CHEMML

ConTEXt XML

Pragma ADE / Hasselt NL

Description

The chemical XML markup dialect provided by ConTeXt is relatively simple, but sufficient for everyday chemistry. Of course we have elements that represent the building blocks of chemistry:

- atoms
- ions
- molecules

In addition there are methods for:

- reactions
- bonds

Reactions, molecules and ions can be annotated. For this we provide:

- captions

For the moment there are no provisions for structure formulas, but there will be some day (probably build on top of the ConTeXt module PPCHTeX).

Beware: the spacing may be improved and therefore can change slightly in future versions.

Structure

The simplest building block is the atom:

```
<chem>
  <atom> H </atom>
</chem>
```

$$\mathrm{H}$$

You can dress up an atom with a couple of ornaments:

```
<chem>
  <atom n="6" charge="-5" weight="652" protons="339"> Rx </atom>
</chem>
```

$${}^{652}_{339}\mathrm{Rx}^{-5}_{6}$$

You (or nature) can combine atoms in molecules:

```
<chem> <molecule>
  <atom n="2"> H </atom>
  <atom>       O </atom>
</molecule> </chem>
```

$$\mathrm{H_2O}$$

An efficient way of identifying multiple molecules is the following:

```
<chem> <molecule n="2">
  <atom n="2"> H </atom>
  <atom>       O </atom>
</molecule> </chem>
```

$$\mathrm{2H_2O}$$

As you can see, a molecule is just a series of atoms and again, we can add a couple of ornaments.

```
<chem> <molecule n="2">
  <atom n="2" charge="+1"> H </atom>
  <atom       charge="-2"> O </atom>
</molecule> </chem>
```

$$\mathrm{2H_2^{+1}O^{-2}}$$

Atoms with a charge are called ions. Because a charge can be associated to a combination of atoms, you can also package the atoms in an ion element.

```
<chem> <molecule n="2">
  <ion charge="+2"> <atom n="2"> H </atom> </ion>
  <ion charge="-2"> <atom>       O </atom> </ion>
</molecule> </chem>
```

$$\mathrm{2H_2^{+2}O^{-2}}$$

You can influence the appearance of a ion. Take the following acid:

```
<chem> <ion charge="-1">
  <atom> C </atom>
  <atom> O </atom>
  <atom> O </atom>
  <atom> H </atom>
</ion> </chem>
```

$$\mathrm{COOH^{-1}}$$

A different way to visualize the charge is to use brackets around an ion. You can force this with a directive.

```
<chem>
  <?context-chemml-directive ion alternative b ?>
  <molecule>
    <ion charge="-1">
      <atom> C </atom>
      <atom> O </atom>
      <atom> O </atom>
      <atom> H </atom>
    </ion>
  </molecule>
</chem>
```

$$[\mathrm{COOH}]^{-1}$$

As you can see in the next example, the negative charge of the whole end up above the number of Y atoms.

```
<chem> <molecule>
  <ion charge="-1">
    <atom> X </atom>
    <atom n="3"> Y </atom>
  </ion>
</molecule> </chem>
```

$$\mathrm{XY}_3^{-1}$$

A molecule seldom comes alone. This is why we have an encapsulating element dealing with reactions. This is a presentational element, which means that we just have a sequence of items to be represented.

```
<formula>
  <chem>
    <reaction>
      <molecule n="2">
        <atom n="2"> H </atom>
      </molecule>
    <plus/>
      <molecule>
        <atom n="2"> O </atom>
      </molecule>
    <equilibrium/>
      <molecule n="2">
        <atom n="2"> H </atom>
        <atom>       O </atom>
      </molecule>
    <gives>
      <caption> wet feet </caption>
    </gives>
      <molecule n="2">
        <atom n="2"> H </atom>
        <atom>       O </atom>
      </molecule>
    </reaction>
  </chem>
</formula>
```

$$2H_2 \quad + \quad O_2 \quad \rightleftharpoons \quad 2H_2O \quad \xrightarrow[\text{wet feet}]{} \quad 2H_2O$$

The following special symbols are available:

element	representation
plus	$+$
minus	$-$
equal	$=$
gives	$\longrightarrow$
equilibrium	$\rightleftharpoons$
mesomeric	$\longleftrightarrow$

You can put some text (often expressing conditions) on top or below the arrows. In that case you need to add a couple or more elements and non empty alternatives of the arrow elements.

```
<formula>
  <chem>
    <reaction>
    <gives>
    </gives>
    <gives>
      <caption>first entry</caption>
    </gives>
    <gives>
      <caption>first entry</caption>
      <caption>second entry</caption>
    </gives>
    <gives/>
    </reaction>
  </chem>
</formula>
```

$$\xrightarrow{} \qquad \xrightarrow[\text{first entry}]{} \qquad \xrightarrow[\text{first entry}]{\text{second entry}} \qquad \xrightarrow{}$$

You can also add captions to molecules and ions. If you want a caption to an atom, you need to encapsulate it in a molecule.

```
<chem>
  <reaction>
    <molecule n="2">
      <atom n="2"> H </atom>
      <caption> hydrogen </caption>
    </molecule>
  <plus/>
    <molecule>
      <atom n="2"> O </atom>
      <caption> oxygen </caption>
    </molecule>
  <gives>
    <caption> hefty </caption>
  </gives>
    <molecule n="2">
      <atom n="2"> H </atom>
      <atom> O </atom>
      <caption> water </caption>
    </molecule>
  </reaction>
</chem>
```

$$\underset{\text{hydrogen}}{2H_2} \quad + \quad \underset{\text{oxygen}}{O_2} \quad \xrightarrow[\text{hefty}]{} \quad \underset{\text{water}}{2H_2O}$$

Another way to dress up a chemical formula is to visualize bonds. Therefore we provide a simple bond element.

```
<chem> <molecule>
  <atom> H </atom>
    <bond n="1"/>
  <atom> C </atom>
    <bond n="2"/>
  <atom> C </atom>
    <bond n="1"/>
  <atom> H </atom>
</molecule> </chem>
```

$$H{=}C{\equiv}C{=}H$$

You can also use a more verbose series of commands to achieve this visualization.

```
<chem> <molecule>
  <atom> H </atom>
    <singlebond/>
  <atom> C </atom>
    <doublebond/>
  <atom> C </atom>
    <singlebond/>
  <atom> H </atom>
</molecule> </chem>
```

H—C═C—H

Normally the typesetting engine will adapt itself automatically to either in–line or display chemistry. The next example shows in–line usage.

```
When we manage to bring <chem> <atom> H </atom> </chem>
(hydrogen) in contact with <chem> <atom> O </atom> </chem>
(oxygen) we get a bit of noise and fire but we end up with
<chem> <molecule> <atom n="2"> H </atom> <atom> O </atom>
</molecule> </chem> (water).
```

When we manage to bring H (hydrogen) in contact with O (oxygen) we get a bit of noise and fire but we end up with H_2O (water).

However, if you want to have a bit more control, you should use one of the following capsules. The normal `<chem>` element acts chooses one of these, depending on the circumstances.

element	meaning
ichem	in–line Chemistry
dchem	display Chemistry

Usage

This module is loaded as any module:

```
\usemodule[chemml]
```

XML example

Here we will collect a few examples.

Configuring

We will add some more control over spacing, lettering and color later.

Documentation

There is no additional documentation. The TEX counterpart of this module, namely PPCHTEX, uses a representation more in tune with the way one codes documents in TEX.

Colofon

This manual is part of the CONTEXT distribution, and is authored and maintained by Hans Hagen. CONTEXT is developed at PRAGMA ADE, Hasselt, The Netherlands. This manual is produced on October 26, 2001.