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:

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

H

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

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

\[ {^{652}_{339}}RX^-5 \]

You (or nature) can combine atoms in molecules:
An efficient way of identifying multiple molecules is the following:

\[ \text{H}_2\text{O} \]

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

\[ \text{2H}_2\text{O} \]

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.

\[ \text{2H}^+\text{O}^- \]

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

\[ \text{COOH}^- \]

A different way to visualize the charge is to use brackets around an ion. You can force this with a directive.
As you can see in the next example, the negative charge of the whole end up above the number of \( Y \) atoms.

\[
[\text{COOH}]^{-1}
\]

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.

\[
\text{XY}_3^{-1}
\]
<gives>
  <caption> wet feet </caption>
</gives>

<gives>
  <molecule n="2">
    <atom n="2"> H </atom>
    <atom> O </atom>
  </molecule>
</gives>

<reaction>
  <gives>
    <caption> first entry </caption>
  </gives>
  <gives>
    <caption> first entry </caption>
    <caption> second entry </caption>
  </gives>
</reaction>

<formula>
  \[
  2H_2 + O_2 \overset{\text{wet feet}}{\longrightarrow} 2H_2O \overset{\text{wet feet}}{\longrightarrow} 2H_2O
  \]
</formula>

The following special symbols are available:

<table>
<thead>
<tr>
<th>element</th>
<th>representation</th>
</tr>
</thead>
<tbody>
<tr>
<td>plus</td>
<td>+</td>
</tr>
<tr>
<td>minus</td>
<td>–</td>
</tr>
<tr>
<td>equal</td>
<td>=</td>
</tr>
<tr>
<td>gives</td>
<td>\hline</td>
</tr>
<tr>
<td>equilibrium</td>
<td>\hline</td>
</tr>
<tr>
<td>mesomeric</td>
<td>\hline</td>
</tr>
</tbody>
</table>

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.
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.

\[
\begin{align*}
\text{hydrogen} + \text{oxygen} & \rightarrow \text{hefty} \\
2\text{H}_2 + \text{O}_2 & \rightarrow 2\text{H}_2\text{O}
\end{align*}
\]

Another way to dress up a chemical formula is to visualize bonds. Therefore we provide a simple bond element.
You can also use a more verbose series of commands to achieve this visualization.

\[
\begin{aligned}
\text{<chem> <molecule> }
\text{ <atom> H </atom> }
\text{ <singlebond/> }
\text{ <atom> C </atom> }
\text{ <doublebond/> }
\text{ <atom> C </atom> }
\text{ <singlebond/> }
\text{ <atom> H </atom> }
\text{ </molecule> </chem>}
\end{aligned}
\]

\[
\text{H—C═C—H}
\]

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 $\text{<chem> <atom> H </atom> </chem>}$ (hydrogen) in contact with $\text{<chem> <atom> O </atom> </chem>}$ (oxygen) we get a bit of noise and fire but we end up with $\text{<chem> <molecule> <atom n="2"> H </atom> <atom> O </atom> </molecule> </chem>}$ (water).

When we manage to bring $\text{H}$ (hydrogen) in contact with $\text{O}$ (oxygen) we get a bit of noise and fire but we end up with $\text{H}_2\text{O}$ (water).

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

<table>
<thead>
<tr>
<th>element</th>
<th>meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>ichem</td>
<td>in-line Chemistry</td>
</tr>
<tr>
<td>dchem</td>
<td>display Chemistry</td>
</tr>
</tbody>
</table>

**Usage**

This module is loaded as any module:

\usemodule[chemml]

**XML example**

Here we will collect a few examples.
We will add some more control over spacing, lettering and color later.

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

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.