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# HAXPES reference spectra of bulk Mo and MoSe<sub>2</sub> with Cr K<sub>α</sub> excitation

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(Received day Month year; accepted day Month year; published day Month year)

Monochromatic Cr K<sub>α</sub> radiation (5414.8 eV) was used to acquire high-energy photoelectron spectroscopy (HAXPES) data on pure Mo and bulk MoSe<sub>2</sub> compound with special attention paid to binding energy scale correction and quantification. The reported spectra include a survey scan and high-resolution Mo 2s, Mo 2p<sub>1/2</sub>, Mo 2p<sub>3/2</sub>, Mo 3d, Mo 3p<sub>1/2</sub>, Mo 3p<sub>3/2</sub>, Mo 3s, Mo 4s, Mo 4p, Se 2s, Se 2p<sub>1/2</sub>, Se 2p<sub>3/2</sub>, Se 3s, Se 3p<sub>1/2</sub>, Se 3p<sub>3/2</sub>, and Se 3d core-levels. The data will be useful as reference core-level spectra for HAXPES studies on molybdenum and its compounds.

**Keywords:** Mo, MoSe<sub>2</sub>, HAXPES, Cr K<sub>α</sub>

## INTRODUCTION

Mo and its compounds are widely used in mechanics, electronics and phototonics, as well as in chemistry and catalysis. Recently developed laboratory based hard x-ray photoelectron spectrometers (HAXPES) allow to excite deeper core-levels, enabling different probing depths as a function of the studied core-level. In the case of Mo and MoSe<sub>2</sub>, Cr K<sub>α</sub> radiation (5414.8 eV) allows to ionize all Mo and Se core-levels of principal quantum numbers N=2, 3 and 4. In this work, we report HAXPES spectra recorded on pure bulk Mo and MoSe<sub>2</sub> compound. The data include a survey scan and high-resolution spectra of Mo 2s, Mo 2p<sub>1/2</sub>, Mo 2p<sub>3/2</sub>, Mo 3d, Mo 3p<sub>1/2</sub>, Mo 3p<sub>3/2</sub>, Mo 3s, Mo 4s, Mo 4p, Se 2s, Se 2p<sub>1/2</sub>, Se 2p<sub>3/2</sub>, Se 3s, Se 3p<sub>1/2</sub>, Se 3p<sub>3/2</sub>, and Se 3d.

## SPECIMEN DESCRIPTION (ACCESSION # 01900)

**Specimen:** Mo

**CAS Registry #:** (Mo) 1317-33-5

**Specimen Characteristics:** Homogeneous; solid; polycrystalline; conductor; metal; Other

**Chemical Name:** Molybdenum

**Composition:** Mo

**Form:** Polycrystalline solid

**Structure:** Body-centered cubic

**History & Significance:** Air exposed thick Mo and bulk MoSe<sub>2</sub> samples

**As Received Condition:** Bulk Mo metal

**Analyzed Region:** Same as specimen

**Ex Situ Preparation/Mounting:** The sample was mounted on the sample holder using double sided conductive tape.

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**Accession#:** 01900, 01901

**Technique:** XPS

**Specimen:** Mo, MoSe<sub>2</sub>

**Instrument:** ULVAC-PHI Quantes

**Major Elements in Spectra:** Mo, Se

**Minor Elements in Spectra:** O, C

**Published Spectra:** 22

**Spectral Category:** Reference

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**In Situ Preparation:** The Mo sample was sputter cleaned by Ar<sup>+</sup> ions (2 keV) for 5 minutes prior to measurements to remove carbon and oxygen contamination.

**Charge Control:** Low-energy electrons (1 eV, filament 1.1 A) and low-energy Ar<sup>+</sup> ions (100 eV)

**Temp. During Analysis:** 300 K

**Pressure During Analysis:** < 2×10<sup>-7</sup> Pa

**Pre-analysis Beam Exposure:** 0 s

## SPECIMEN DESCRIPTION (ACCESSION # 01901)

**Specimen:** MoSe<sub>2</sub>

**CAS Registry #:** (MoSe<sub>2</sub>) 12058-18-3

**Specimen Characteristics:** Homogeneous; solid; polycrystalline; semiconductor -

**Chemical Name:** Molybdenum diselenide

**Composition:** MoSe<sub>2</sub>

**Form:** Polycrystalline solid

**Structure:** Hexagonal

**History & Significance:** Air exposed bulk MoSe<sub>2</sub> sample

**As Received Condition:** Bulk MoSe<sub>2</sub>

**Analyzed Region:** Same as specimen

**Ex Situ Preparation/Mounting:** The sample was mounted on the sample holder using double sided conductive tape.

**In Situ Preparation:** None

**Charge Control:** Low-energy electrons (1 eV, filament 1.1 A) and low-energy Ar<sup>+</sup> ions (100 eV)

**Temp. During Analysis:** 300 K

**Pressure During Analysis:** < 2×10<sup>-7</sup> Pa

<sup>a)</sup>Electronic mail: olivier.renault@cea.fr

**Pre-analysis Beam Exposure:** 0 s

## **INSTRUMENT DESCRIPTION**

**Manufacturer and Model:** ULVAC-PHI Quantex

**Analyzer Type:** spherical sector

**Detector:** multichannel resistive plate

**Number of Detector Elements:** 32

## **INSTRUMENT PARAMETERS COMMON TO ALL SPECTRA**

### **■ Spectrometer**

**Analyzer Mode:** constant pass energy

**Throughput ( $T=E^N$ ):** The energy dependence can be modeled using the following equation:  $\frac{A}{E_p} = \left(\frac{a^2}{a^2+R^2}\right)^b$ , where a and b are constants,  $E_p$  is the pass energy, A is the peak area and R is the retard ratio equal to  $E/E_p$ , where E is the kinetic energy. Three spectral regions are recorded on a sputter cleaned sample at different pass energies. The values of a and b are then determined by a linear least square fit of the data applying the equation described above.

**Excitation Source Window:** Al

**Excitation Source:** Cr  $K_\alpha$  monochromatic

**Source Energy:** 5414.8 eV

**Source Strength:** 50 W

**Source Beam Size:** 100  $\mu\text{m}$  x 100  $\mu\text{m}$

**Signal Mode:** multichannel direct

### **■ Geometry**

**Incident Angle:** 22 °

**Source-to-Analyzer Angle:** 46 °

**Emission Angle:** 45 °

**Specimen Azimuthal Angle:** 0 °

**Acceptance Angle from Analyzer Axis:** 0 °

**Analyzer Angular Acceptance Width:** 20 ° x 20 °

### **■ Ion Gun**

**Manufacturer and Model:** ULVAC-PHI Quantex

**Energy:** 2000 eV

**Current:** 0.001 mA

**Current Measurement Method:** Faraday cup

**Sputtering Species:** Ar

**Spot Size (unrastered):** 100  $\mu\text{m}$

**Raster Size:** 3000  $\mu\text{m}$  x 3000  $\mu\text{m}$

**Incident Angle:** 45 °

**Polar Angle:** 45 °

**Azimuthal Angle:** 45 °

**Comment:** Differentially pumped ion gun used for pre-sputtering of the sample and to prevent reoxidation during analysis.

## **DATA ANALYSIS METHOD**

**Energy Scale Correction:** The decrease of photoionization cross-sections in HAXPES (Refs. 1 and 2) leads to a very low intensity of the C 1s core-level peak which is often used to correct the energy scale. Also, in the case of metals, great care must be taken regarding the reliability of energy scale correction relying on the C 1s binding energy of adventitious carbon (Ref. 3). Therefore, the binding energy correction of the data of pure Mo was performed by first considering the binding energy of the Mo 3d<sub>5/2</sub> peak recorded with Al  $K_\alpha$  radiation on the sputter-clean surface referenced to the Fermi level, as determined from a fitting of the band onset. Then, the correction factor was found by aligning on this value the Mo 3d<sub>5/2</sub> binding energy measured with Cr  $K_\alpha$  radiation. Doing so, the Mo 3d<sub>5/2</sub> binding energy was 227.8 eV, in agreement with an average of 24 binding energy values published in the NIST Database (Ref. 4). The spectra recorded with the Cr  $K_\alpha$  source were then rescaled by shifting the Mo 3d<sub>5/2</sub> to 227.8 eV. Regarding bulk MoSe<sub>2</sub>, the C 1s peak in HAXPES is too weak to be considered for correction of the energy scale. In XPS, the strong Se Auger line completely overlaps the C 1s core line. Therefore, the energy correction of the HAXPES data is made by applying to all spectra an energy shift which is the difference between the Mo 3d<sub>5/2</sub> binding energy measured by XPS and the Mo 3d<sub>5/2</sub> binding energy measured by HAXPES. Doing so, the Mo 3d<sub>5/2</sub> binding energy was 228.9 eV, in good agreement with other data (Ref. 5). The spectra recorded with the Cr  $K_\alpha$  source were then rescaled by shifting the Mo 3d<sub>5/2</sub> to 228.9 eV.

**Recommended Energy Scale Shift:** -0.6 eV for bulk Mo and +0.4 eV for bulk MoSe<sub>2</sub>.

**Peak Shape and Background Method:** Shirley background was employed for peak area determination. No curve fitting was performed on the spectra.

**Quantitation Method:** PHI Multipak software Version 9.9.0.8 was used to perform quantification. The determined intensities were checked for repeatability by comparing, before and after acquisition, the intensities of the Mo 2s core-line of both samples on the one hand, and on the other hand the intensity of the Ag 3d line of a sputter-clean, bulk silver sample mounted on the same holder. In all cases the standard deviation in intensity was below 6%. Empirically determined sensitivity factors (RSFs) were provided by the software, from the most recently released RSF database. The RSFs were derived from the pure-element relative sensitivity factor as defined in ISO 18118:2015 (Ref 6) which were measured on pure element samples using a Cr  $K_\alpha$  source. They therefore account for the decrease of cross-section and different escape depth of photoelectrons using higher energy photons. RSFs are reported proportional to the RSF of F 1s equal to 1. Using the determined pure element RSF's leads to quantification error of ~5% for the MoSe<sub>2</sub> compound.

## **ACKNOWLEDGMENTS**

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## **AUTHOR DECLARATION**

*The authors have no conflict to disclose.*

## **DATA AVAILABILITY STATEMENT**

*The data that supports the findings of this study are available within the article and its supplementary material.*

## **REFERENCES**

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4. NIST X-ray Photoelectron Spectroscopy Database, ver 4.1, <http://dx.doi.org/10.18434/T4T88K>.
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6. International Organization for Standardization 2015, *Surface chemical analysis - Auger electron spectroscopy and X-ray photoelectron spectroscopy - Guide to the use of experimentally determined relative sensitivity factors for the quantitative analysis of homogeneous materials*, ISO 18118:2015.

| SPECTRAL FEATURES TABLE |                      |                  |                      |                        |                    |                       |                 |
|-------------------------|----------------------|------------------|----------------------|------------------------|--------------------|-----------------------|-----------------|
| Spectrum ID #           | Element/ Transition  | Peak Energy (eV) | Peak Width FWHM (eV) | Peak Area (eV x cts/s) | Sensitivity Factor | Concentration (at. %) | Peak Assignment |
| 01900-02                | Mo 2p <sub>3/2</sub> | 2521.0           | 2.36                 | 36812                  | 9.584              | ...                   | ...             |
| 01900-03                | Mo 2p <sub>1/2</sub> | 2625.8           | 2.40                 | 20306                  | 4.969              | ...                   | ...             |
| 01900-04                | Mo 2s                | 2866.7           | 4.17                 | 16358                  | 3.805              | ...                   | ...             |
| 01900-05                | Mo 3d                | 227.8            | 1.26                 | 3360                   | 1.103              | ...                   | ...             |
| 01900-06                | Mo 3p <sub>3/2</sub> | 393.7            | 2.81                 | 7093                   | 2.063              | ...                   | ...             |
| 01900-06                | Mo 3p <sub>1/2</sub> | 411.0            | 2.60                 | 3222                   | 1.134              | ...                   | ...             |
| 01900-07                | Mo 3s                | 505.3            | 6.25                 | 3969                   | 0.971              | ...                   | ...             |
| 01900-08                | Mo 4s                | 62.7             | 4.76                 | 1158                   | 0.284              | ...                   | ...             |
| 01900-09                | Mo 4p                | 35.4             | 3.54                 | 1558                   | 0.425              | ...                   | ...             |
| 01901-02                | Mo 2p <sub>3/2</sub> | 2521.9           | 2.37                 | 7307                   | 9.584              | ...                   | ...             |
| 01901-03                | Mo 2p <sub>1/2</sub> | 2626.9           | 2.36                 | 3897                   | 4.969              | ...                   | ...             |
| 01901-04                | Mo 2s                | 2867.9           | 4.47                 | 3459                   | 3.805              | ...                   | ...             |
| 01901-05                | Mo 3d, Se 3s         | 229.1            | 2.34                 | 1610                   | 1.103, 0.708       | ...                   | ...             |
| 01901-06                | Mo 3p <sub>3/2</sub> | 394.7            | 2.86                 | 1311                   | 2.063              | ...                   | ...             |
| 01901-06                | Mo 3p <sub>1/2</sub> | 412.3            | 2.58                 | 803                    | 1.134              | ...                   | ...             |
| 01901-07                | Mo 3s                | 506.8            | 4.93                 | 734                    | 0.971              | ...                   | ...             |
| 01901-08                | Mo 4s                | 63.2             | 3.04                 | 149                    | 0.284              | ...                   | ...             |
| 01901-08                | Se 3d                | 54.9             | 1.75                 | 216                    | 1.245              | ...                   | ...             |
| 01901-09                | Mo 4p                | 36.9             | 3.49                 | 311                    | 0.425              | ...                   | ...             |
| 01901-10                | Se 2p <sub>3/2</sub> | 1433.7           | 1.69                 | 6956                   | 5.135              | ...                   | ...             |
| 01901-11                | Se 2p <sub>1/2</sub> | 1474.6           | 1.69                 | 3915                   | 2.773              | ...                   | ...             |
| 01901-12                | Se 2s                | 1653.7           | 4.85                 | 5183                   | 3.355              | ...                   | ...             |
| 01901-13                | Se 3p <sub>3/2</sub> | 161.0            | 2.16                 | 841                    | 0.809              | ...                   | ...             |
| 01901-13                | Se 3p <sub>1/2</sub> | 166.6            | 2.24                 | 357                    | 0.436              | ...                   | ...             |

| ANALYZER CALIBRATION TABLE |                      |                  |                      |                        |                    |                       |                 |
|----------------------------|----------------------|------------------|----------------------|------------------------|--------------------|-----------------------|-----------------|
| Spectrum ID #              | Element/ Transition  | Peak Energy (eV) | Peak Width FWHM (eV) | Peak Area (eV x cts/s) | Sensitivity Factor | Concentration (at. %) | Peak Assignment |
| ...                        | Ag 3d <sub>5/2</sub> | 368.17           | 1.00                 | 724121                 | ...                | ...                   | ...             |
| ...                        | Cu 2p <sub>3/2</sub> | 932.61           | 0.99                 | 65630                  | ...                | ...                   | ...             |
| ...                        | Au 4f <sub>7/2</sub> | 83.96            | 0.83                 | 73825                  | ...                | ...                   | ...             |

Comment to Analyzer Calibration Table: The spectra in the analyzer calibration table were recorded using Al K<sub>α</sub> photons.

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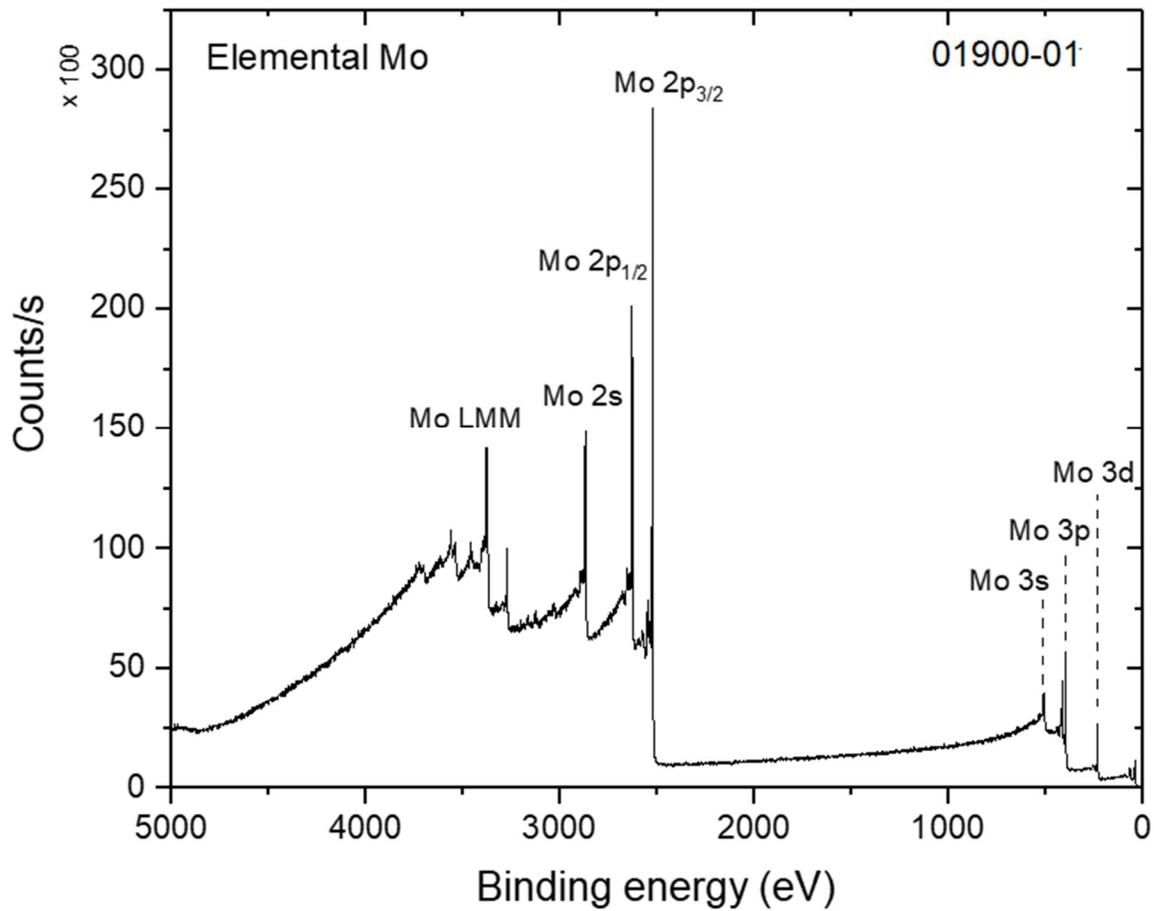
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**GUIDE TO FIGURES**

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| <b>Spectrum<br/>(Accession) #</b> | <b>Spectral Region</b>        | <b>Voltage Shift*</b> | <b>Multiplier</b> | <b>Baseline</b> | <b>Comment #</b> |
|-----------------------------------|-------------------------------|-----------------------|-------------------|-----------------|------------------|
| 01900-01                          | Survey                        | 0                     | 1                 | 0               | ...              |
| 01900-02                          | Mo $2p_{3/2}$                 | +0.6                  | 1                 | 0               | ...              |
| 01900-03                          | Mo $2p_{1/2}$                 | +0.6                  | 1                 | 0               | ...              |
| 01900-04                          | Mo 2s                         | +0.6                  | 1                 | 0               | ...              |
| 01900-05                          | Mo 3d                         | +0.6                  | 1                 | 0               | ...              |
| 01900-06                          | Mo 3p                         | +0.6                  | 1                 | 0               | ...              |
| 01900-07                          | Mo 3s                         | +0.6                  | 1                 | 0               | ...              |
| 01900-08                          | Mo 4s                         | +0.6                  | 1                 | 0               | ...              |
| 01900-09                          | Mo 4p                         | +0.6                  | 1                 | 0               | ...              |
| 01901-01                          | Survey                        | 0                     | 1                 | 0               |                  |
| 01901-02                          | Mo $2p_{3/2}$                 | -0.4                  | 1                 | 0               |                  |
| 01901-03                          | Mo $2p_{1/2}$                 | -0.4                  | 1                 | 0               |                  |
| 01901-04                          | Mo 2s                         | -0.4                  | 1                 | 0               |                  |
| 01901-05                          | Mo 3d, Se 3s                  | -0.4                  | 1                 | 0               |                  |
| 01901-06                          | Mo 3p                         | -0.4                  | 1                 | 0               |                  |
| 01901-07                          | Mo 3s                         | -0.4                  | 1                 | 0               |                  |
| 01901-08                          | Mo 4s, Se 3d                  | -0.4                  | 1                 | 0               |                  |
| 01901-09                          | Mo 4p                         | -0.4                  | 1                 | 0               |                  |
| 01901-10                          | Se $2p_{3/2}$                 | -0.4                  | 1                 | 0               |                  |
| 01901-11                          | Se $2p_{1/2}$                 | -0.4                  | 1                 | 0               |                  |
| 01901-12                          | Se 2s                         | -0.4                  | 1                 | 0               |                  |
| 01901-13                          | Se $3p_{3/2}$ , Se $3p_{1/2}$ | -0.4                  | 1                 | 0               |                  |

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Accession #

01900-01

■ Specimen

Mo

■ Technique

XPS

■ Spectral Region

Survey

Instrument

ULVAC-PHI Quantes

Excitation Source

Cr K<sub>α</sub> monochromatic

Source Energy

5414.8 eV

Source Strength

50 W

Source Size

0.1 mm x 0.1 mm

Analyzer Type

spherical sector analyzer

Incident Angle

22°

Emission Angle

45°

Analyzer Pass Energy

280 eV

Analyzer Resolution

2.33 eV

Total Signal Accumulation Time

5205 s

Total Elapsed Time

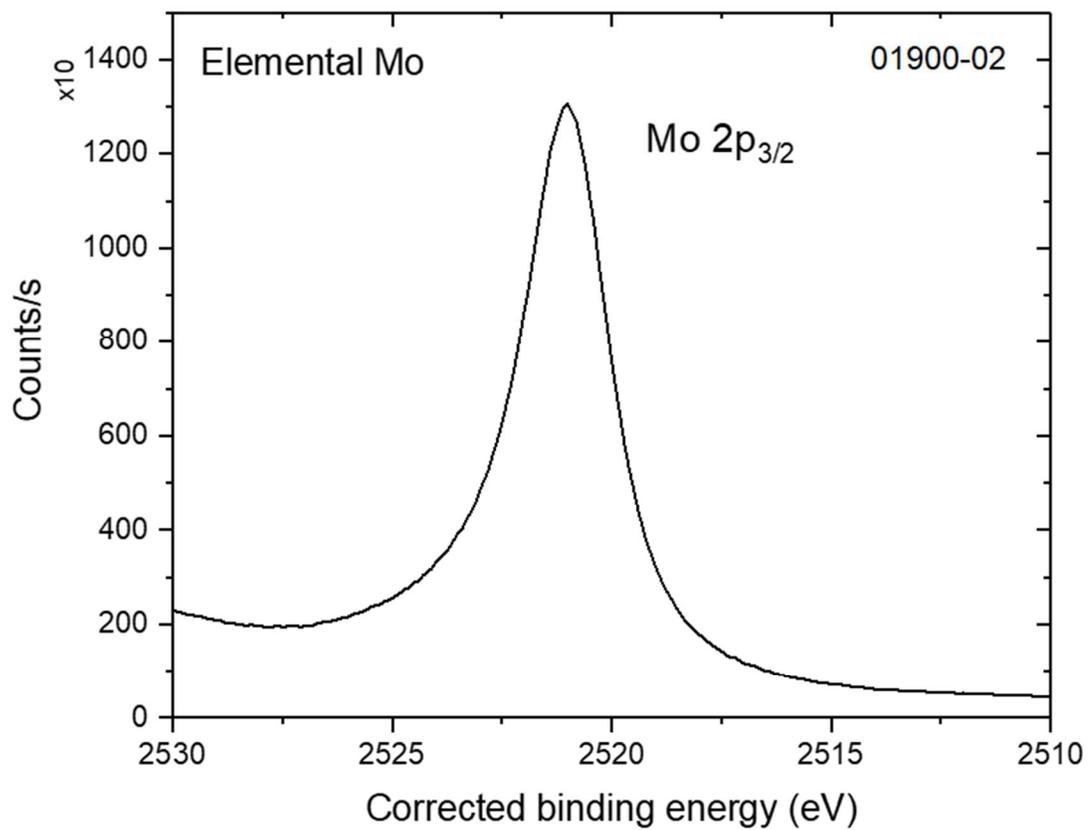
5760 s

Number of Scans

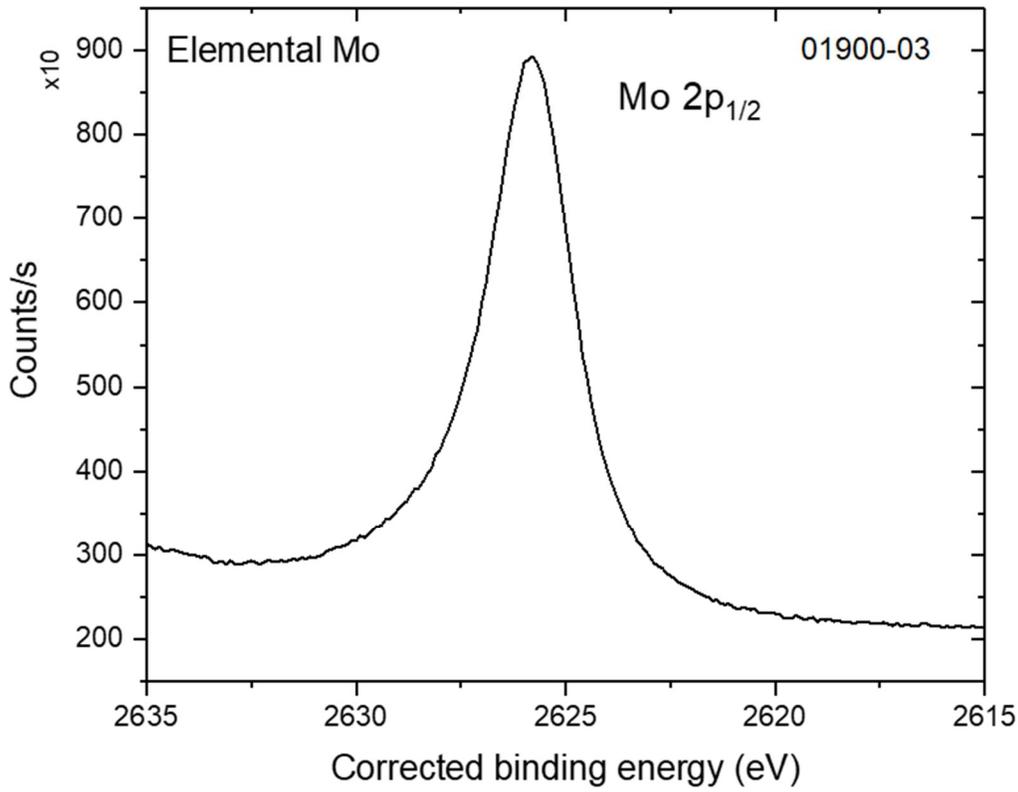
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Effective Detector Width

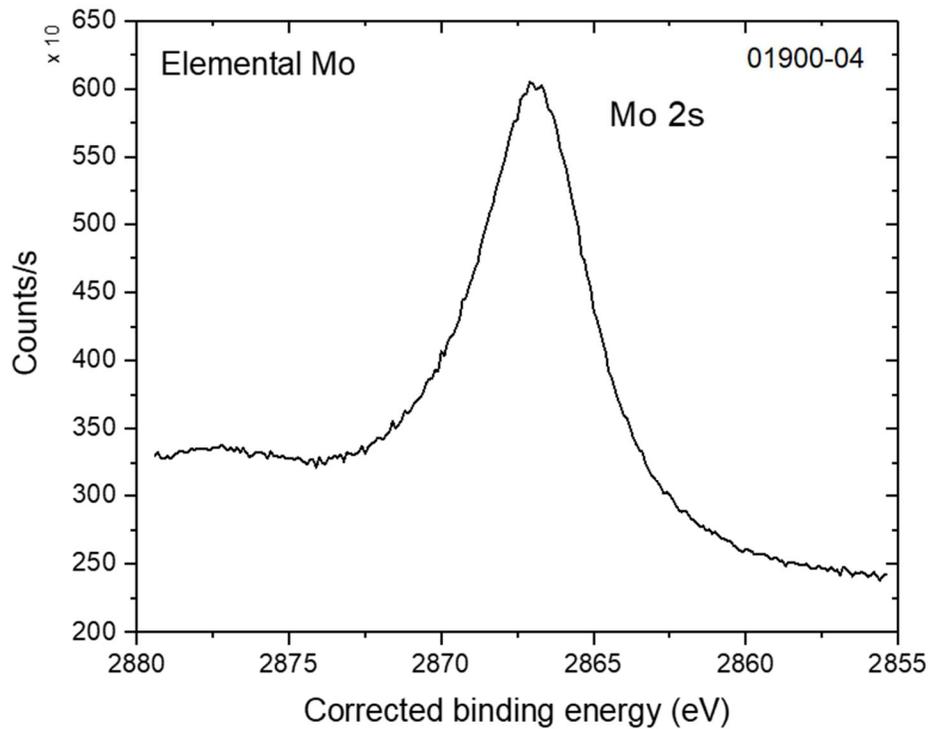
31 eV



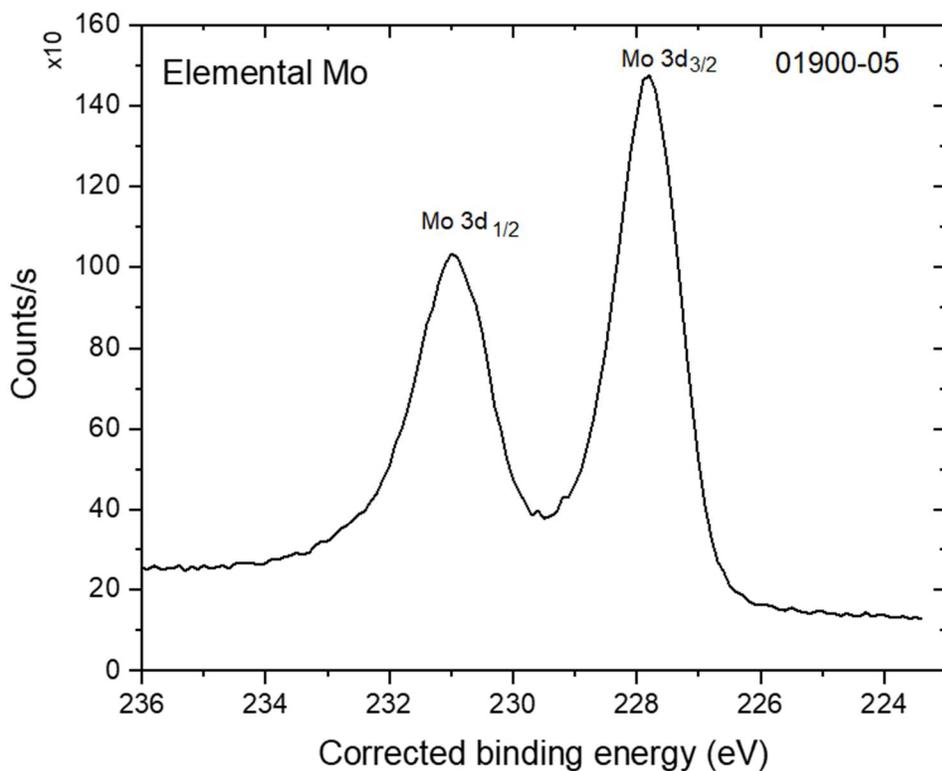
■ **Accession #:** 01900-02  
■ **Specimen:** Mo  
■ **Technique:** XPS  
■ **Spectral Region:** Mo  
*2p<sub>3/2</sub>*  
Instrument: ULVAC-PHI  
Quantes  
Excitation Source: Cr *K<sub>α</sub>*  
monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1  
mm  
Analyzer Type: spherical  
sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112  
eV  
Analyzer Resolution: 1.17  
eV  
Total Signal Accumulation  
Time: 3606 s  
Total Elapsed Time: 3978 s  
  
Number of Scans: 27  
  
Effective Detector Width:  
12.4 eV



■ **Accession #:** 01900-03  
■ **Specimen:** Mo  
■ **Technique:** XPS  
■ **Spectral Region:** Mo 2p<sub>1/2</sub>  
Instrument: ULVAC-PHI Quantes  
Excitation Source: Cr K<sub>α</sub> monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal  
Accumulation Time: 3606 s  
Total Elapsed Time: 3978 s  
Number of Scans: 27  
Effective Detector Width: 12.4 eV



■ **Accession #:** 01900-04  
■ **Specimen:** Mo  
■ **Technique:** XPS  
■ **Spectral Region:** Mo 2s  
Instrument: ULVAC-PHI  
Quantes  
Excitation Source: Cr  $K_{\alpha}$   
monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation  
Time: 876 s  
Total Elapsed Time: 960 s  
  
Number of Scans: 25  
  
Effective Detector Width: 12.4  
eV



■ **Accession #:** 01900-05

■ **Specimen:** Mo

■ **Technique:** XPS

■ **Spectral Region:** Mo 3d

Instrument: ULVAC-PHI  
Quantes

Excitation Source: Cr  $K_{\alpha}$   
monochromatic

Source Energy: 5414.8 eV

Source Strength: 50 W

Source Size: 0.1 mm x 0.1  
mm

Analyzer Type: spherical  
sector

Incident Angle: 22 °

Emission Angle: 45 °

Analyzer Pass Energy 112 eV

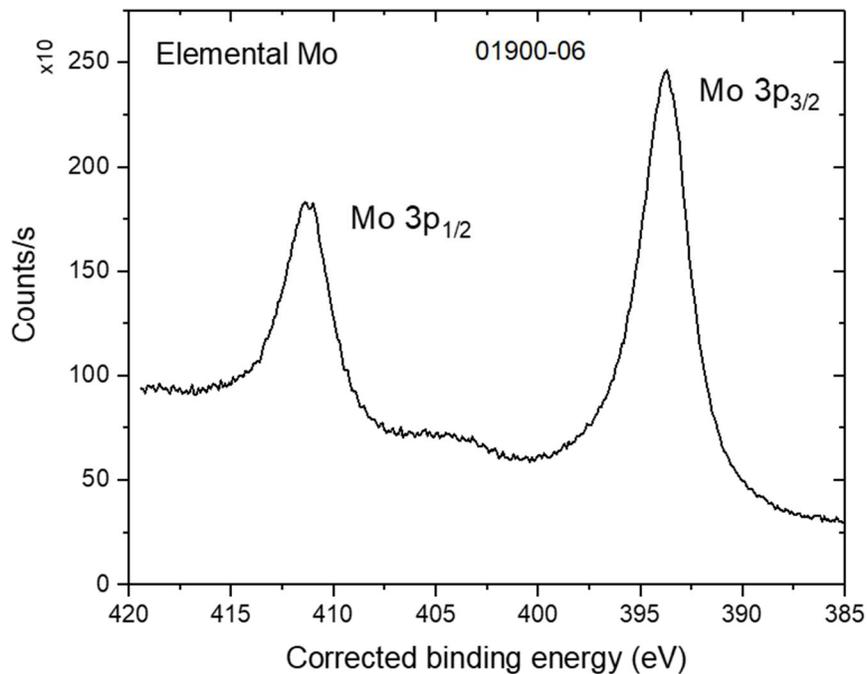
Analyzer Resolution: 1.17 eV

Total Signal Accumulation  
Time: 3660 s

Total Elapsed Time: 4032 s

Number of Scans: 36

Effective Detector Width: 12.4  
eV



■ **Accession #:** 01900-06

■ **Specimen:** Mo

■ **Technique:** XPS

■ **Spectral Region:** Mo 3p

Instrument: ULVAC-PHI  
Quantes

Excitation Source: Cr  $K_{\alpha}$   
monochromatic

Source Energy: 5414.8 eV

Source Strength: 50 W

Source Size: 0.1 mm x 0.1 mm

Analyzer Type: spherical sector

Incident Angle: 22 °

Emission Angle: 45 °

Analyzer Pass Energy 112 eV

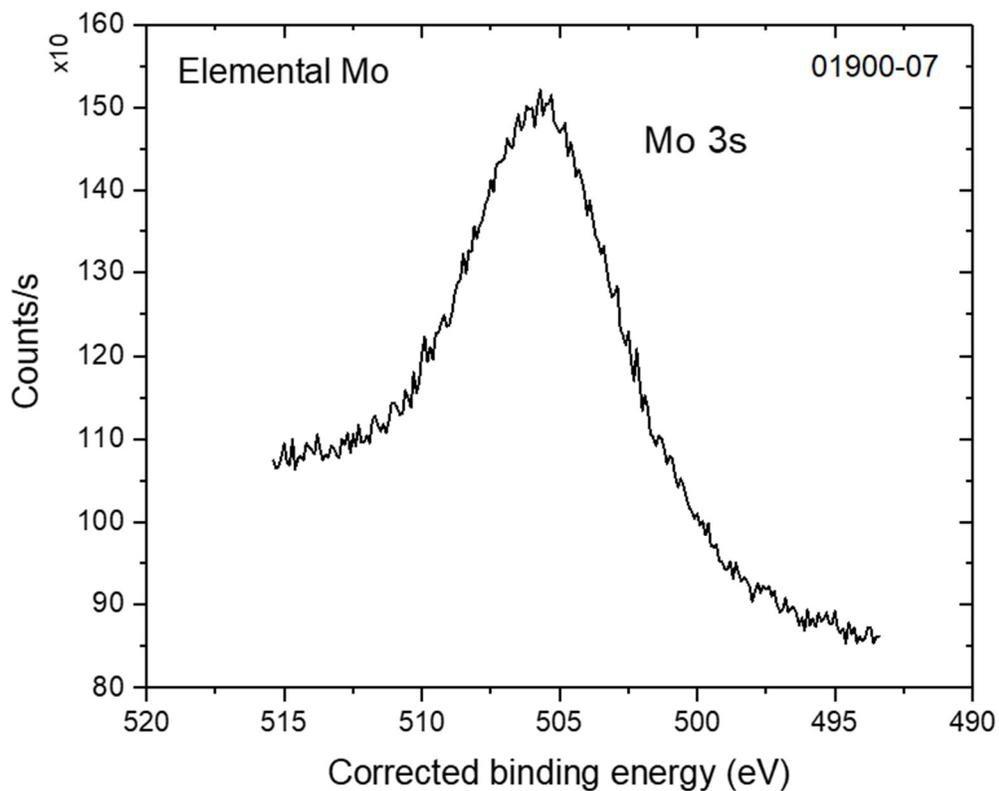
Analyzer Resolution: 1.17 eV

Total Signal Accumulation Time:  
3600 s

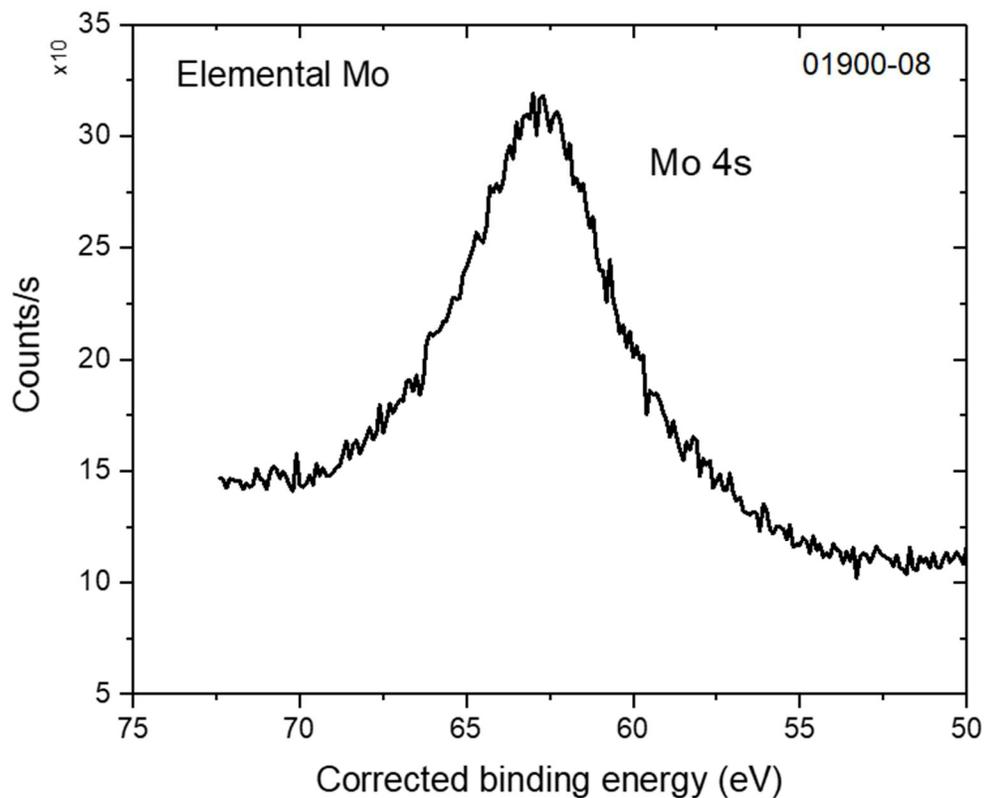
Total Elapsed Time: 3966 s

Number of Scans: 19

Effective Detector Width: 12.4  
eV



■ **Accession #:** 01900-07  
■ **Specimen:** Mo  
■ **Technique:** XPS  
■ **Spectral Region:** Mo 3s  
Instrument: ULVAC-PHI  
Quantes  
Excitation Source: Cr  $K_{\alpha}$   
monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation Time: 3576 s  
Total Elapsed Time: 3942 s  
Number of Scans: 26  
Effective Detector Width: 12.4 eV



■ Accession #: 01900-08

■ Specimen: Mo

■ Technique: XPS

■ Spectral Region: Mo 4s

Instrument: ULVAC-PHI Quantes

Excitation Source: Cr  $K_{\alpha}$  monochromatic

Source Energy: 5414.8 eV

Source Strength: 50 W

Source Size: 0.1 mm x 0.1 mm

Analyzer Type: spherical sector

Incident Angle: 22 °

Emission Angle: 45 °

Analyzer Pass Energy 112 eV

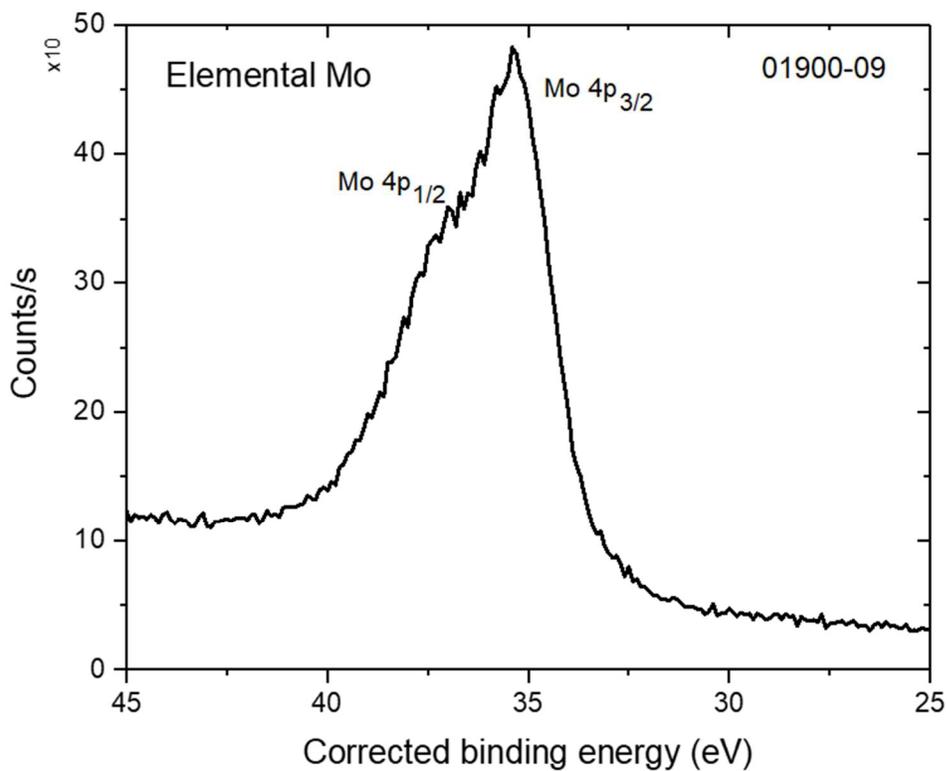
Analyzer Resolution: 1.17 eV

Total Signal Accumulation Time: 3684 s

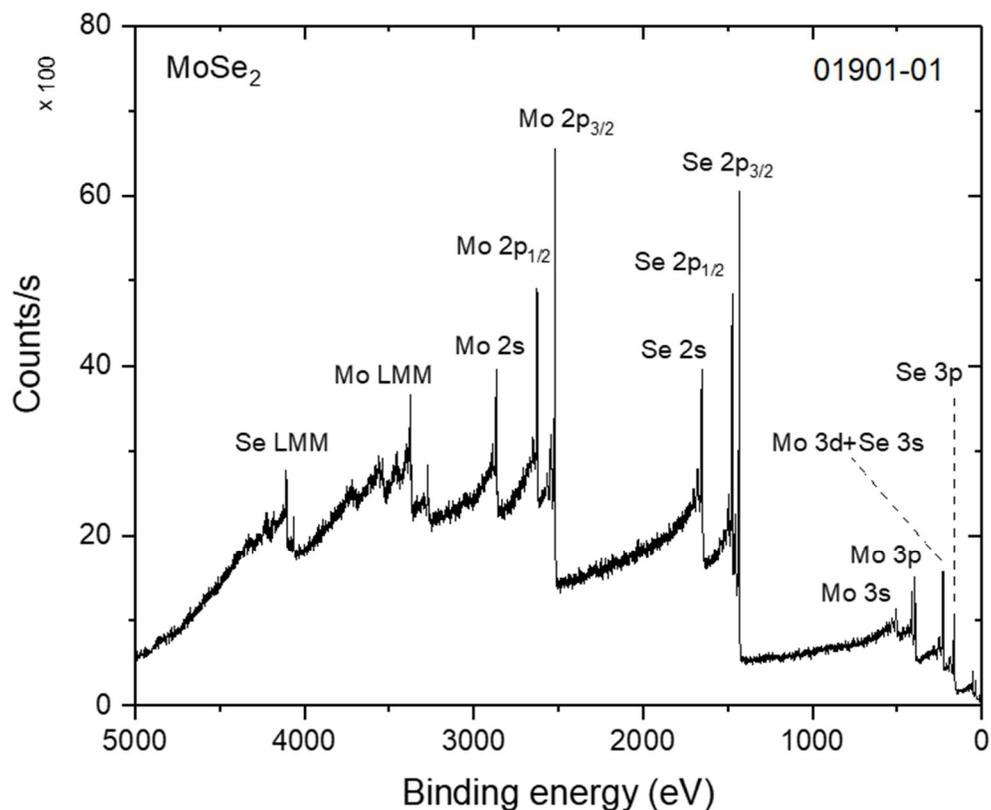
Total Elapsed Time: 4056 s

Number of Scans: 26

Effective Detector Width: 12.4 eV

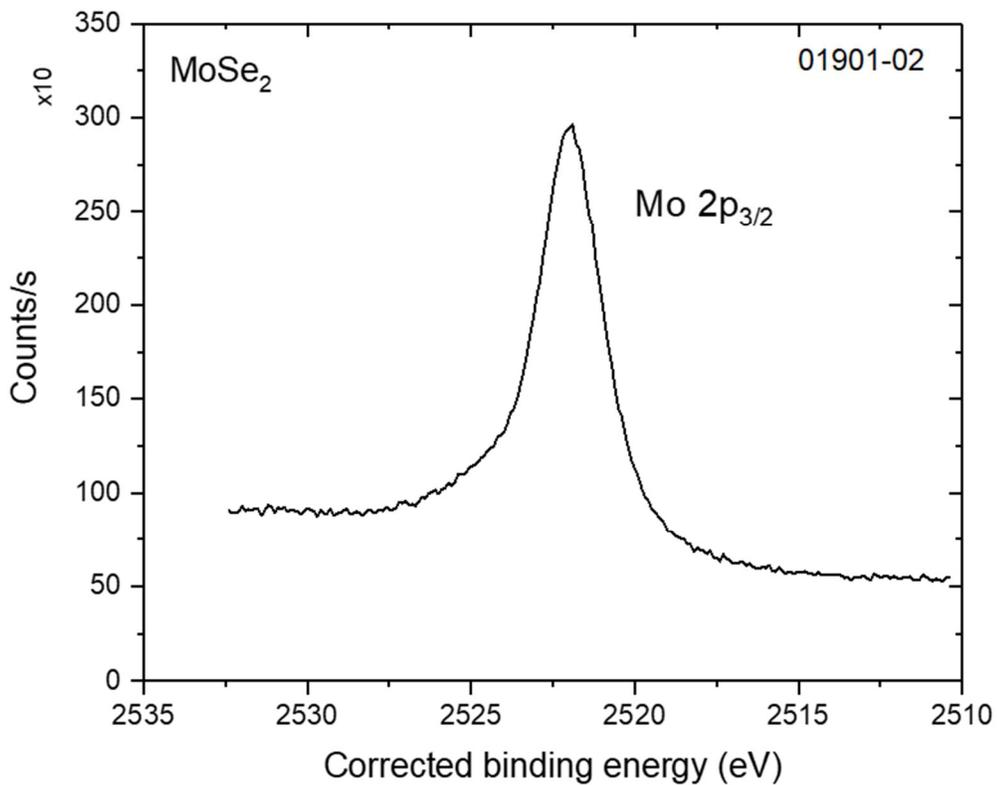


■ **Accession #:** 01900-09  
■ **Specimen:** Mo  
■ **Technique:** XPS  
■ **Spectral Region:** Mo 4p  
Instrument: ULVAC-PHI  
Quantes  
Excitation Source: Cr  $K_{\alpha}$   
monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation Time: 3576 s  
Total Elapsed Time: 3942 s  
Number of Scans: 26  
Effective Detector Width: 12.4 eV

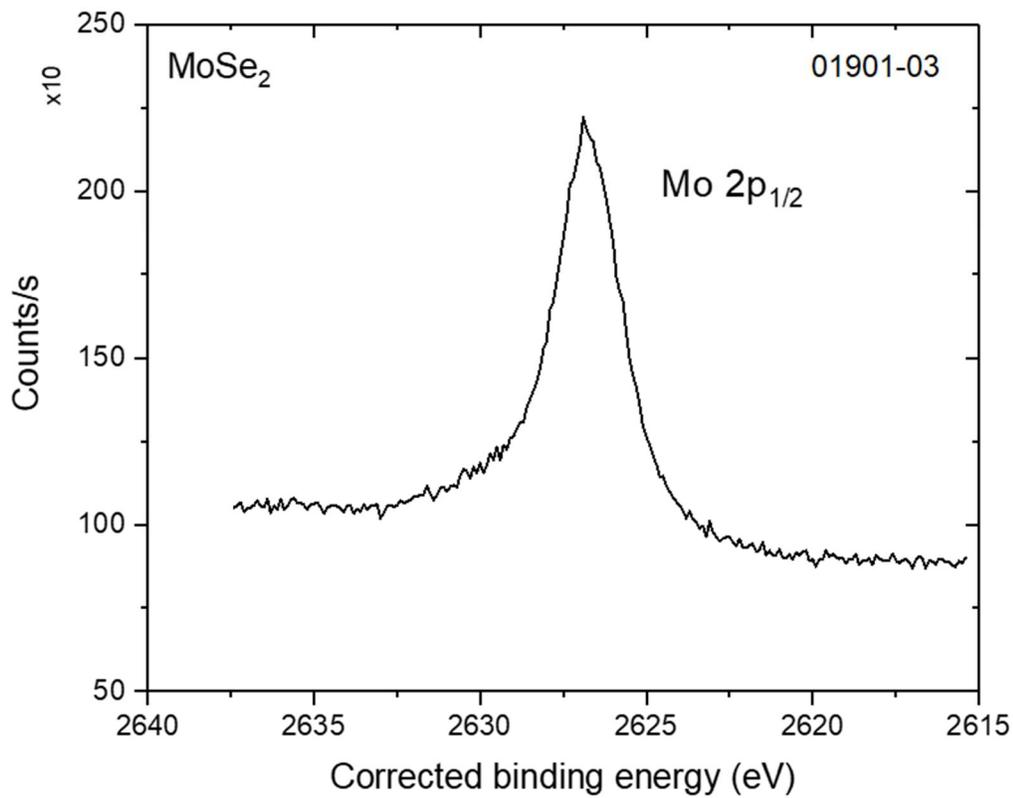


Accession # 01901-01

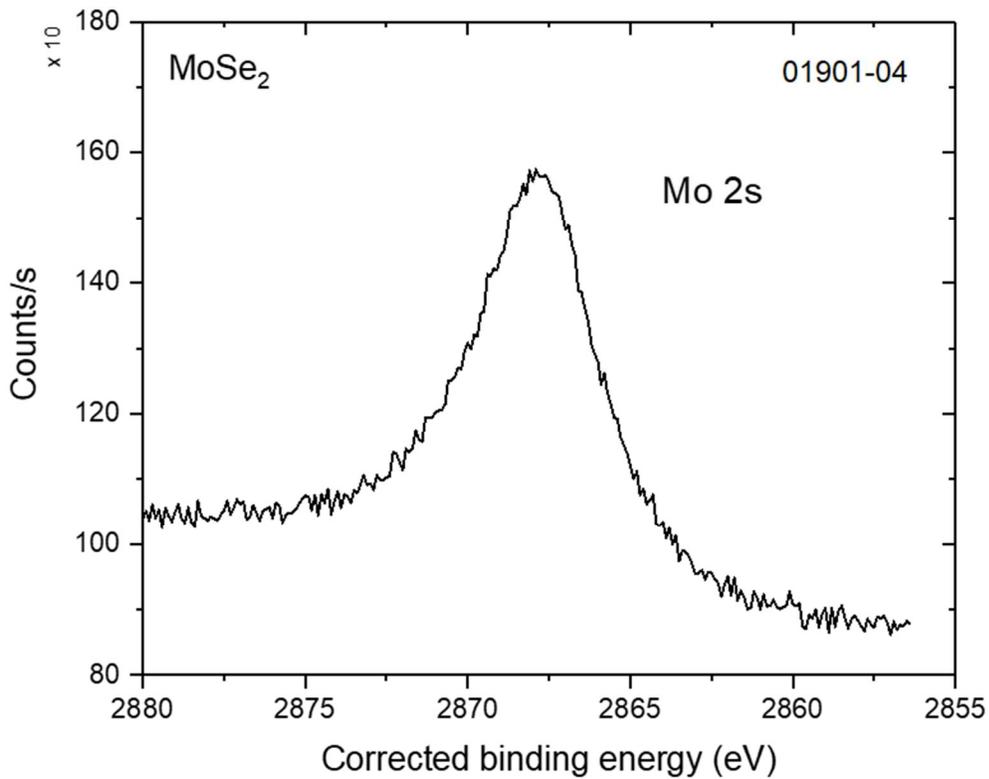
|                                |                                 |
|--------------------------------|---------------------------------|
| ■ Specimen                     | MoSe <sub>2</sub>               |
| ■ Technique                    | XPS                             |
| ■ Spectral Region              | Survey                          |
| Instrument                     | ULVAC-PHI Quantes               |
| Excitation Source              | Cr K <sub>α</sub> monochromatic |
| Source Energy                  | 5414.8 eV                       |
| Source Strength                | 50 W                            |
| Source Size                    | 0.1 mm x 0.1 mm                 |
| Analyzer Type                  | spherical sector analyzer       |
| Incident Angle                 | 22°                             |
| Emission Angle                 | 45°                             |
| Analyzer Pass Energy           | 280 eV                          |
| Analyzer Resolution            | 2.33 eV                         |
| Total Signal Accumulation Time | 5238 s                          |
| Total Elapsed Time             | 5760 s                          |
| Number of Scans                | 10                              |
| Effective Detector Width       | 31 eV                           |



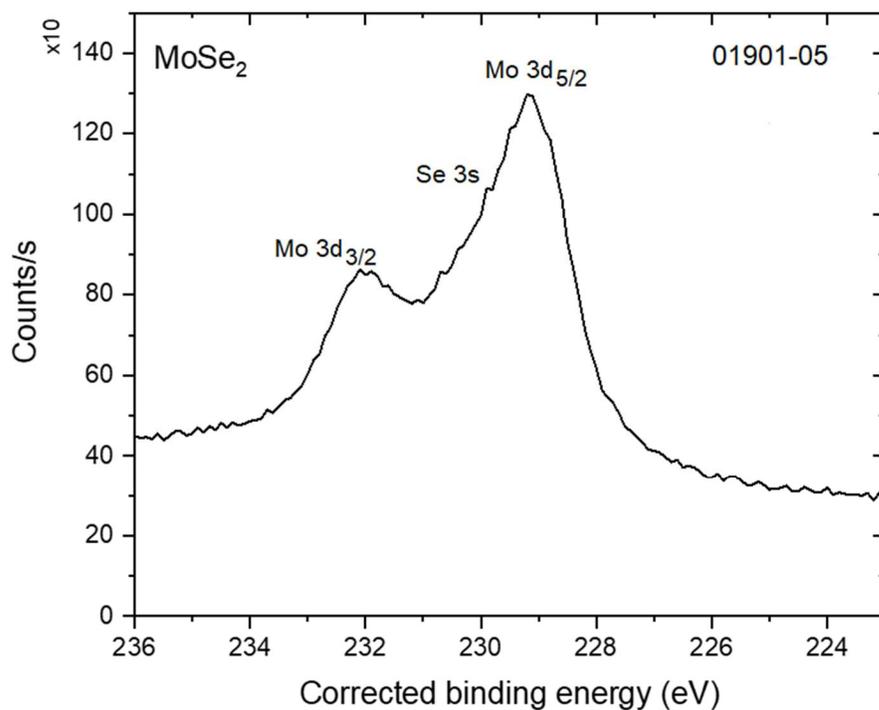
■ **Accession #:** 01901-02  
■ **Specimen:** MoSe<sub>2</sub>  
■ **Technique:** XPS  
■ **Spectral Region:** Mo 2p<sub>3/2</sub>  
Instrument: ULVAC-PHI Quantes  
Excitation Source: Cr K<sub>α</sub> monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation Time: 3300 s  
Total Elapsed Time: 3642 s  
Number of Scans: 24  
Effective Detector Width: 12.4 eV



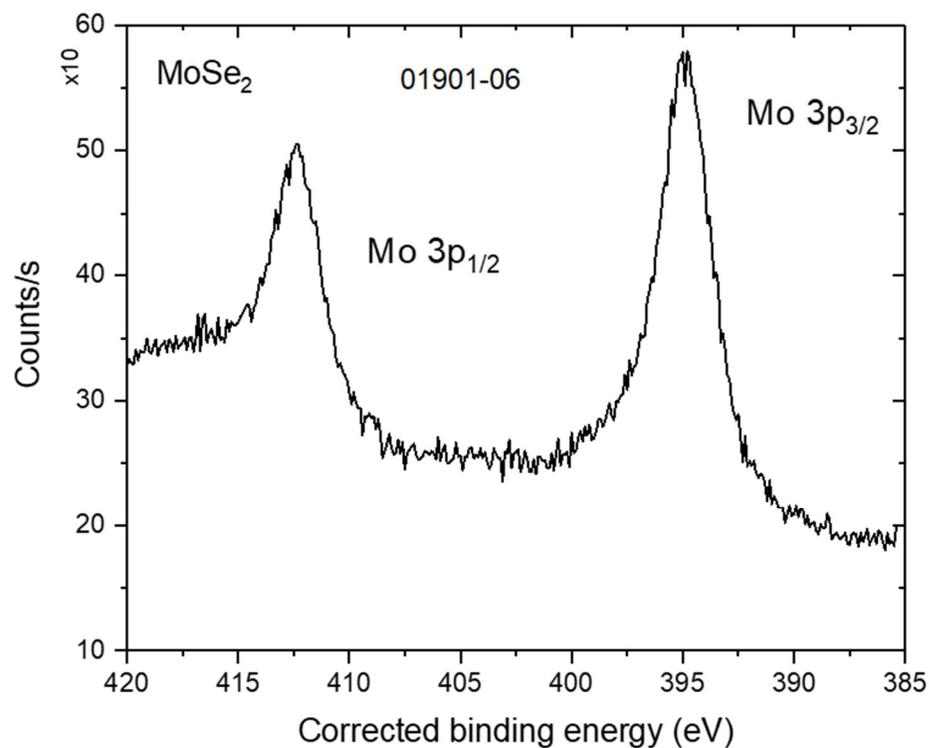
■ **Accession #:** 01901-03  
■ **Specimen:** MoSe<sub>2</sub>  
■ **Technique:** XPS  
■ **Spectral Region:** Mo 2p<sub>1/2</sub>  
Instrument: ULVAC-PHI Quantes  
Excitation Source: Cr K<sub>α</sub> monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation Time: 3300 s  
Total Elapsed Time: 3642 s  
Number of Scans: 24  
Effective Detector Width: 12.4 eV



■ **Accession #:** 01901-02  
■ **Specimen:** MoSe<sub>2</sub>  
■ **Technique:** XPS  
■ **Spectral Region:** Mo 2s  
Instrument: ULVAC-PHI  
Quantes  
Excitation Source: Cr  $K_{\alpha}$   
monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1  
mm  
Analyzer Type: spherical  
sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112  
eV  
Analyzer Resolution: 1.17  
eV  
Total Signal Accumulation  
Time: 3492 s  
Total Elapsed Time: 3852 s  
Number of Scans: 24  
Effective Detector Width:  
12.4 eV



■ **Accession #:** 01901-05  
■ **Specimen:** MoSe<sub>2</sub>  
■ **Technique:** XPS  
■ **Spectral Region:** Mo 3d, Se 3s  
Instrument: ULVAC-PHI Quantes  
Excitation Source: Cr K<sub>α</sub> monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation Time: 7146 s  
Total Elapsed Time: 7878 s  
  
Number of Scans: 64  
  
Effective Detector Width: 12.4 eV



■ Accession #: 01901-06

■ Specimen: MoSe<sub>2</sub>

■ Technique: XPS

■ Spectral Region: Mo 3p

Instrument: ULVAC-PHI

Quantes

Excitation Source: Cr  $K_{\alpha}$   
monochromatic

Source Energy: 5414.8 eV

Source Strength: 50 W

Source Size: 0.1 mm x 0.1  
mm

Analyzer Type: spherical  
sector

Incident Angle: 22 °

Emission Angle: 45 °

Analyzer Pass Energy 112  
eV

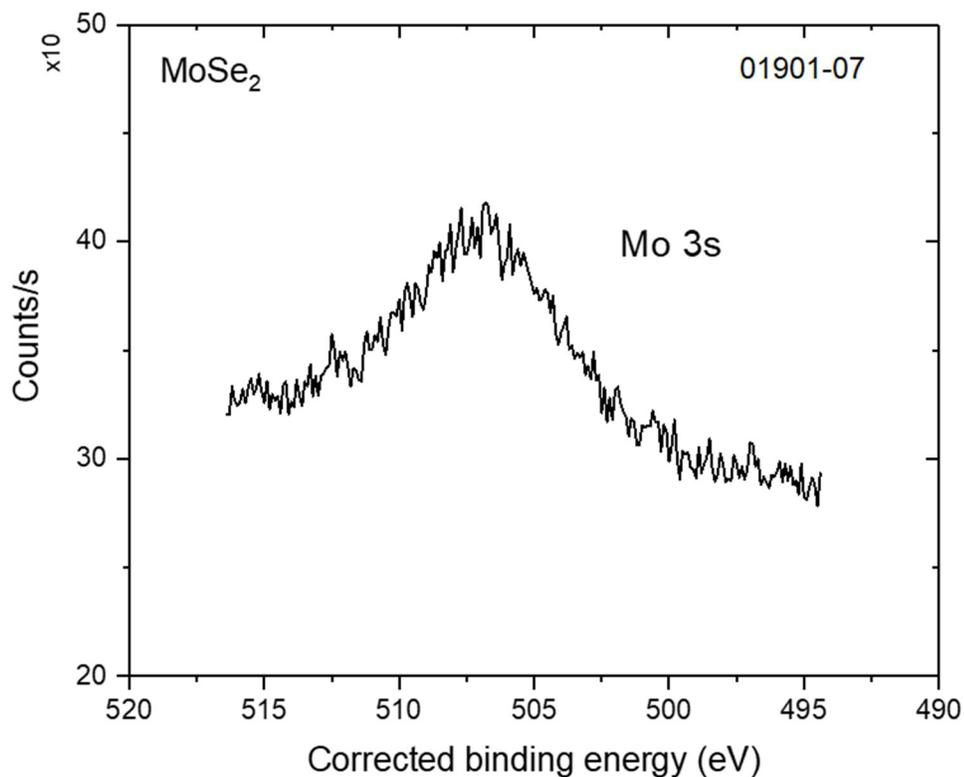
Analyzer Resolution: 1.17 eV

Total Signal Accumulation  
Time: 3792 s

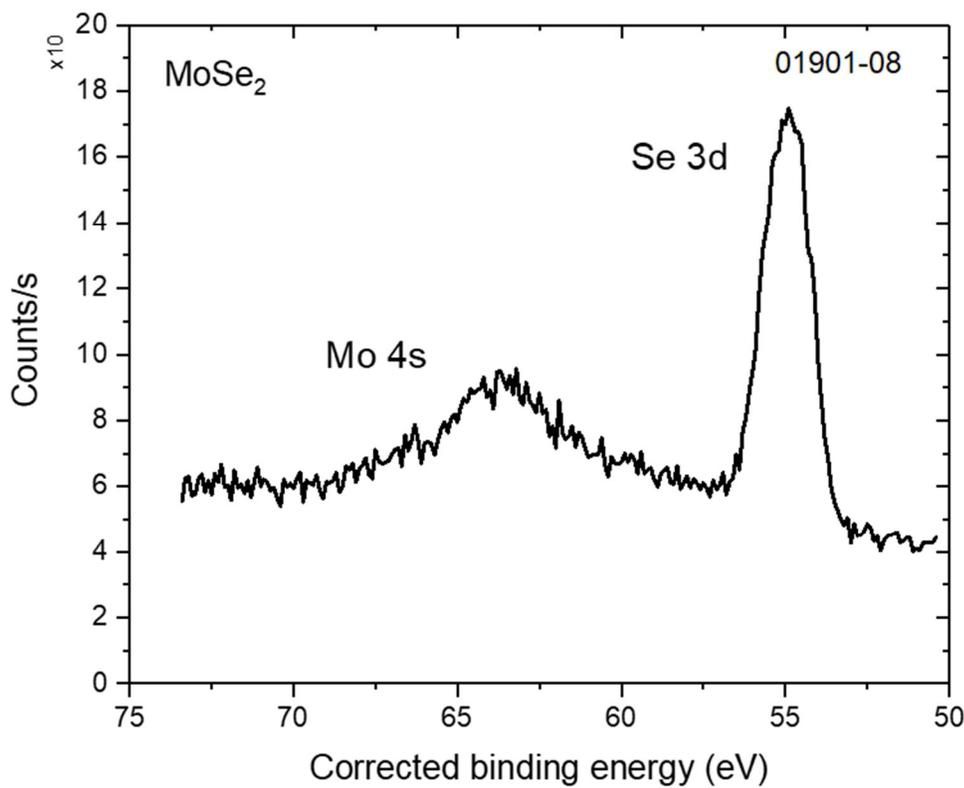
Total Elapsed Time: 4176 s

Number of Scans: 20

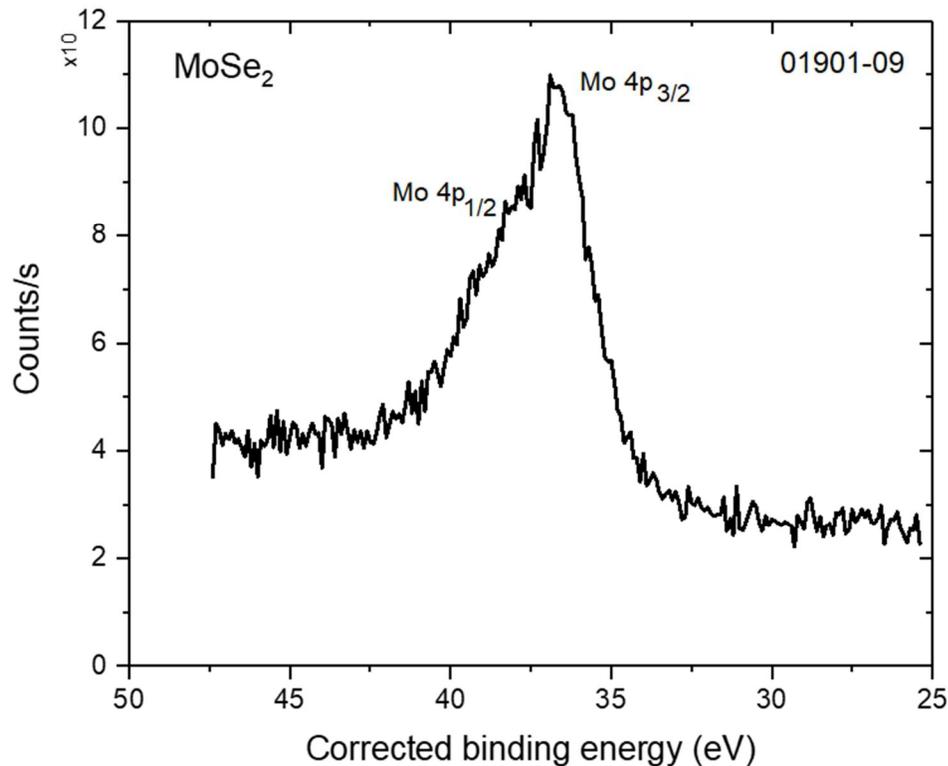
Effective Detector Width:  
12.4 eV



■ **Accession #:** 01901-07  
■ **Specimen:** MoSe<sub>2</sub>  
■ **Technique:** XPS  
■ **Spectral Region:** Mo 3s  
Instrument: ULVAC-PHI  
Quantes  
Excitation Source: Cr K<sub>α</sub>  
monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation Time: 3300 s  
Total Elapsed Time: 3642 s  
Number of Scans: 24  
Effective Detector Width: 12.4 eV



■ **Accession #:** 01901-08  
■ **Specimen:** MoSe<sub>2</sub>  
■ **Technique:** XPS  
■ **Spectral Region:** Mo 4s, Se 3d  
Instrument: ULVAC-PHI Quantes  
Excitation Source: Cr K<sub>α</sub> monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation Time: 3396 s  
Total Elapsed Time: 3744 s  
Number of Scans: 24  
Effective Detector Width: 12.4 eV



■ **Accession #:** 01901-09

■ **Specimen:** MoSe<sub>2</sub>

■ **Technique:** XPS

■ **Spectral Region:** Mo 4p

Instrument: ULVAC-PHI  
Quantes

Excitation Source: Cr K $\alpha$   
monochromatic

Source Energy: 5414.8 eV

Source Strength: 50 W

Source Size: 0.1 mm x 0.1  
mm

Analyzer Type: spherical  
sector

Incident Angle: 22 °

Emission Angle: 45 °

Analyzer Pass Energy 112 eV

Analyzer Resolution: 1.17 eV

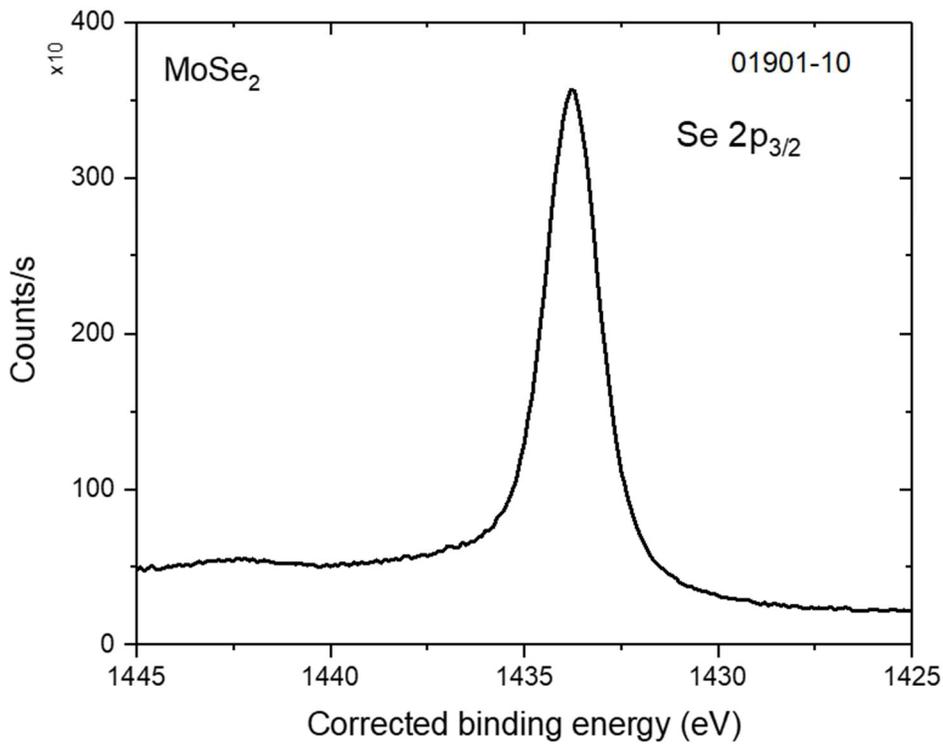
Total Signal Accumulation

Time: 3300 s

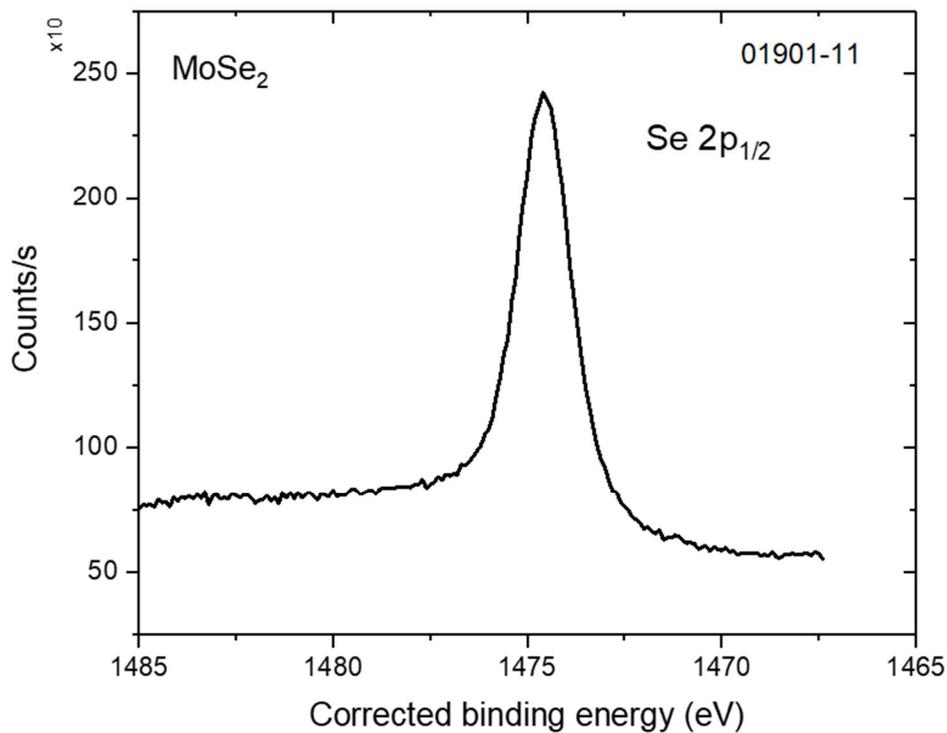
Total Elapsed Time: 3642 s

Number of Scans: 24

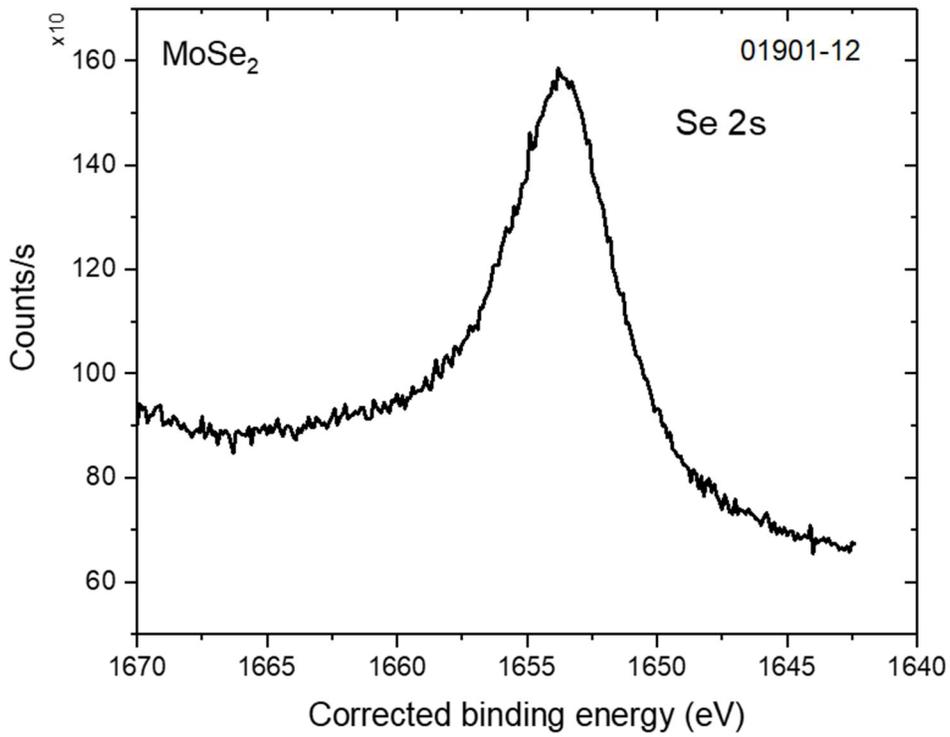
Effective Detector Width: 12.4  
eV



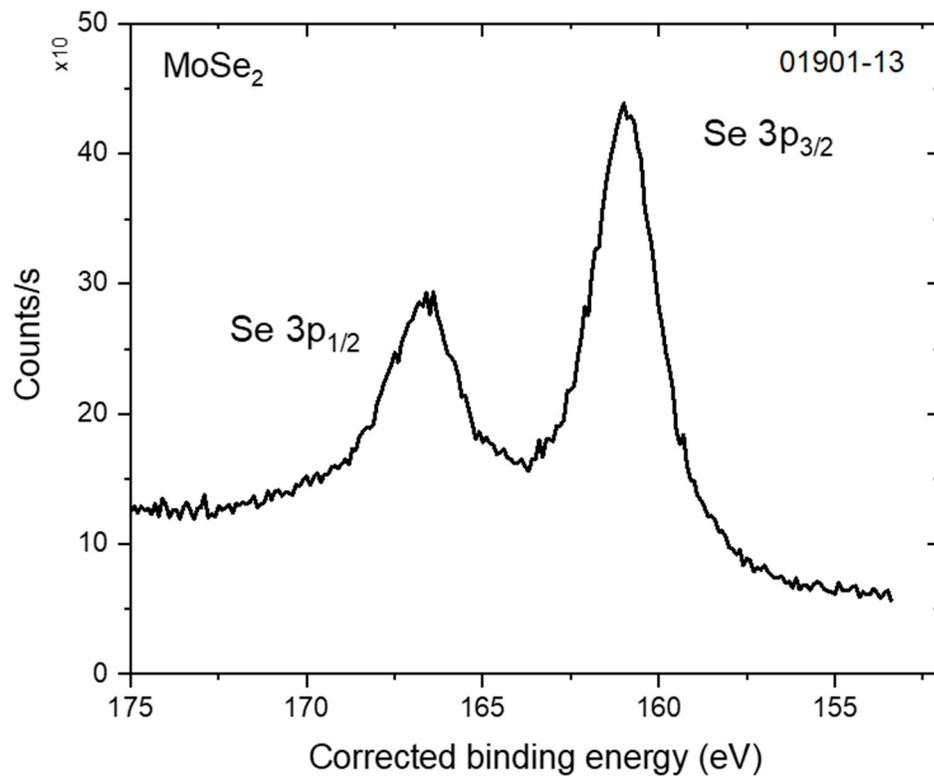
■ **Accession #:** 01901-10  
■ **Specimen:** MoSe<sub>2</sub>  
■ **Technique:** XPS  
■ **Spectral Region:** Se 2p<sub>3/2</sub>  
Instrument: ULVAC-PHI Quantes  
Excitation Source: Cr K<sub>α</sub>  
monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation Time:  
3588 s  
Total Elapsed Time: 3954 s  
  
Number of Scans: 24  
  
Effective Detector Width: 12.4 eV



■ **Accession #:** 01901-11  
■ **Specimen:** MoSe<sub>2</sub>  
■ **Technique:** XPS  
■ **Spectral Region:** Se 2p<sub>1/2</sub>  
Instrument: ULVAC-PHI Quantes  
Excitation Source: Cr K<sub>α</sub>  
monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation Time:  
3630 s  
Total Elapsed Time: 4002 s  
  
Number of Scans: 28  
  
Effective Detector Width: 12.4 eV



■ **Accession #:** 01901-12  
■ **Specimen:** MoSe<sub>2</sub>  
■ **Technique:** XPS  
■ **Spectral Region:** Se 2s  
Instrument: ULVAC-PHI Quantes  
Excitation Source: Cr  $K_{\alpha}$  monochromatic  
Source Energy: 5414.8 eV  
Source Strength: 50 W  
Source Size: 0.1 mm x 0.1 mm  
Analyzer Type: spherical sector  
Incident Angle: 22 °  
Emission Angle: 45 °  
Analyzer Pass Energy 112 eV  
Analyzer Resolution: 1.17 eV  
Total Signal Accumulation Time: 3234 s  
Total Elapsed Time: 3564 s  
Number of Scans: 20  
Effective Detector Width: 12.4 eV



■ **Accession #:** 01901-13

■ **Specimen:** MoSe<sub>2</sub>

■ **Technique:** XPS

■ **Spectral Region:** Se 3p

Instrument: ULVAC-PHI Quantes

Excitation Source: Cr K<sub>α</sub>  
monochromatic

Source Energy: 5414.8 eV

Source Strength: 50 W

Source Size: 0.1 mm x 0.1 mm

Analyzer Type: spherical sector

Incident Angle: 22 °

Emission Angle: 45 °

Analyzer Pass Energy 112 eV

Analyzer Resolution: 1.17 eV

Total Signal Accumulation Time:  
3492 s

Total Elapsed Time: 3852 s

Number of Scans: 24

Effective Detector Width: 12.4 eV