SLAP evolution proposal

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Why updating the standard ?

Conclusions of Interop in Trieste :

- Aiming at a convergence between VAMDC and IVOA standards for spectral lines search

- VAMDC will provide a SLAP output for its services

- SLAP needs to be completed

Evolution proposed in Trieste

- Introduction of a file-creation timestamp into each output file produced.

- Providing information about the version of the database used for generating the output file (a database may evolve over time and having different versions. For the reproducibility of a scientific procedure, the final user should be informed about the version of data he/she is using).

- Providing the references to the scientific sources (in the bibliographic sense) used for compiling the data contained into an output file.

- Explicitly define the units used for expressing the energies.

Additional modifications

- A new ION_CHARGE parameter to complete the already existing CHEMICAL_ELEMENT, containing an interval of charge

- Replacing optional CHEMICAL_ELEMENT in the output fields by optional INITIAL_CHEMICAL_ELEMENT and FINAL_CHEMICAL_ELEMENT

- Adding optional INITIAL_ION_CHARGE and FINAL_ION_CHARGE in output fields

- Adding InChi and InChiKey as optional output fields

- A specific request to get the complete list of species available in the service, without querying spectral lines
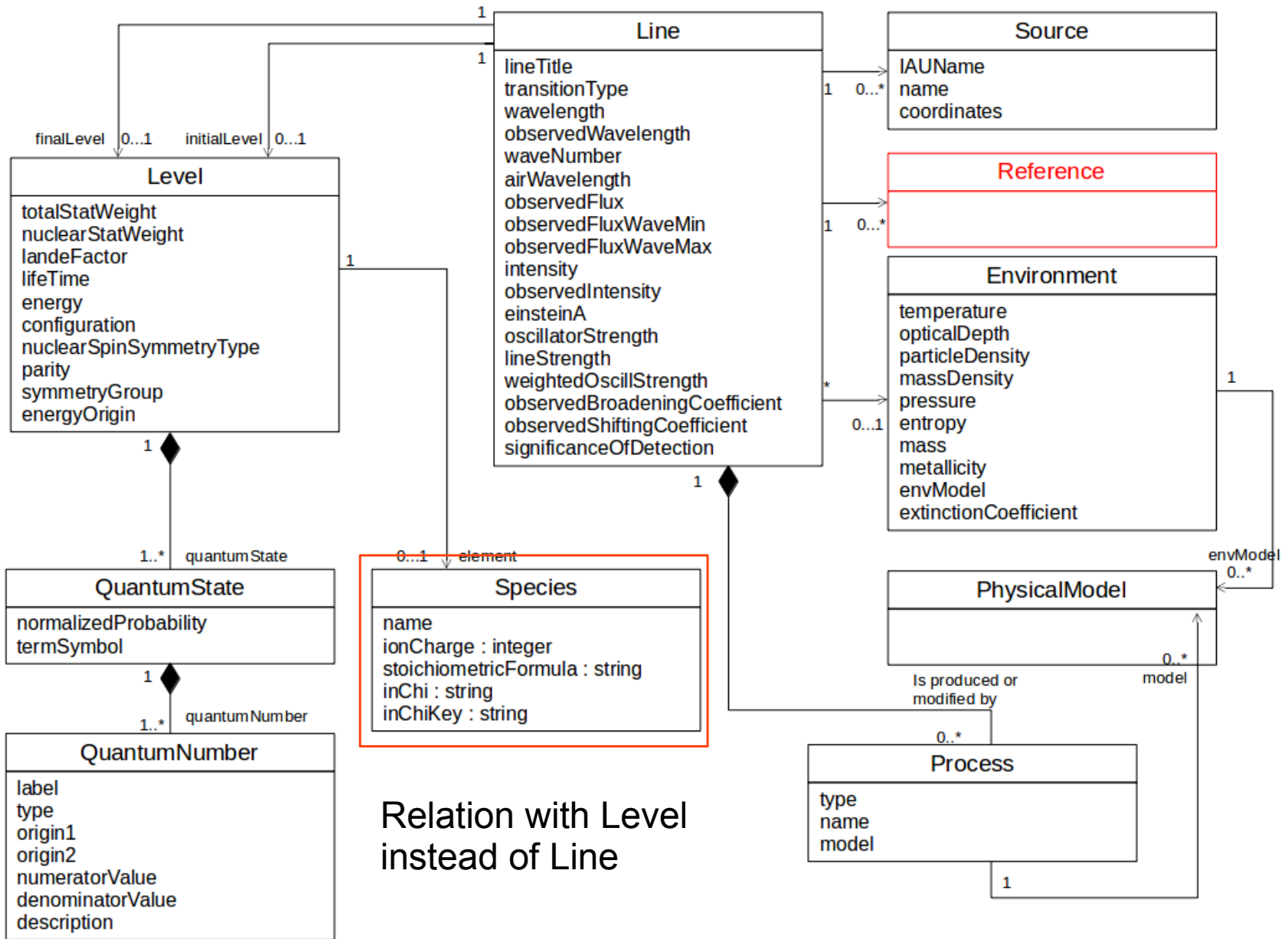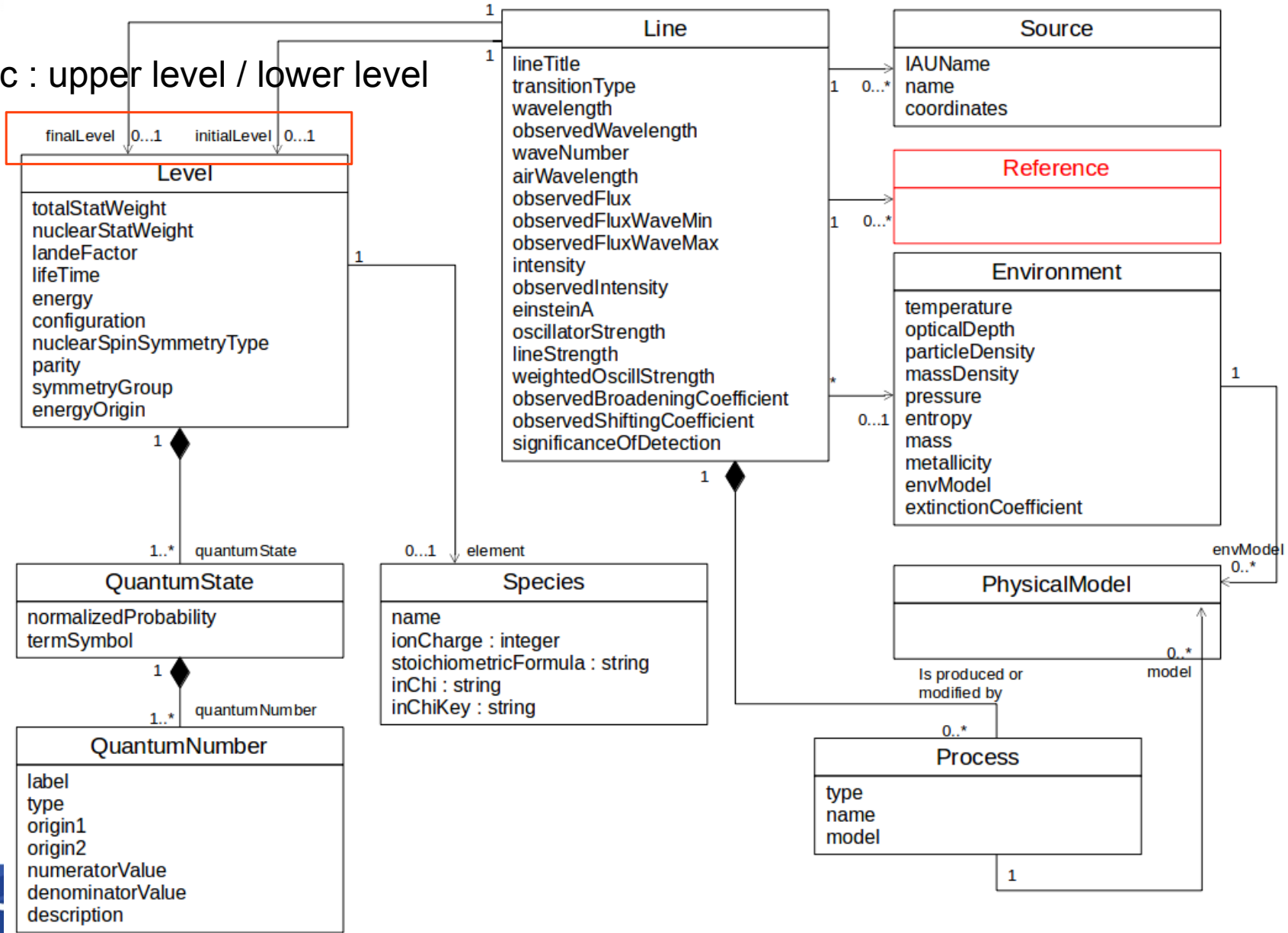
Modifications in SSLDM

Shanghai Interop meeting 2017
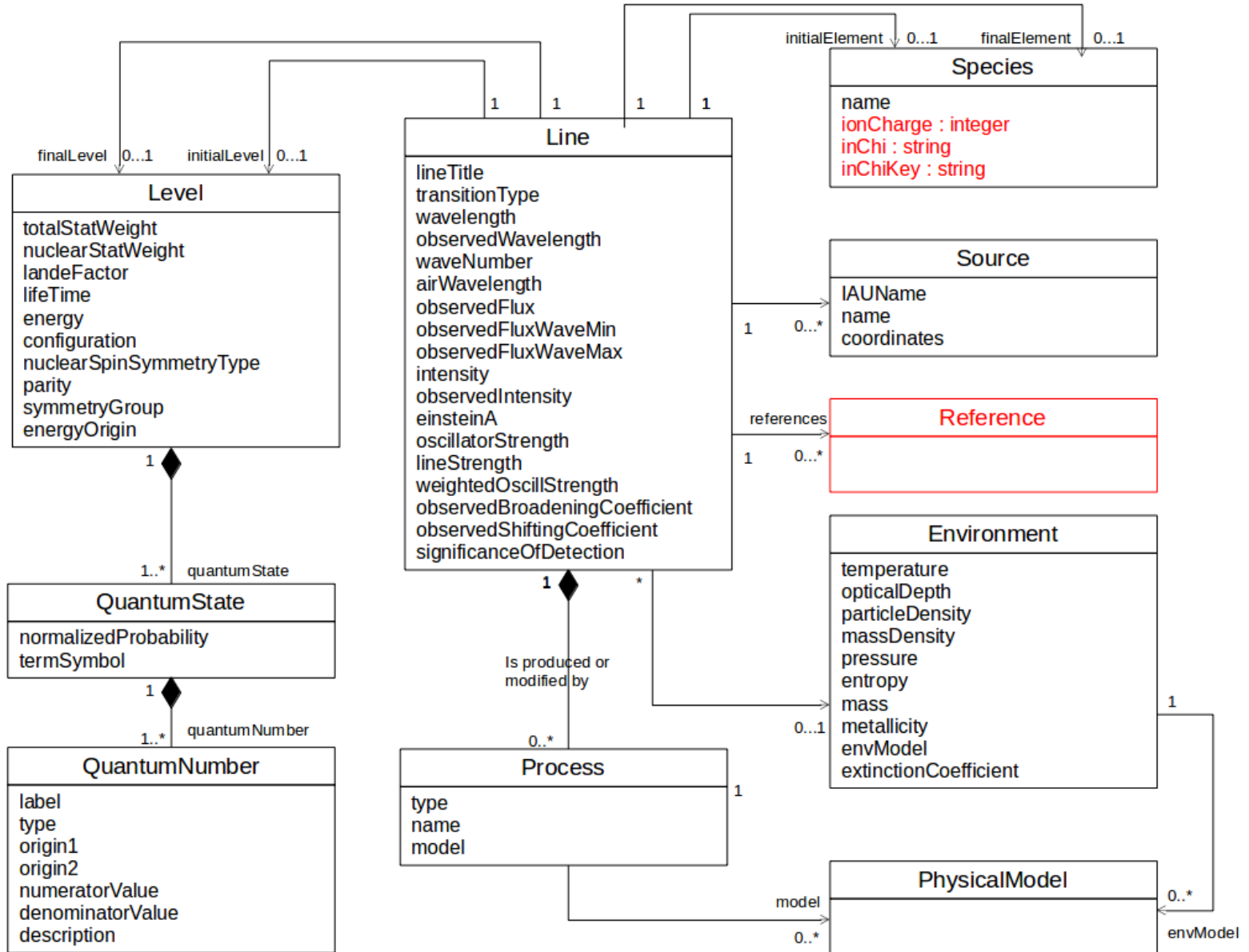
Modifications in SSLDM

Reference
title : string
category : string
authors : string
year : integer
volume : int
sourcename : string
pageBegin : int
pageEnd : int
uniformResourceIdentifier : string
digitalObjectIdentifier : string

• Reference object is equivalent to source object in XSAMS, there already is a Source object in SSLDM

• In XSAMS, possible categories are : book, database, journal, preprint, private communication, proceedings, report, theses. Content would be free in SLAP.

Other possible modifications in SSLDM (only remark for now)

Relation with Level instead of Line

Other possible modifications in SSLDM (only remark for now)

Vamdc : upper level / lower level

Standard evolution
(Trieste interop)

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- Explicitly define the units used for expressing the energies.

Modifications in SLAP output : INFO Fields

New INFO elements in <RESOURCE id="results">

- The RESOURCE element SHOULD contain an INFO with name="FILE_TIMESTAMP". Its value attribute contains the UNIX timestamp in seconds when the file was created by the service.

- The RESOURCE element SHOULD contain an INFO with name="DATABASE_VERSION".

  - Its value attribute contains the version of the database on which the service rely
  - The format of this value is managed by the data provider.
  - It must be updated each time the database content evolves.

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Modifications in SLAP output : References

New TABLE element containing references in <RESOURCE ID="results">


```
<TABLE ID="references">
  <FIELD ID="reference_id" name="reference_id" datatype="char" arraysize="25">
    <DESCRIPTION>An integer identifier for this reference</DESCRIPTION>
  </FIELD>
  <FIELD name="title" datatype="char" arraysize="*" utype="ssldm:Reference.title" ucd="meta.title" >
    <DESCRIPTION>Title of the reference</DESCRIPTION>
  </FIELD>
  <FIELD name="category" datatype="char" arraysize="*" utype="ssldm:Reference.category">
    <DESCRIPTION>Type of the reference</DESCRIPTION>
  </FIELD>
  <FIELD name="authors" datatype="char" arraysize="*" utype="ssldm:Reference.authors" ucd="meta.bib.author">
    <DESCRIPTION></DESCRIPTION>
  </FIELD>
  <FIELD name="year" datatype="int" utype="ssldm:Reference.year">
    <DESCRIPTION></DESCRIPTION>
  </FIELD>
  <GROUP ID="reference" name="primaryKey">
    <DESCRIPTION>reference linked to published data</DESCRIPTION>
    <FIELDref ref="reference_id"/>
  </GROUP>
  <DATA>
```

Mandatory

Shanghai Interop meeting 2017

Modifications in SLAP output :
Relations between data and references

```
<TABLE ID="lines">
  <FIELD name="title" datatype="char" ucd="em.line" utype="ssldm:Line.title" arraysize="*">
    <DESCRIPTION>small description identifying the line</DESCRIPTION>
  </FIELD>
  <FIELD  ID="line_references" name="references" datatype="char" arraysize="25s," ucd="meta.bib">
    <DESCRIPTION></DESCRIPTION>
  </FIELD>
```

Foreign key declaration

List of reference IDs

```
<GROUP  name="foreignKey" ref="references">
  <DESCRIPTION>a reference where data have been published</DESCRIPTION>
  <PARAM name="local_field" datatype="char" arraysize="*" value="line_references"/>
  <FIELDref ref="reference_id"/>
</GROUP>
```

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Modifications in SLAP output :
Unit attribute mandatory for energies


```
<FIELD name="initial_energy" datatype="double"
  utype="ssldm:Line.initialLevel.energy.value"
  ucd="phys.energy;phys.atmol.initial;phys.atmol.level" unit="joules">
</FIELD>
<FIELD name="final_energy" datatype="double"
  utype="ssldm:Line.finalLevel.energy.value"
  ucd="phys.energy;phys.atmol.final;phys.atmol.level" unit="joules">
</FIELD>
```

Mandatory unit attribute

Standard evolution (additional changes)

- A new ION_CHARGE parameter to complete the already existing CHEMICAL_ELEMENT, containing an interval of charge

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Modifications in SLAP parameters : ION_CHARGE

- Current SLAP version only has CHEMICAL_ELEMENT to look for species

- Not precise enough for searching, CHARGE can only be concatenated into species

- Needs to be parsed

- Examples of requests with new parameter :

  - Neutral CO :
  http://someservice/slap.jsp?
      REQUEST=queryData&**CHEMICAL_ELEMENT=CO&ION_CHARGE=0**

  - CO+ :
  http://someservice/slap.jsp?
      REQUEST=queryData&**CHEMICAL_ELEMENT=CO&ION_CHARGE=1**

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Modifications in SLAP output
Element name FIELD

Exactly one field SHOULD have utype="ssldm:Line.species.name" with datatype="char", arraysize="*" and ucd="phys.atmol.element", containing a name of the chemical element source of this line.

REPLACED BY

Exactly one field SHOULD have utype="ssldm:Line.initialElement.name" with datatype="char", arraysize="*" and ucd="phys.atmol.element;phys.atmol.initial", containing a name of the chemical element source of the initial level of this line.

Exactly one field SHOULD have utype="ssldm:Line.finalElement.name" with datatype="char", arraysize="*" and ucd="phys.atmol.element;phys.atmol.final", containing a name of the chemical element source of the final level of this line. If only one of initial and final element name has been specified, it is assumed that the other one is identical.

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Modifications in SLAP output
New optional FIELDs

- Exactly one field SHOULD have utype="ssldm:**Line.initialElement.inChiKey**" with datatype="char", arraysize="*" and ucd="phys.atmol.initial", containing the inchikey of the chemical element source of this line.

- Exactly one field SHOULD have utype="ssldm:**Line.finalElement.inChiKey** " with datatype="char", arraysize="*" and ucd="phys.atmol.final", containing the name of the chemical element source of this line. If only one of initial and final element inChiKey has been specified, it is assumed that the other one is identical.

- Exactly one field SHOULD have utype="ssldm:**Line.initialElement.ionCharge**" with datatype="int", containing the charge of the chemical element source of this line.

- Exactly one field SHOULD have utype="ssldm:**Line.finalElement.ionCharge**" with datatype="int", containing the name of the chemical element source of this line. If only one of initial and final element ion charge has been specified, it is assumed that the other one is identical.

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Modifications in SLAP parameters : QuerySpecies operation

- Client applications needs to know what species are available to :
  - Suggest species existing in a service to the user
  - Suggest services for a given species

- VAMDC has a specific request "select species"

- In addition to already defined REQUEST=queryData, we propose REQUEST=querySpecies

- It will return a list of species for which spectral lines are available in the service

Modifications in SLAP parameters : QuerySpecies operation

```xml
<VOTABLE xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.ivoa.net/xml/VOTable/v1.3" version="1.3">
  <RESOURCE type="results">
    <INFO name="QUERY_STATUS" value="OK"/>
    <INFO name="FILE_TIMESTAMP" value="1487063789" />

    <INFO name="DATABASE_VERSION" value="2017_01_25"/>
    <TABLE ID="results">
      <FIELD name="species_name" datatype="char" arraysize="*" ucd="phys.atmol.element" utype="ssldm:Species.name">
        <DESCRIPTION></DESCRIPTION>
      </FIELD>
      <FIELD name="ion_charge" datatype="int" ucd="phys.atmol.ionization" utype="ssldm:Species.ionCharge">
        <DESCRIPTION></DESCRIPTION>
      </FIELD>
      <DATA>
        <TABLEDATA>
          <TR>
            <TD>C</TD>
            <TD>0</TD>
          </TR>
          <TR>
            <TD>CO</TD>
            <TD>0</TD>
          </TR>
          <TR>
            <TD>CO</TD>
            <TD>1</TD>
          </TR>
        </TABLEDATA>
      </DATA>
    </TABLE>
  </RESOURCE>
</VOTABLE>
```

Mandatory → (points to the FIELD name="species_name" line)

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    <INFO name="DATABASE_VERSION" value="2017_01_25"/>
    <TABLE ID="results">
    <FIELD name="species_name" datatype="char" arraysize="*" ucd="phys.atmol.element" utype="ssldm:Species.name">
       <DESCRIPTION></DESCRIPTION>
    </FIELD>
    <FIELD name="ion_charge" datatype="int" ucd="phys.atmol.ionization" utype="ssldm:Species.ionCharge">
       <DESCRIPTION></DESCRIPTION>
    </FIELD>
    <DATA>
      <TABLEDATA>
        <TR>
          <TD>C</TD>
          <TD>0</TD>
        </TR>
        <TR>
          <TD>CO</TD>
          <TD>0</TD>
        </TR>
        <TR>
          <TD>CO</TD>
          <TD>1</TD>
        </TR>
      </TABLEDATA>
    </DATA>
    </TABLE>
  </RESOURCE>
</VOTABLE>
```

Mandatory → (species_name FIELD)

Optional → (ion_charge FIELD)