

Russian Federal Nuclear Centre – All-Russian Institute of Technical Physics (RFNC-VNIITF)



WP7: JRA2 Publishing Tools

WP7 Tasks Steps for Period 1 involving RFNC-VNIITF activities:

Task 3: Preparing the prototype of the import tool (lead by UU)

Task 4: Prototype development and deployment of the VAMDC XSAMS interface for the Spectr-W³ & VALD (?-should have been discussed in detail @ the meeting) databases (lead by RFNC-VNIITF)

Local version of the Spectr-W³ database

For off-line use on PCs under Windows. Previous interface was completely rewritten in C# ➔ flexibility & improved functionality.

Setup package will be made downloadable from the Spectr-W³ homepage in autumn, 2010.

Also employed for the development & testing of export/ import options to XML & plain text formats.

Local version of the Spectr-W³: selection of energy levels of Co-like W

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Ionization potentials

Energy levels

Spectral lines

Collisional data

◀ ▶ ×

Enter search conditions:

Atom: W (74)

Isoelectronic sequence: Co (27)

Method:

Reference:

Level configuration

Term [2S+1]: L: J:

Ground configuration

Sort result records by:

First: Energy

Second: Ion

Third:

Ascending

Descending

Ascending

Descending

Ascending

Descending

Fields to include:

This is multiply choice.

Use <Ctrl> and <left mouse button> for select/deselect the item.

Or use these buttons for include:

All

Default

Inverse

Zspec

Level name

Level configuration

M

L

J

g

Energy

Accuracy

Ground state

Ground configuration

Gamma rad, s-1

Gamma auto, s-1

Search

Reset

How to use

Search results

Found records: 266 Page: 1 from: 3 Page size: 100

Export to XSAMS

Energy levels

N	Atom	Ion	Znuc	Zspec	Level name	Level configuration	J	g	Energy cm ⁻¹	Method	Reference	Comment
1	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ (1)4s _{1/2}) J=3/2	3p(5)3d(9)4s	3/2	4	1.977482e7	Thr	R415	MCDF-EAL calculation, GRASP ² code
2	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ (1)4s _{1/2}) J=1/2	3p(5)3d(9)4s	1/2	2	1.977207e7	Thr	R415	MCDF-EAL calculation, GRASP ² code
3	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ _{3/2} (2) 4s _{1/2})J=5/2	3p(5)3d(9)4s	5/2	6	1.950803e7	Thr	R415	MCDF-EAL calculation, GRASP ² code
4	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ _{3/2} (2) 4s _{1/2})J=3/2	3p(5)3d(9)4s	3/2	4	1.949055e7	Thr	R415	MCDF-EAL calculation, GRASP ² code
5	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ (3)4s _{1/2}) J=5/2	3p(5)3d(9)4s	5/2	6	1.917006e7	Thr	R415	MCDF-EAL calculation, GRASP ² code
6	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ (3)4s _{1/2}) J=7/2	3p(5)3d(9)4s	7/2	8	1.916337e7	Thr	R415	MCDF-EAL calculation, GRASP ² code
7	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ _{5/2} (2) 4s _{1/2})J=3/2	3p(5)3d(9)4s	3/2	4	1.911693e7	Thr	R415	MCDF-EAL calculation, GRASP ² code
8	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ _{5/2} (2) 4s _{1/2})J=5/2	3p(5)3d(9)4s	5/2	6	1.909545e7	Thr	R415	MCDF-EAL calculation, GRASP ² code
9	W	Co	74	48	(3d ² _{3/2} 3d ⁶ _{5/2} (0) 4f _{5/2})J=5/2	3d(8)4f	5/2	6	1.856746e7	Thr	R415	MCDF-EAL calculation, GRASP ² code
10	W	Co	74	48	(3d ² _{3/2} 3d ⁶ _{5/2} (0) 4f _{7/2})J=7/2	3d(8)4f	7/2	8	1.854365e7	Thr	R415	MCDF-EAL calculation, GRASP ² code
11	W	Co	74	48	(3d ² _{3/2} 3d ⁶ _{5/2} (2) 4f _{5/2})J=3/2	3d(8)4f	3/2	4	1.847033e7	Thr	R415	MCDF-EAL calculation, GRASP ² code

Ready

C:\Program Files\Spectr-CD\exe\database.mdb | 21 апреля 2010 г. | 17:20:42

xSAMS export tool for Spectr-W³.

Example 1: Export of selected data to XML under xSAMS

All fields should be highlighted in the *Fields to include* output selector & XML output filename specified with the xSAMS xsd file attached

The screenshot displays the SpectrCD-2010 application window. The 'Energy levels' tab is active, showing a table of search results. A dialog box titled 'Select the source of XSAMS scheme, please' is overlaid on the table. The dialog has two sections: 'XSAMS schema' and 'Output XML file'. In the 'XSAMS schema' section, the radio button for 'the file on my computer' is selected, and the text box shows the path 'C:\xsams-0.1.xsd'. In the 'Output XML file' section, the text box shows the path 'd:\Мои Документы\Co-like_W_level_energies_xSAMS.xml'. The 'OK' button is highlighted.

Energy levels

N	Atom	Ion	Znuc	Zspec	Level name	Level configuration	M	L	J	g	Energy cm ⁻¹	Accu
1	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ (1)4s _{1/2}) J=3/2	3p(5)3d(9)4s			3/2	4	1.977482e7	
2	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ (1)4s _{1/2}) J=1/2	3p(5)3d(9)4s			1/2	2	1.977207e7	
3	W											
4	W											
5	W											
6	W											
7	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ _{5/2} (2)) 4s _{1/2} J=3/2	3p(5)3d(9)4s			3/2	4	1.911693e7	
8	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ _{5/2} (2)) 4s _{1/2} J=5/2	3p(5)3d(9)4s			5/2	6	1.909545e7	
9	W	Co	74	48	(3d ² _{3/2} 3d ⁶ _{5/2} (0)) 4f _{5/2} J=5/2	3d(8)4f			5/2	6	1.856746e7	
10	W	Co	74	48	(3d ² _{3/2} 3d ⁶ _{5/2} (0)) 4f _{7/2} J=7/2	3d(8)4f			7/2	8	1.854365e7	

xSAMS export tool for Spectr-W³.

Example 1: xSAMS-gauged XML file successfully generated

SpectrCD-2010

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Ionization potentials Energy levels Spectral lines Collisional data Bibliography How to use XML Viewer

d:\Мои Документы\Co-like_W_level_energies_xSAMS.xml

```
<?xml version="1.0" encoding="UTF-8" ?>
<XSAMSData xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
- <States>
- <Atoms>
- <Atom sourceRef="B001" methodRef="M1">
  <Comments>MCDF-EAL calculation, GRASP<sup>2</sup></sup> code
- <ChemicalElement>
  <NuclearCharge>74</NuclearCharge>
  <ElementSymbol>W</ElementSymbol>
</ChemicalElement>
- <Isotope>
- <IonState>
  <IonCharge>47</IonCharge>
  <IsoelectronicSequence>Co</IsoelectronicSequence>
- <AtomicState stateID="S1">
- <AtomicNumericalData>
  <StateEnergy>
    <Value units="1/cm">1.977482e7</Value>
  </StateEnergy>
  <StatisticalWeight>4</StatisticalWeight>
</AtomicNumericalData>
- <AtomicQuantumNumbers>
  <TotalAngularMomentum>1.5</TotalAngularMomentum>
</AtomicQuantumNumbers>
- <AtomicComposition>
- <Component>
- <Configuration>
  - <Shells>
  - <Shell>
    <PrincipalQuantumNumber>3</PrincipalQuantumNumber>
    - <OrbitalAngularMomentum>
      <Value>1</Value>
      <Symbol>p</Symbol>
    </OrbitalAngularMomentum>
    <NumberOfElectrons>5</NumberOfElectrons>
  </Shell>
  - <Shell>
    <PrincipalQuantumNumber>3</PrincipalQuantumNumber>
    - <OrbitalAngularMomentum>
      <Value>2</Value>
      <Symbol>d</Symbol>
    </OrbitalAngularMomentum>
    <NumberOfElectrons>9</NumberOfElectrons>
  </Shell>
  - <Shell>
    <PrincipalQuantumNumber>4</PrincipalQuantumNumber>
    - <OrbitalAngularMomentum>
      <Value>0</Value>
      <Symbol>s</Symbol>
    </OrbitalAngularMomentum>
```

Search results

Found records: 266 Page: 1 from: 3 Page size: 100 Export to XSAMS

Energy levels

N	Atom	Ion	Znuc	Zspec	Level name	Level configuration	M	L	J	g	Energy cm ⁻¹	Accu
1	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ (1)4s _{1/2}) J=3/2	3p(5)3d(9)4s			3/2	4	1.977482e7	
2	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ (1)4s _{1/2}) J=1/2	3p(5)3d(9)4s			1/2	2	1.977207e7	
3	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ _{3/2} (2) 4s _{1/2})J=5/2	3p(5)3d(9)4s			5/2	6	1.950803e7	
4	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ (3)4s _{1/2}) J=7/2	3p(5)3d(9)4s			7/2	8	1.949055e7	
5	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ _{5/2} (2) 4s _{1/2})J=3/2	3p(5)3d(9)4s			3/2	4	1.911693e7	
6	W	Co	74	48	(3p ⁵ _{1/2} 3d ⁹ _{5/2} (2) 4s _{1/2})J=5/2	3p(5)3d(9)4s			5/2	6	1.909545e7	
7	W	Co	74	48	(3d ² _{3/2} 3d ⁶ _{5/2} (0) 4f _{5/2})J=5/2	3d(8)4f			5/2	6	1.856746e7	
8	W	Co	74	48	(3d ² _{3/2} 3d ⁶ _{5/2} (0) 4f _{7/2})J=7/2	3d(8)4f			7/2	8	1.854365e7	
9	W	Co	74	48	(3d ² _{3/2} 3d ⁶ _{5/2} (2)							

Verifying of the XML-document

The document 'd:\Мои Документы\Co-like_W_level_energies_xSAMS.xml' has been verified successfully, OK

XSAMS schema path: 'C:\xsams-0.1.xsd'

OK

xSAMS export tool for Spectr-W³.

Example 2: xSAMS-export of selected data on 3p-3s transitions of Ne-like Ge

SpectrCD-2010

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Ionization potentials Energy levels **Spectral lines** Collisional data Bibliography

Enter search conditions:

Like:

Atom:

Isoelectronic sequence:

Nuclear charge:

Method:

Reference:

Upper level
Configuration: Term [2S+1]:

Lower level
Configuration: Term [2S+1]:

Optical electron transition:

Wavelength from: to Å

Sort result records by:

First: ☐ Ascending ☒ Descending

Second: ☒ Ascending ☐ Descending

Third: ☒ Ascending ☐ Descending

Fields to include:

This is multiply choice.
Use <Ctrl> and <left mouse button> for select/deselect the item.
Or use these buttons for include:

Search results

Found records: 21 Page: 1 from: 1 Page size: 100

Spectral lines

N	Atom	Ion	Znuc	Zspec	Wavelength Å	Accuracy Å	Transition	Upper level	Upper configuration	2S _u + 1	L _u	J _u	g _u	Lower level
1	Ge	Ne	32	23	192		3p-3s	(2p ⁵ _{3/2} 3p _{3/2}) 3p ₀	2p3p	3	P	0		(2p ⁵ _{3/2} 3s _{1/2}) 1p ₁
2	Ge	Ne	32	23	131		3p-3s	(2p ⁵ _{1/2} 3p _{1/2}) 1s ₀	2p3p	1	S	0		(2p ⁵ _{3/2} 3s _{1/2}) 1p ₁
3	Ge	Ne	32	23	196		3p-3s	(2p ⁵ _{1/2} 3p _{1/2}) 1s ₀	2p3p	1	S	0		(2p ⁵ _{1/2} 3s _{1/2}) 3p ₁
4	Ge	Ne	32	23	248		3p-3s	(2p ⁵ _{3/2} 3p _{3/2}) 1p ₁	2p3p	1	P	1		(2p ⁵ _{3/2} 3s _{1/2}) 1p ₁
5	Ge	Ne	32	23	286		3p-3s	(2p ⁵ _{1/2} 3p _{1/2}) 3D ₁	2p3p	3	D	1		(2p ⁵ _{1/2} 3s _{1/2}) 3p ₁
6	Ge	Ne	32	23	241		3p-3s	(2p ⁵ _{3/2} 3p _{3/2}) 3p ₁	2p3p	3	P	1		(2p ⁵ _{1/2} 3s _{1/2}) 3p ₁
7	Ge	Ne	32	23	287		3p-3s	(2p ⁵ _{3/2} 3p _{1/2}) 3D ₂	2p3p	3	D	2		(2p ⁵ _{3/2} 3s _{1/2}) 1p ₁
8	Ge	Ne	32	23	233		3p-3s	(2p ⁵ _{3/2} 3p _{3/2}) 3p ₂	2p3p	3	P	2		(2p ⁵ _{3/2} 3s _{1/2}) 1p ₁
9	Ge	Ne	32	23	237		3p-3s	(2p ⁵ _{1/2} 3p _{3/2}) 3D ₂	2p3p	3	D	2		(2p ⁵ _{1/2} 3s _{1/2}) 3p ₁
10	Ge	Ne	32	23	232.24	4.e-2	3p-3s	(2p ⁵ _{3/2} 3p _{3/2}) J=2	2p(5)3p			2		(2p ⁵ _{3/2} 3s _{1/2}) J=1
11	Ge	Ne	32	23	236.26	4.e-2	3p-3s	(2p ⁵ _{1/2} 3p _{3/2}) J=2	2p(5)3p			2		(2p ⁵ _{1/2} 3s _{1/2}) J=1
12	Ge	Ne	32	23	286.46	4.e-2	3p-3s	(2p ⁵ _{3/2} 3p _{1/2}) J=2	2p(5)3p			2		(2p ⁵ _{3/2} 3s _{1/2}) J=1
13	Ge	Ne	32	23	247.32	4.e-2	3p-3s	(2p ⁵ _{3/2} 3p _{3/2}) J=1	2p(5)3p			1		(2p ⁵ _{3/2} 3s _{1/2}) J=1
14	Ge	Ne	32	23	196.06	4.e-2	3p-3s	(2p ⁵ _{1/2} 3p _{1/2}) J=0	2p(5)3p			0		(2p ⁵ _{1/2} 3s _{1/2}) J=1

xSAMS export tool for Spectr-W³.

Example 2: xSAMS-gauged XML file successfully generated

SpectrCD-2010

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Ionization potentials Energy levels Spectral lines Collisional data Bibliography How to use XML Viewer

d:\Мои Документы\Co-like_W_level_energies_xSAMS.xml

```
<?xml version="1.0" encoding="UTF-8" ?>
<XSAMSData xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:
- <States>
- <Atoms>
- <Atom sourceRef="B001" methodRef="M1">
- <ChemicalElement>
<NuclearCharge>32</NuclearCharge>
<ElementSymbol>Ge</ElementSymbol>
</ChemicalElement>
- <Isotope>
- <IonState>
<IonCharge>22</IonCharge>
<IsoelectronicSequence>Ne</IsoelectronicSequence>
- <AtomicState stateID="S1">
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- <AtomicComposition>
- <Component>
- <Configuration>
- <Shells>
- <Shell>
<PrincipalQuantumNumber>2</PrincipalQuantumNumber>
- <OrbitalAngularMomentum>
<Value>1</Value>
<Symbol>p</Symbol>
</OrbitalAngularMomentum>
<NumberOfElectrons>1</NumberOfElectrons>
</Shell>
- <Shell>
<PrincipalQuantumNumber>3</PrincipalQuantumNumber>
- <OrbitalAngularMomentum>
<Value>1</Value>
<Symbol>p</Symbol>
</OrbitalAngularMomentum>
<NumberOfElectrons>1</NumberOfElectrons>
</Shell>
</Shells>
</Configuration>
- <Term>
- <LS>
- <L>
<Value>1</Value>
</L>
<Multiplicity>3</Multiplicity>
<S>0</S>
</LS>
</Term>
</Component>
</AtomicComposition>
</AtomicState>
</IonState>
```

Search results

Found records: 21 Page: 1 from: 1 Page size: 100 Export to XSAMS

Spectral lines

N	Atom	Ion	Znc	Zspec	Wavelength Å	Accuracy Å	Transition	Upper level	Upper configuratic
1	Ge	Ne	32	23	192		3p-3s	(2p ⁵ _{3/2} 3p _{3/2}) 3p ₀	2p3p
2	Ge	Ne	32	23	131		3p-3s	(2p ⁵ _{1/2} 3p _{1/2}) 1s ₀	2p3p
3	Ge	Ne	32	23	196		3p-3s	(2p ⁵ _{1/2} 3p _{1/2}) 1s ₀	2p3p
4	Ge	Ne	32	23	248		3p-3s	(2p ⁵ _{3/2} 3p _{3/2}) 1p ₁	2p3p
5	Ge	Ne	32	23	286		3p-3s	(2p ⁵ _{1/2} 3p _{1/2}) 3p ₀	2p3p
6								(2p ⁵ _{1/2} 3p _{3/2}) 3p ₂	2p3p
7								(2p ⁵ _{3/2} 3p _{1/2}) 3p ₂	2p3p
8								(2p ⁵ _{3/2} 3p _{3/2}) 3p ₂	2p3p
9	Ge	Ne	32	23	237		3p-3s	(2p ⁵ _{1/2} 3p _{3/2}) 3p ₂	2p3p
10	Ge	Ne	32	23	232.24	4.e-2	3p-3s	(2p ⁵ _{3/2} 3p _{3/2}) j=2	2p(5)3p
11	Ge	Ne	32	23	236.26	4.e-2	3p-3s	(2p ⁵ _{1/2} 3p _{3/2}) j=2	2p(5)3p
12	Ge	Ne	32	23	286.46	4.e-2	3p-3s	(2p ⁵ _{3/2} 3p _{1/2}) j=2	2p(5)3p
13	Ge	Ne	32	23	247.32	4.e-2	3p-3s	(2p ⁵ _{3/2} 3p _{3/2}) j=1	2p(5)3p
14	Ge	Ne	32	23	196.06	4.e-2	3p-3s	(2p ⁵ _{1/2} 3p _{1/2}) j=0	2p(5)3p

Verifying of the XML-document

The document 'd:\Мои Документы\Co-like_W_level_energies_xSAMS.xml' has been verified successfully, OK

XSAMS schema path: 'C:\xsams-0.1.xsd'

OK

Preparing the prototype of the import tool for Spectr-W³

Content viewer of the input xSAMS-gauged xml file: energy levels of Ne-like Si

The screenshot displays the 'XSAMS Import Demo Tool' interface. The main window shows the XML content of the file 'C:\Program Files\Spectr-CD\exe\asd2.xml'. The XML structure includes metadata such as the source (Gaithersburg, MD, USA), authors (Yu. Ralchenko, A. Kramida, J. Reader, NIST ASD Team), year (2010), version (3.1.3), and source name (NIST Atomic Spectra Database Version 3.1.3). The XML also contains data for the element Silicon (Si) with nuclear charge 14 and ion charge 4, representing Ne-like Si.

Overlaid on the XML view is a table titled 'Import XSAMS' showing the first 9 records of the data. The table has the following columns: N, StateID (string), ElementSymbol (string), NuclearCharge (decimal), IonCharge (decimal), IsoelectronicSequence (string), AtomicStateDescription (string), and StateEnergy (double).

N	StateID (string)	ElementSymbol (string)	NuclearCharge (decimal)	IonCharge (decimal)	IsoelectronicSequence (string)	AtomicStateDescription (string)	StateEnergy (double)
1	S014005.000001	Si	14	4	Ne	Conf 2s2.2p6; Term: 1S	0
2	S014005.000006	Si	14	4	Ne	Conf 2s2.2p5.3s; Term: 3P*	838017,
3	S014005.000007	Si	14	4	Ne	Conf 2s2.2p5.3s; Term: 3P*	840590
4	S014005.000008	Si	14	4	Ne	Conf 2s2.2p5.3s; Term: 3P*	843070,
5	S014005.000009	Si	14	4	Ne	Conf 2s2.2p5.3s; Term: 1P*	848511,
6	S014005.000010	Si	14	4	Ne	Conf 2s2.2p5.3p; Term: 3S	906252,
7	S014005.000011	Si	14	4	Ne	Conf 2s2.2p5.3p; Term: 3D	917928,
8	S014005.000012	Si	14	4	Ne	Conf 2s2.2p5.3p; Term: 3D	918959,
9	S014005.000013	Si	14	4	Ne	Conf 2s2.2p5.3p; Term: 3D	920863,

Initial selection of energy levels of Ne-like Si: 109 records in Spectr-W³

SpectrCD-2010

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Ionization potentials **Energy levels** Spectral lines Collisional data

Enter search conditions:

Atom: Si (14) Isoelectronic sequence: Ne (10) Method: Reference:

Level configuration: Term (2S+1): L: J: Ground configuration:

Sort result records by:

First: Energy Ascending Descending Second: Ascending Descending Third: Ascending Descending

Fields to include:

This is multiply choice. Use <Ctrl> and <left mouse button> for select/deselect the item. Or use these buttons for include: All Default Inverse

Search

Reset

How to use

Search results

Found records: 109 Page: 1 from: 11 Page size: 10 Export to XSAMS

Energy levels

N	Atom	Ion	Znuc	Zspec	Level name	Level configuration	M	L	J	g	Energy cm ⁻¹	Accuracy cm ⁻¹	Γ_{rad} s ⁻¹	Γ_{auto} s ⁻¹	Method	Refer
1	Si	Ne	14	5	((2p ² 3p)4d) ⁴ P _{5/2}	2p(2)4d	4	P	5/2	6	4.4215e5				Comp	R001
2	Si	Ne	14	5	(2p ⁵ 3s) ³ P ₁	2p(5)3s	3	P	1	3	8.31271e5				Thr	R048
3	Si	Ne	14	5	((2p ⁵ 2p)3s) ³ P ₂	2p(5)3s	3	P	2	5	8.3802e5				Comp	R001
4	Si	Ne	14	5	(2p ⁵ 3s) ¹ P ₁	2p(5)3s	1	P	1	3	8.39532e5				Thr	R048
5	Si	Ne	14	5	((2p ⁵ 2p)3s) ³ P ₁	2p(5)3s	3	P	1	3	8.4059e5				Comp	R001
6	Si	Ne	14	5	((2p ⁵ 2p)3s) ³ P ₀	2p(5)3s	3	P	0	1	8.4307e5				Comp	R001
7	Si	Ne	14	5	((2p ⁵ 2p)3s) ¹ P ₁	2p(5)3s	1	P	1	3	8.4851e5				Comp	R001
8	Si	Ne	14	5	((2p ⁵ 2p)3p) ³ S ₁	2p(5)3p	3	S	1	3	9.0625e5				Comp	R001
9	Si	Ne	14	5	((2p ⁵ 2p)3p) ³ D ₃	2p(5)3p	3	D	3	7	9.1793e5				Comp	R001
10	Si	Ne	14	5	((2p ⁵ 2p)3p) ³ D ₂	2p(5)3p	3	D	2	5	9.1896e5				Comp	R001

Search cond

Isoelectronic s

First s

Search results Import XSAMS

R001

reference

Reference code : R001

Author: Kelly R.L., Palumbo L.J.

Journal: NRL Report 7599, 1973, v.1-2, p.750

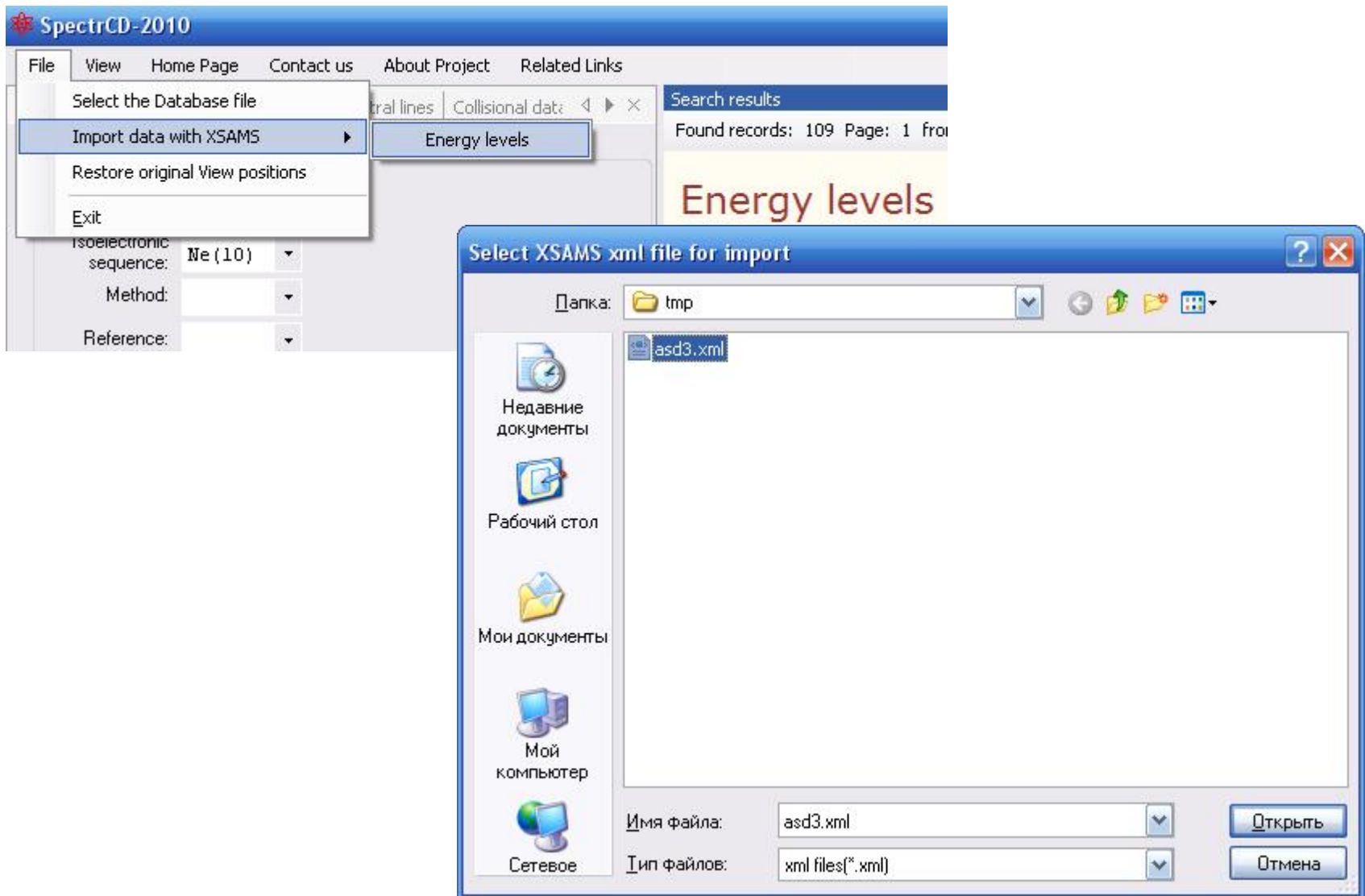
Title: Atomic and ionic emission lines below 2000 angstroms

Status protocol

Ready

D:\Projects\SpectrProject\exe\database.mdb Tuesday, April 20, 2010 21:52:39

Selection of the input-data file for importing into Spectr-W³



93 records are obtained from the selected input-data file

SpectrCD-2010

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XML Viewer

D:\tmp\asd3.xml

```
<?xml version="1.0" encoding="UTF-8" ?>
<XSAMSData
  xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
  xsi:noNamespaceSchemaLocation="http://www-amdis.iaea.org/xsams/schema/xsams-0.1.xsd">
  <Sources>
    <Source sourceID="B1">
      <City>Gaithersburg, MD, USA</City>
      <UniformResourceIdentifier>
        <Authors>
          <Author>
            <Name>Yu.Ralchenko</Name>
          </Author>
          <Author>
            <Name>A.Kramida</Name>
          </Author>
          <Author>
            <Name>J.Reader</Name>
          </Author>
          <Name>NIST ASD Team</Name>
        </Authors>
        <Year>2010</Year>
        <Version>3.1.3</Version>
        <SourceName>NIST Atomic Spectra Database Version 3.1.3</SourceName>
      </UniformResourceIdentifier>
    </Source>
  </Sources>
</XSAMSData>
```

Import XSAMS

Found records: 93 Page: 1 from: 2 Page size: 50

Write to database Table for Spectr-CD

SPE_ENERGY

N	Atom	Ion	Znuc	Level name	Level configuration	M	L	J	g	Energy cm ⁻¹	Accuracy cm ⁻¹	Γ_{rad} s ⁻¹	Γ_{auto} s ⁻¹	Method	Reference	Co
1	Si	Ne	14	(2S(2)2P(6)) ¹ s ₀	2S(2)2P(6)	1	s	0	1 0					Unkn	B1	
2	Si	Ne	14	(2S(2)2P(5)3S) ³ p ₁	2S(2)2P(5)3S	3	p	1	5	838017.4				Unkn	B1	
3	Si	Ne	14	(2S(2)2P(5)3S) ³ p ₁	2S(2)2P(5)3S	3	p	1	3	840590				Unkn	B1	
4	Si	Ne	14	(2S(2)2P(5)3S) ³ p ₁	2S(2)2P(5)3S	3	p	1	1	843070.6				Unkn	B1	
13	Si	Ne	14	(2S(2)2P(5)3P) ³ p ₁	2S(2)2P(5)3P	3	p	1	1	927805.7				Unkn	B1	
14	Si	Ne	14	(2S(2)2P(5)3P) ³ p ₁	2S(2)2P(5)3P	3	p	1	3	928405.4				Unkn	B1	

Verifying of the XML-document

The document 'D:\tmp\asd3.xml' has been verified successfully, OK

XSAMS schema path: 'http://www-amdis.iaea.org/xsams/schema/xsams-0.1.xsd'

OK

Search results Import XSAMS

B1

reference

Reference code : B1

Author: Yu.Ralchenko, A.Kramida, J.Reader, NIST ASD Team

Journal: NIST Atomic Spectra Database Version 3.1.3, 2010

Title:

Ready

D:\Projects\SpectrProject\exe\database.mdb Tuesday, April 20, 2010 23:26:22

But only 16 new records are added to Spectr-W³: duplications in the key fields of the input-data file found (to be analyzed). Also 1 bibliography reference is added

SpectrCD-2010

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Import X5AMS

Found records: 93 Page: 1 from: 2 Page size: 50 Write to database Table for Spectr-CD

SPE_ENERGY

N	Atom	Ion	Znuc	Level name	Level configuration	M	L	J	g	Energy cm ⁻¹	Accuracy cm ⁻¹	Γ_{rad} s ⁻¹	Γ_{auto} s ⁻¹	Method	Reference	Co
1	Si	Ne	14	(2S(2)2P(6)) ¹ s ₀	2S(2)2P(6)	1	s	0	1	0				Unkn	B1	
2	Si	Ne	14	(2S(2)2P(5)3S) ³ p ₁	2S(2)2P(5)3S	3	p	1	5	838017.4				Unkn	B1	
3	Si	Ne	14	(2S(2)2P(5)3S) ³ p ₁	2S(2)2P(5)3S	3	p	1	3	840590				Unkn	B1	
4	Si	Ne	14	(2S(2)2P(5)3S) ³ p ₁	2S(2)2P(5)3S	3	p	1	1	843070.6				Unkn	B1	
5	Si	Ne	14	(2S(2)2P(5)3S) ³ p ₁	2S(2)2P(5)3S	3	p	1	3	848511.2				Unkn	B1	
6	Si	Ne	14	(2S(2)2P(5)3P) ³ s ₁	2S(2)2P(5)3P	3	s	1	3	906252.3				Unkn	B1	
7	Si					3	d	1	7	917928.5				Unkn	B1	
8	Si					3	d	1	5	918959.4				Unkn	B1	
9	Si					3	d	1	3	920863.9				Unkn	B1	
10	Si					3	d	1	5	924291.7				Unkn	B1	
11	Si					3	d	1	3	925947.3				Unkn	B1	
12	Si					3	d	1	5	927398.2				Unkn	B1	
13	Si	Ne	14	(2S(2)2P(5)3P) ³ p ₁	2S(2)2P(5)3P	3	p	1	1	927805.7				Unkn	B1	
14	Si	Ne	14	(2S(2)2P(5)3P) ³ p ₁	2S(2)2P(5)3P	3	p	1	3	928405.4				Unkn	B1	

Writing into SPE_ENERGY

Not all records have been written into the tables:

Table SPE_REF2: 1 records were added
Table SPE_METHOD: 1 records were added
Table SPE_ENERGY: 16 records were added

OK

Error message

reference

Reference code : B1

Author: Yu.Ralchenko, A.Kramida, J.Reader, NIST ASD Team

Journal: NIST Atomic Spectra Database Version 3.1.3, 2010

Title:

Record 93. Error message: Изменения не были успешно внесены из-за повторяющихся значений в индексе, ключевых полях или связях. Измените

D:\Projects\SpectrProject\exe\database.mdb Tuesday, April 20, 2010 23:28:17

Follow-on selection of energy levels of Ne-like Si: 125 records are found in Spectr-W³ for energy levels of Ne-like Si

SpectrCD-2010

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Ionization potentials **Energy levels** Spectral lines Collisional data

Enter search conditions:

Atom: **Si (14)**
 Isoelectronic sequence: **Ne (10)**
 Method:
 Reference:

Level configuration
 Term (2S+1): L: J:

Ground configuration

Sort result records by:

First: **Energy** ☒ Ascending ☐ Descending
 Second: ☐ Ascending ☐ Descending
 Third: ☐ Ascending ☐ Descending

Fields to include:

This is multiply choice.
 Use <Ctrl> and <left mouse button> for select/deselect the item.
 Or use these buttons for include:

☐ L ☐ J ☐ g ☐ Energy ☐ Accuracy ☐ Ground state ☐ Ground configuration ☐ Gamma rad, s⁻¹ ☐ Gamma auto, s⁻¹ ☐ Ionization potential ☐ Method ☐ Reference ☐ Comment

Search results

Found records: 125 Page: 1 from: 13 Page size: 10 Export to XSAMS

Energy levels

N	Atom	Ion	Znuc	Zspec	Level name	Level configuration	M	L	J	g	Energy cm ⁻¹	Accuracy cm ⁻¹	$\Gamma_{\text{rad}} \text{ s}^{-1}$	$\Gamma_{\text{auto}} \text{ s}^{-1}$	Method	Refer	
1	Si	Ne	14	5	(2S(2)2P(6)) ¹ s ₀	2S(2)2P(6)	1	s	0	1	0.					Unkn	B1
2	Si	Ne	14	5	((2p ² 3p)4d) ⁴ p _{5/2}	2p(2)4d	4	p	5/2	6	4.4215e5					Comp	R001
3	Si	Ne	14	5	(2p ⁵ 3s) ³ p ₁	2p(5)3s	3	p	1	3	8.31271e5					Thr	R048
4	Si	Ne	14	5	(2S(2)2P(5)3S) ³ p ₁	2S(2)2P(5)3S	3	p	1	5	8.380174e5					Unkn	B1
5	Si	Ne	14	5	((2p ⁵ 2p)3s) ³ p ₂	2p(5)3s	3	p	2	5	8.3802e5					Comp	R001
6	Si	Ne	14	5	(2p ⁵ 3s) ¹ p ₁	2p(5)3s	1	p	1	3	8.39532e5					Thr	R048
7	Si	Ne	14	5	((2p ⁵ 2p)3s) ³ p ₁	2p(5)3s	3	p	1	3	8.4059e5					Comp	R001
8	Si	Ne	14	5	((2p ⁵ 2p)3s) ³ p ₀	2p(5)3s	3	p	0	1	8.4307e5					Comp	R001
9	Si	Ne	14	5	((2p ⁵ 2p)3s) ¹ p ₁	2p(5)3s	1	p	1	3	8.4851e5					Comp	R001
10	Si	Ne	14	5	((2p ⁵ 2p)3p) ³ s ₁	2p(5)3p	3	s	1	3	9.0625e5					Comp	R001

Search conditions:

Atom: **Si (14)**
 Isoelectronic sequence: **Ne (10)**
 Method:
 Reference:

reference

Reference code : B1

Author: Yu.Ralchenko, A.Kramida, J.Reader, NIST ASD Team
 Journal: NIST Atomic Spectra Database Version 3.1.3, 2010
 Title: