular Geometry Comments**

\*

**Section E. Variable Instrument Parameters**

**Line 4. Source Beam Size**

X Value (µm): . . . . . *>25 mm* . . . . . Conventional X-ray source (flood source)  
 . . . . . *2 mm* . . . . . Model 10-400 monochromator  
 . . . . . *1 mm* . . . . . 10-410 and 10-420 monochromator (point mode)  
 . . . . . *2 mm* . . . . . 10-410 and 10-420 monochromator (area mode)  
 Y Value (µm): . . . . . *>25 mm* . . . . . Conventional X-ray source (flood source)  
 . . . . . *2 mm* . . . . . Model 10-400 monochromator  
 . . . . . *1.2 mm* . . . . . 10-410 and 10-420 monochromator (point mode)  
 . . . . . *5 mm* . . . . . 10-410 and 10-420 monochromator (area mode)

**Line 5. Source Raster**

*NO*

**Line 6. Source Beam Size at Specimen Surface**

\* (Note: For all systems, beam size varies as the sine of the angle in X and is unchanged in Y from the values given in Line 4.)

**Line 7. Raster Frame Rate**

No Answer

**Line 8. Analyzer Resolution**

In % (constant retarding ratio): . . . . . \*

In eV (constant pass): . . . . . 1% of the pass energy (SCD and MCD)  
 . . . . . 1.5% of the pass energy (PSD)

**Line 9. Analyzer Constants**

\*

**Line 10. Analyzer Width**

Energy Dependent: . . . . . *NO*

X and Y Values: . . . . . *3x10 mm* . . . . . Four-element len  
 . . . . . \* (See tables below) . . . . . Omni Focus lens

At Energy: . . . . . *ALL*

X and Y Values for the Omni Focus and Omni Focus II Lenses:

Aperture Number	Software Setting	
	Small-Area Mode	Large-Area Mode
1	200 µm	500 µm
2	600 µm	2 mm
3	1.1 mm	4 mm
4	1 x 3.5 mm	3 x 10 mm

**Section E. Variable Instrument Parameters (continued)**

X and Y Values for the Omni Focus III Lens:

Aperture Number	Software Setting		
	Minimum-Area Mode	Small-Area Mode	Large-Area Mode
1	75 μm	—	—
2	150 μm	200 μm	500 μm
3	400 μm	600 μm	2 mm
4	800 μm	1.1 mm	4 mm
5	0.8 x 2 mm	1 x 3.5 mm	3 x 10 mm

X and Y Values for the Omni Focus IV and V Lenses:

Aperture Number	Software Setting		
	Minimum-Area Mode	Small-Area Mode	Large-Area Mode
1	30 μm	—	—
2	120 μm	175 μm	400 μm
3	400 μm	600 μm	2 mm
4	800 μm	1.1 mm	4 mm
5	0.8 x 2 mm	1 x 3.5 mm	3 x 10 mm

**Line 11. Analyzer Angular Acceptance Width**

Constant with Energy: . . . . . **NO**<sup>@</sup>

X and Y Angles: . . . . . **4**<sup>°</sup> . . . . . Four-element lens

. . . . . \*(See tables below) . . . . . Omni Focus lens

At Energy. . . . . **ALL**<sup>@</sup>

<sup>@</sup>Acceptance angles are constant at low retard ratios and decrease at high retard ratios. The acceptance angles noted in the following tables are the largest possible values and are most accurate in the regime where the acceptance angle is constant.

Omni Focus and Omni Focus II Lenses:

	Software Setting	
	Small-Area Mode	Large-Area Mode
<b>Solid Angle</b>	20°	6°

**Section E. Variable Instrument Parameters (continued)**

Omni Focus III, IV, and V Lenses:

	Software Setting		
	Minimum-Area Mode	Small-Area Mode	Large-Area Mode
<b>Solid Angle</b>	14°	10°	4°

Note: 75 μm analysis area has a solid angle of 10°.  
 30 μm analysis area has a solid angle of 8°.

**Section F. Spectral Parameters**

**Line 16. Signal Mode**

*DIRECT ANALOG* . . . . . SCD  
*MULTICHANNEL PULSE* . . . . . PSD and MCD

**Line 17. Detector Width**

1% of the pass energy (SCD and MCD)  
 1.5% of the pass energy (PSD)

**Line 20. Signal Intensity Correction**

*NO* (Displayed raw data does not contain corrections. The user may specify additional corrections and these are noted in the original Y axis label.)

**Line 21. Signal Modulation Method**

*NONE*

**Line 22. Lock-in Parameters**

*NONE*