Incorporation of Meta-Data in Content Management & eLearning

Horst Bögel

Martin-Luther-University, Institute of Organic Chemistry, D-06120 Halle (GERMANY)  boegel@chemie.uni-halle.de

From Gutenberg Printing to WEB Publishing and eLearning

- Traditional printed Textbook
- Electronic Books and Journals
- Online Searching & Reading
- WEB - Publishing (Re-use of data)
- New Media and eLearning
- Virtual laboratories
Client - Server Architecture

- HTML documents (Server / Browser)
- dynamic HTML (JavaScript, CSS)
- Pictures (SVG), Animations, Videos (MPEG4)
- 3D molecular structures and dynamics (Chime plugin)
- Flash & Shockwave animations (Macromedia)
- VRML 1 & 2 (Cosmo-, Cortona- player)
- Java, Java Applet, Java2, Java3D
- online calculations (Perl Scripts, Servlets, CGI)
- XML (eXtensible ML, DTD, XSLT)

Navigation & User Interactivity

Using concepts & models instead of memorizing facts
Multimedia Publication:
Chemical Innovations on the Web

- High Quality Content
  - Presented the way the users want (Re-use, extensible)
  - Searchable the way the users expect (on-line)
  - New and Novel features (not just page integrity)
  - Three-dimensional objects (3D with CHIME)
  - Visualization of Object Dynamics (VRML 1.0 / 2.0)
  - Editable content
  - Highly structured data (CML, MathML)
  - Finely Grained data
  - Collaborative
  - Content separated from Layout (+DTD, Meta-Data)
  - XML and Java --> HTML, PDF, User Interactivity
- Emphasis on Content over Style Leads to Quality!

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3D Structure of Molecules - the most important data in chemistry
### Structure and Dynamics

<table>
<thead>
<tr>
<th>Geometric</th>
<th>Electronic</th>
<th>Energetic</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Position of Nuclei</strong></td>
<td>'Position' of Electrons</td>
<td>Interactions ( n - e )</td>
</tr>
<tr>
<td>Cartesian coordinates</td>
<td>Electron density</td>
<td>Total energy</td>
</tr>
<tr>
<td>Internal coordinates (Z-mat)</td>
<td>Atomic Charge</td>
<td>Orbital energies (Frontier orb)</td>
</tr>
<tr>
<td>Shape</td>
<td>Polarity</td>
<td>Atomisation energies</td>
</tr>
<tr>
<td>vdw-Surface</td>
<td>Dipole moment (Vector)</td>
<td>Dissoziation energies</td>
</tr>
<tr>
<td>Volume</td>
<td>Polarisability (Tensor)</td>
<td>Binding energies</td>
</tr>
<tr>
<td><strong>Rendering</strong></td>
<td>Electronegativity</td>
<td>Heat of Formation</td>
</tr>
<tr>
<td>Wire - Modell</td>
<td>Hard- and Softness (HSAB)</td>
<td></td>
</tr>
<tr>
<td>Ball &amp; Stick</td>
<td>MEP</td>
<td></td>
</tr>
<tr>
<td>CPK</td>
<td>MLP</td>
<td></td>
</tr>
<tr>
<td>Iso-Surface (Connolly)</td>
<td>Donor- und Acceptor-numbers</td>
<td></td>
</tr>
<tr>
<td>PovRay (light, shadow, reflex)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Properties** (microscopic/macroscopic)

**Catalysis, biochemical activity**

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Here are some applications of VRML.
About CML

In particular we note here how the original CML specification can be extended by modularisation into a **Core namespace**, and extended via other schemas into e.g.

- **CMLReact**. A reaction, containing *reactantLists, productLists* and *links* between them.
- **CMLComp**. A container for computational and simulation input and results
- **CMLQuery**. A generic query language
- **Hooks** for other Schemas such as e.g. **SpectHook**, for spectral parameters and data, and links to molecular details (assignment)

[see: Peter Murray-Rust]
XML-Editor and Server

- XML-Editor (XMLSpy) + CML + MathML + DTD
- Cocoon / Apache -Server + CSS --> HTML or PDF (Client-Browser)
- SQL-DB Java-Servlets
- Online Computation (Quantum Mechanics: G98) Servlet ---> XML
- Java-Applets and Java Interactions (Orbital-Iso-Surfaces)
- Problems in XML (types: multiple choice ...)
- User data (overview about inspected modules and solved problems)
Metadata Standards

- IMS Global Learning Consortium
  - XML, schema, DTD (examples)
  - http://www.imsglobal.org/
- Dublin Core Metadata Initiative DCMI
  - development of interoperable online metadata standards (Registry)
  - Working Group
  - http://dublincore.org/....
- Shared Content Object Reference Model SCORM
  - Advanced Distributed Learning (ADLNet)
  - "Content Aggregation Model" in XML
  - http://www.adlnet.org/
- IEEE Learning Technology Standards Committee LTSC
  - IEEE P1484.12 Learning Object Metadata Working Group LOM
  - http://ltsc.ieee.org/

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Summary and Conclusions

- XML, CML, MatML, .... for data in the WWW
- Meta-data for qualified Search and Access
- New Data Types: 2D Maps, 3D-Structures, 3D-Dynamics
- These will be available for individual Inspection and Re-use
- This enables for better way of Learning and to improve our KNOWLEDGE
- Online Computing and Modeling in the network is possible
- This enables for world-wide Collaboration and Research (team work)
- user-friedly interactive Visualizations