

Applying AnI ML to UV/Vis Data

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- Samples and their Roles
- Measurement Data
- Instrument Parameters

```
<?xml version="1.0" encoding="UTF-8"?>
<AnIML xmlns="urn:org:astm:animl:schema:core:draft:0.2" xmlns:ds="http://www.w3.org/2000/09/xmldsig#" xmlns:xsi="
http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="urn:org:astm:animl:schema:core:draft:0.2
C:\DOCUME~1\MarenF.CLCDOM\MYDOCU~1\Projekte\AnIML\AnIML CVS\schema\animl-core.xsd" version="0.2">
  <SampleSet>
  <ExperimentStepSet>
  <AuditTrail>
</AnIML>
```

- **Test Sample**
 - Solvent
 - Blank
 - Reference Sample
- Qualification Reference
 - Proficiency Reference
 - Transmittance Reference
 - Wavelength Reference



Standard
Reference
Materials, e.g.
from NIST

- **Name** "Holmium Oxide Wavelength Standard"
- **Descriptive Name** "NIST SRM 2034"
- **Mass**
- **Volume** "3.5 mL"
- **Concentration**
- **State** "liquid"
- **Disposal Procedure**
- **Handling Precautions** "Should a leak in the cuvette develop or if the cuvette is accidentally broken, carefully treat the spill immediately with generous amounts of water"
- **Storage Information** "stored in the container provided at a temperature between 20°C and 30°C"
- **Storage Location**

- Receipt Time Stamp
- Preparation Procedure

“The holmium oxide solution was prepared by dissolving the powder Holmium Oxide (4 percent by weight) in a 10% perchloric acid. This solution was contained in a flame-sealed, non-fluorescent, fused-silica cuvette”
- Pressure
- Temperature

“25°C”
- Density
- Lot or Batch Name/Number
- Origin/Supplier

“NIST”
- Boiling Point
- Melting Point
- Refractive Index



<http://www.cstl.nist.gov/acd/839.04/wavelength.htm>

- Name "Holmium Oxide"
- Descriptive Name
- Concentration "40 g/L"
- Molecular Formula "Ho2O3"
- Molecular Mass
- Chemical Structure
 - SMILES
 - Wiswesser
 - MOL File
 - CML
- Chemical Identifier
 - CAS Name
 - CAS Registry Number "12055-62-8"
 - InChI
 - Beilstein Lawson Number
 - CML

```
<ParameterCategory name="Substance Description">  
  <ParameterSet>  
    <Parameter name="Name">  
      <string>Holmium Oxide</string>  
    </Parameter>  
    <Parameter name="Concentration">  
      <float32>40</float32>  
      <Unit label="g/l">  
        <SIUnit exponent="1" factor="0.001" offset="0">kg</SIUnit>  
        <SIUnit exponent="-3" factor="0.001" offset="0">m</SIUnit>  
      </Unit>  
    </Parameter>  
    <Parameter name="Molecular Formula">  
      <string>Ho2O3</string>  
    </Parameter>  
    <Parameter name="CASRegistryNo">  
      <string>12055-62-8</string>  
    </Parameter>  
  </ParameterSet>  
</ParameterCategory>
```

The actual measurement data

```
<?xml version="1.0" encoding="UTF-8"?>
<AniML xmlns="urn:org:astm:animl:schema:core:draft:0.2" xmlns:ds="http://www.w3.org/2000/09/xmldsig#" xmlns:xsi="
http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="urn:org:astm:animl:schema:core:draft:0.2
C:\DOCUME~1\MarenF\CLC\DOM\WY\DOCU~1\Projekte\AniML\AniMLCVS\schem\animl-core.xsd" version="0.2">
  <SampleSet>
    <ExperimentStepSet>
      <ExperimentStep name="UV_Measurement">
        <Author type="device">
          <Name>Lambda 900</Name>
          <EMail>melody.smith@nist.gov</EMail>
          <Phone>301-975-8533</Phone>
          <Location>NIST-Gaithersburg</Location>
        </Author>
        <Timestamp>2004-11-01T14:58:00</Timestamp>
        <SampleReferenceSet>
          <SampleReference sampleID="SRM2034" role="SampleMeasurement" samplePurpose="consumed"/>
        </SampleReferenceSet>
        <Technique name="UV" uri="http://www.animl.org/Techniques/UVTechniqueDefinition.atid"/>
        <ParameterCategorySet>
          <ParameterCategory name="Instrument Description">
            <ParameterCategory name="Instrument Owner">
              <ParameterCategory name="Instrument Location">
            </ParameterCategorySet>
          </ParameterCategorySet>
        <PageSet>
          <Page name="Spectrum">
        </PageSet>
      </ExperimentStep>
    </ExperimentStepSet>
  <AuditTrail>
</AniML>
```

Who did it?

Which sample(s) were used?

Which analytical technique?

Which instrument was used?

The spectrum

- Spectrum

- Intensity vs. Wavelength

Use for time-/temperature-dependent measurements as well

- Interferogram

- Intensity vs. Time

- Peak Table

- Peak Max at Wavelength

- Peak Number

- Peak Start Position

- Peak End Position

- Peak Width

- Peak Height

- Peak Percent Height

- Peak Area

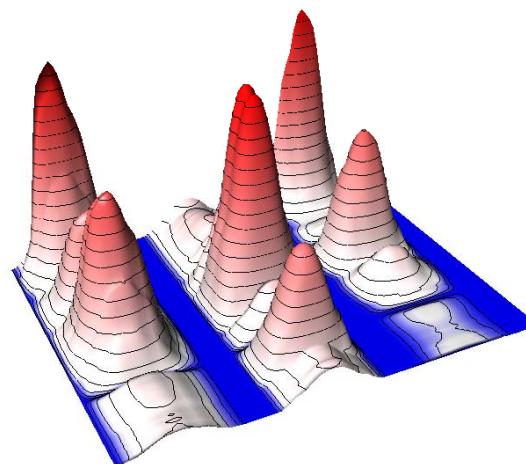
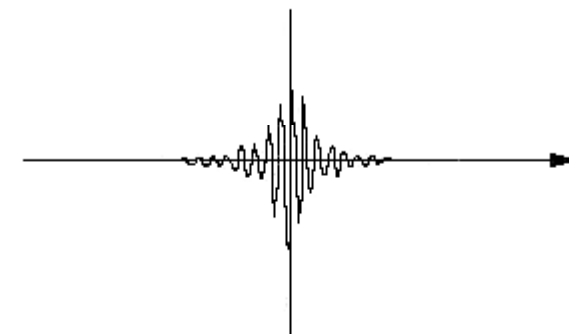
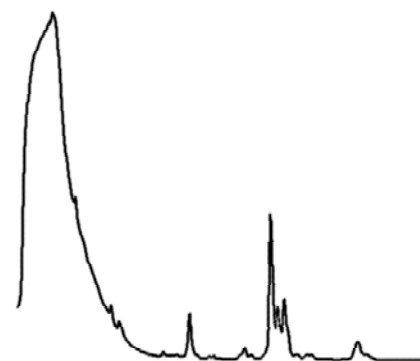
- Peak Percent Area

- Peak Assignment

- Peak Asymmetry

- Peak Baseline Start Value

- Peak Baseline Stop Value



■ Instrument Description

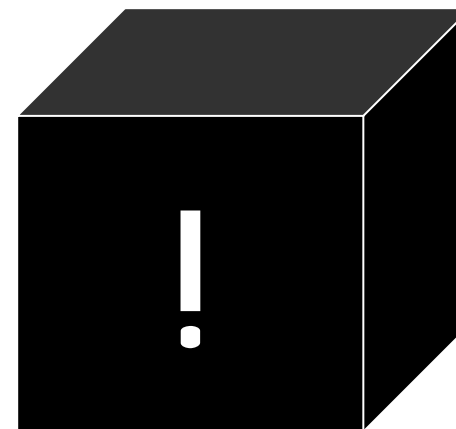
- **Identifier** "101N8061291"
- **Manufacturer** "Perkin Elmer"
- **Model Name** "Lambda 900"
- **Serial Number** "101N8061291"
- **Instrument Type** "double beam"
- **Operating System Name** "Windows 2000"
- **Operating System Version**
- **Control Software Name** "UV WinLab"
- **Control Software Version** "5.1.0"
- **Firmware Version**
- **Linear Dispersion**
- **Resolution** "2.0 nm"
- **Description**
- **Comments**


■ Instrument Owner

- **Name** "NIST"
- **Contact** "301-975-8215"

■ Instrument Location

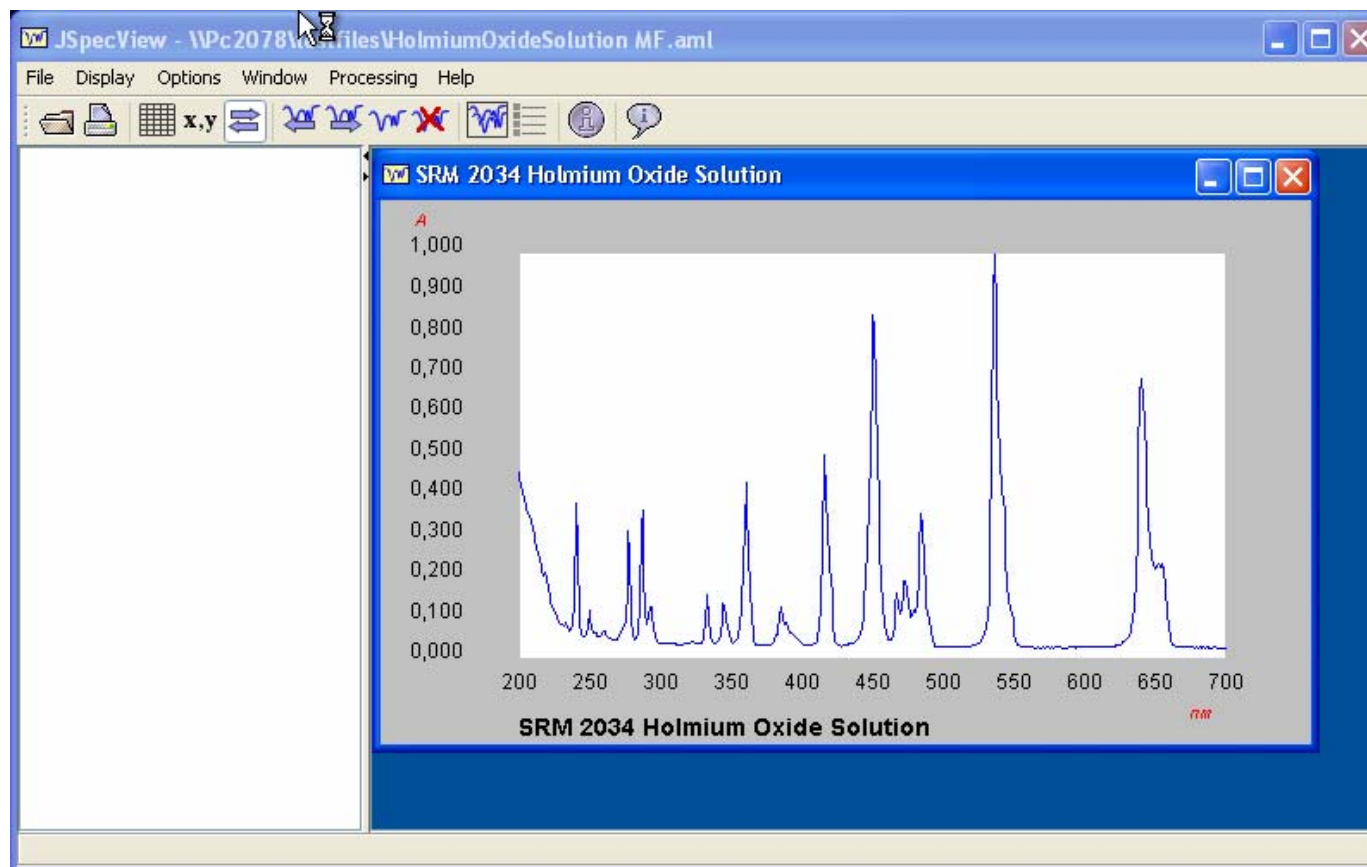
- **Name** "Bldg. 227,
Rm. A322"
- **Contact** "301-975-8215"



- Vector "Wavelength"
 - 200-700 nm, increment 1 nm
 - Vector "Intensity"
 - Absorbance data as base64 encoded stream
 - Parameter Category "Measurement Description"
 - **Identifier** "SRM 2034 Holmium Oxide Solution"
 - Title
 - Project "AnIML"
 - Method Reference
 - Scan Number "1"
 - Scan Duration
 - **Experiment Duration** "1.878 s"
 - **Sample Path Length** "10.0 mm"
 - Temperature Range
- 

- Parameter Category "Instrument Property"
 - **Resolution** "2.0 nm"
 - **Scan Mode** "Spectrum"
 - Spectral Slit Width
 - **Slit Width** "2.0 nm"
 - Integration Period "1.0 s"
 - **Spectrum Derivatization Method** "0"
 - Derivatization Algorithm Description
 - Background Correction Type
 - Straylight Correction
 - Signal to Noise Ratio
 - Filter
 - Detector Types
 - Scan Speed "266.75 nm/s"
 - Point Separation
 - Sample Holder "Carriage"
 - Sample Position "2"
 - Spectral Bandwidth Range "0.1 – 3.0 nm"
 - Wavelength Range "200-700 nm"
 - Absorbance Range
 - Source Used "Deuterium Lamp, 200-400 nm;
Tungsten Lamp, 400-700 nm"

Example



JSPECVIEW by R.J. Lancashire, UWI at Mona, Jamaica
<http://jspecview.sourceforge.net/>

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