Javascript viewer
For NMR and MS experiment

Tutorial to know how it works

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1 Introduction

1.1 What does it do?

The aim is to build a viewer displaying the output of a chemical experiment:

-Mass Spectra experiment

-NMR experiment

Each output experiment provides the information about:

-The molecule studied.

-Its spectra.

-The additional information about the condition of the experiment

Hence, the viewer must **displays** the **molecule** along with its **spectrum**. Besides, we want it to be **interactive** with the user, e.g when the user mouse over one peak, it has to **highlights** and highlights the corresponding atoms it is linked to(in the case of a NMR experiment) and it has to display the corresponding fragment(s) (in case of a MS experiment).

1.2 How do we do it?

The entire viewer is build with JavaScript and use the google closure library

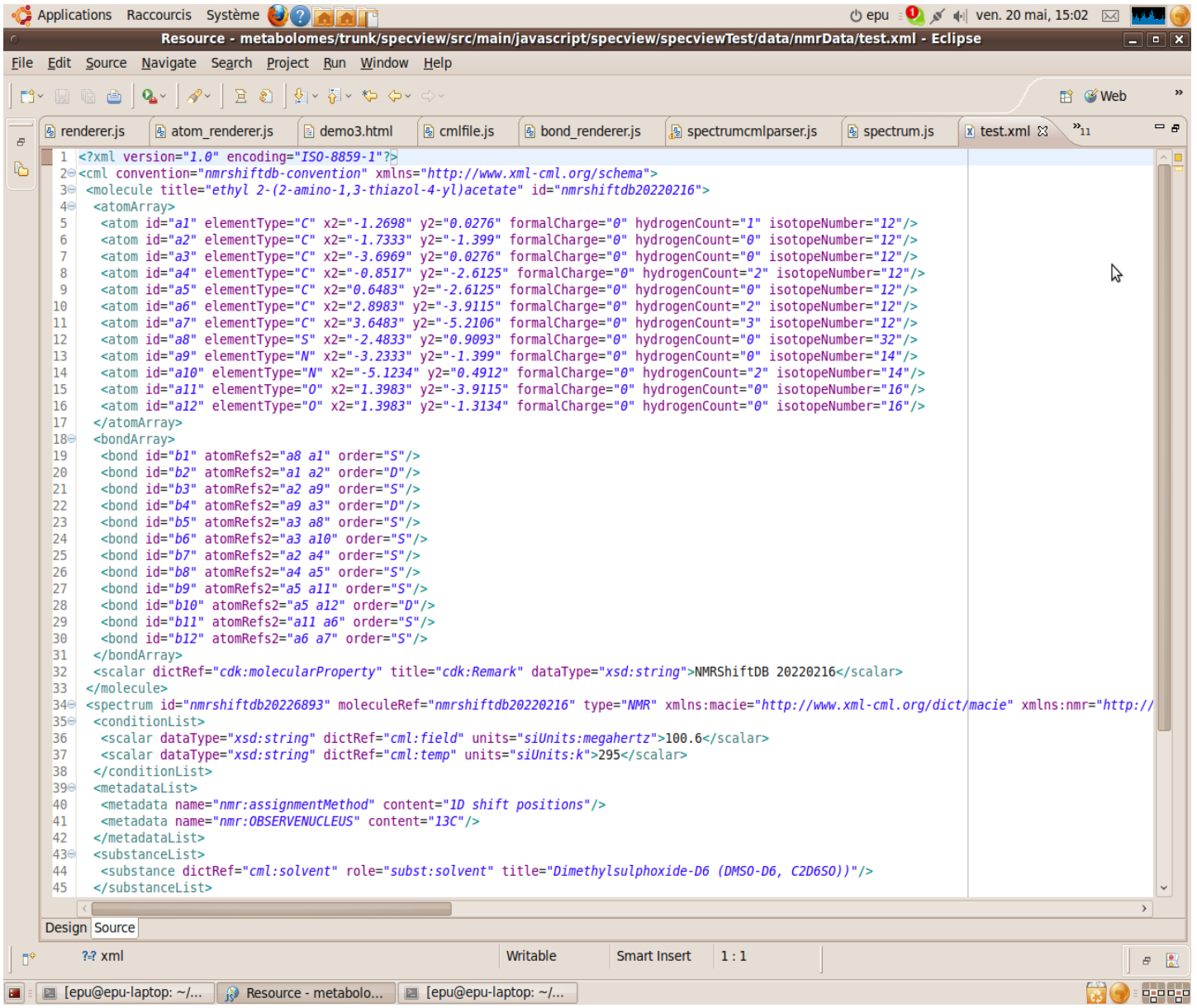
1.2.1 Google Closure

In summary, the Closure Library is a JavaScript library which is based on a modulable architecture. It provides cross-browser functions for DOM manipulations and events, AJAX and JSON, as well as more high-level objects such as User Interface widgets and controls. For instance and in our case, it provides the tools to design a canvas editor, and all the objects to have a control over this canvas.

2 The entry point

Our Input data is a file in a **cml file**, which is a standart of xml. The file contains the information generated by the output of the experiment. It holds either MS data, or NMR data.

Figure 1: Example of cml file



2.1 What does it contain?

This file provides all the information required in order to build a **molecule** and a **spectrum**. THe molecule consists in a liste of ***atoms***:

Figure 2: A list of atoms

```
<atomArray>
 <atom id="a1" elementType="C" x2="-1.2698" y2="0.0276" formalCharge="0" hydrogenCount="1" isotopeNumber="12"/>
 <atom id="a2" elementType="C" x2="-1.7333" y2="-1.399" formalCharge="0" hydrogenCount="0" isotopeNumber="12"/>
 <atom id="a3" elementType="C" x2="-3.6969" y2="0.0276" formalCharge="0" hydrogenCount="0" isotopeNumber="12"/>
 <atom id="a4" elementType="C" x2="-0.8517" y2="-2.6125" formalCharge="0" hydrogenCount="2" isotopeNumber="12"/>
```

The list of atoms contains all the informations to identify the entities of the molecules. The important point is that the coordinates it contains are relative coordinates. In order to display the atoms on the screen, they have to be transformed into actual coordinatesm, "pixel coordinates".

Figure 3: A list of bonds

```
<bondArray>
 <bond id="b1" atomRefs2="a8 a1" order="S"/>
 <bond id="b2" atomRefs2="a1 a2" order="D"/>
 <bond id="b3" atomRefs2="a2 a9" order="S"/>
 <bond id="b4" atomRefs2="a9 a3" order="D"/>
```

The bonds refer to 2 atoms by their id. It is possible, that single order bond have a certain stereo specificity. In that case, the bond "b_i'' would have a tag "*bondStereo*" specifying the orientation of the bond.

Figure 4: Example of peak annotation for a NMR experiment

```
<peakList>
 <peak xValue="103.12" xUnits="units:ppm" peakShape="sharp" peakMultiplicity="D" id="p0" atomRefs="a1"/>
 <peak xValue="14.11" xUnits="units:ppm" peakShape="sharp" peakMultiplicity="Q" id="p1" atomRefs="a7"/>
 <peak xValue="144.37" xUnits="units:ppm" peakShape="sharp" peakMultiplicity="S" id="p2" atomRefs="a2"/>
 <peak xValue="168.24" xUnits="units:ppm" peakShape="sharp" peakMultiplicity="S" id="p3" atomRefs="a3"/>
 <peak xValue="170.18" xUnits="units:ppm" peakShape="sharp" peakMultiplicity="S" id="p4" atomRefs="a5"/>
 <peak xValue="36.93" xUnits="units:ppm" peakShape="sharp" peakMultiplicity="T" id="p5" atomRefs="a4"/>
 <peak xValue="60.16" xUnits="units:ppm" peakShape="sharp" peakMultiplicity="T" id="p6" atomRefs="a6"/>
</peakList>
```

THe most important point of the file is that it is an annotated file. In the case of a file holding NMR experiment, it simply means that one peak refer to one or multiple atoms. In the case of a file holding MS data, the peak refers to one or multiple molecules.

Thanks to these annotation files, it is possible to have a cross talk between the molecule and its spectra.

Figure 5: Example of peak annotation for a MS experiment

```
"    <peakList>\n" +
"      <peak xValue=\"223.075904592\" xUnits=\"units:mz\" yValue=\"100.0\" yUnits=\"units:cps\" id=\"peak0\">\n" +
"        <molecule ref=\"CHEBI:1734_0\"/>\n" +
"      </peak>\n" +
"      <peak xValue=\"147.044604464\" xUnits=\"units:mz\" yValue=\"100.0\" yUnits=\"units:cps\" id=\"peak1\">\n" +
"        <molecule ref=\"CHEBI:1734_1\"/>\n" +
"      </peak>\n" +
```

2.2 Create a JavaScript Object

Now, in order to display the content of the file, we decide to create an object, called "*metaSpecObject*". This object is a generic object that can contains all the data to represent a molecule along with its spectrum and the information to allow the cross talk between the two entities.

2.3 The parser

3 How to display everything?