# Integrating CML and OMDoc

Michael Kohlhase
Jacobs University

Peter Murray Rust
Cambridge University

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**Abstract**

This will revolutionize science.[1] EdNote(1)

## 1 Introduction

[2] EdNote(2)

## 2 Examples

We consider an example from Steininger's Dissertation [Ste05, p.23]

```
<ochemdoc xml:id="disstest" xmlns= "http://www.sciml.org/ochemdoc">

<!-- <symbol name="ester"/>
<molecule for="esther">
  <cml>....</cml>
</molecule>-->

<assertion>
  <CMP>
    Der erste Teil wird nicht wie in Kapitel 2.3.2 als konstante Hintergrundreaktion
    angenommen, sondern die fr diese Reaktion verfgbare Esterkonzentration <math><share
    href="#esterconst"/></math> nimmt durch die Bildung des Ester-Katalysator-Komplexes
    ab.

<math class="display">
  <apply>
    <eq/>
    <csymbol cd="foundations" name="rgas"/>
    <apply>
      <plus/>
      <apply>
        <times/>
        <csymbol cd="rateconstants" name="O"/>
        <apply xml:id="esterconst">
          <csymbol cd="foundations" name="concentration"/>
          <csymbol cd="cml" name="Ester"/>
        </apply>
      </apply>
      <apply>
```

[1] EdNote: continue
[2] EdNote: write something

```
        <times/>
        <csymbol cd="rateconstants" name="Kat"/>
        <apply>
          <csymbol cd="foundations" name="concentration"/>
          <compound>
            <csymbol cd="cml" name="Ester"/>
            <csymbol cd="cml" name="Katstar"/>
          </compound>
        </apply>
      </apply>
    </apply>
  </apply>
</math>

hier kommt der rest
  </CMP>
</assertion>
</ochemdoc>
```

# 3 Conclusion

# References

[Ste05] Harald Steininger. *2-Pyridon-katalysierte Esteraminolyse*. PhD thesis, Ludwig-Maximilians-Universitt Mïchen, 2005.

```
# A RelaxNG schema for Open Chemical Documents (OChemDoc 1.2)
# $Id: omdoc.rnc 6399 2007-05-25 15:07:45Z kohlhase $
# $HeadURL: https://svn.omdoc.org/repos/omdoc/branches/omdoc-1.2/rnc/omdoc.rnc $
# See the documentation and examples at http://www.omdoc.org
# Copyright (c) 2007 Michael Kohlhase, released under the GNU Public License (GPL)

default namespace omdoc = "http://www.sciml.org/ochemdoc"

id.attrib = attribute xml:id {xsd:ID}?,attribute class {xsd:string}?

items = assertion

start = element ochemdoc {id.attrib,items*}

assertion = element assertion {id.attrib,CMP*}
CMP = element CMP {(text|math)*}
mtoken = eq|plus|times
ctoken = notAllowed
ccont = compound
cexp = apply|bind|ci|csymbol|share|mtoken|ctoken|ccont
math = element math {id.attrib,cexp*}

eq = element eq {id.attrib}
plus = element plus {id.attrib}
times = element times {id.attrib}

csymbol = element csymbol {attribute cd {xsd:NCName},attribute name {xsd:NCName}}

compound = element compound {id.attrib,cexp*} #(can also be used in an apply)

apply= element apply {id.attrib,cexp,cexp+}
bind= element bind {id.attrib,cexp,bvar+,condition,cexp}
bvar = element bvar {ci*}
condition = element condition {id.attrib,cexp}
ci = element ci {id.attrib}
```