



Posibilitati de cercetare in domeniul chimiei pe Web

Sabin-Corneliu Buraga

Facultatea de Informatica, Universitatea "A.I.Cuza"

Teodora Rusu

Institutul de Chimie Macromoleculara "P.Poni"

Victor Tarhon-Onu

Facultatea de Automatizari si Calculatoare, Univ.Tehnica

Catalina Elena Aberle

Institutul de Chimie Macromoleculara "P.Poni"

Cuprins

- World-Wide Web
- Cercetarea in domeniul chimiei pe Web
- Concluzii finale



World-Wide Web

- Web, WWW, “pinza de paianjen mondiala”
- Sistem de distributie locala sau globala a informatiilor hipermedia (text, imagini, audio, video)
- Serviciu Internet (**WWW** ≠ **Internet**)
- Dezvoltat la CERN (1989) de fizicianul **Tim Berners-Lee** si echipa sa
- Dezvoltare spectaculoasa (1-2 miliarde de pagini Web - aug.2000)

De ce Web?

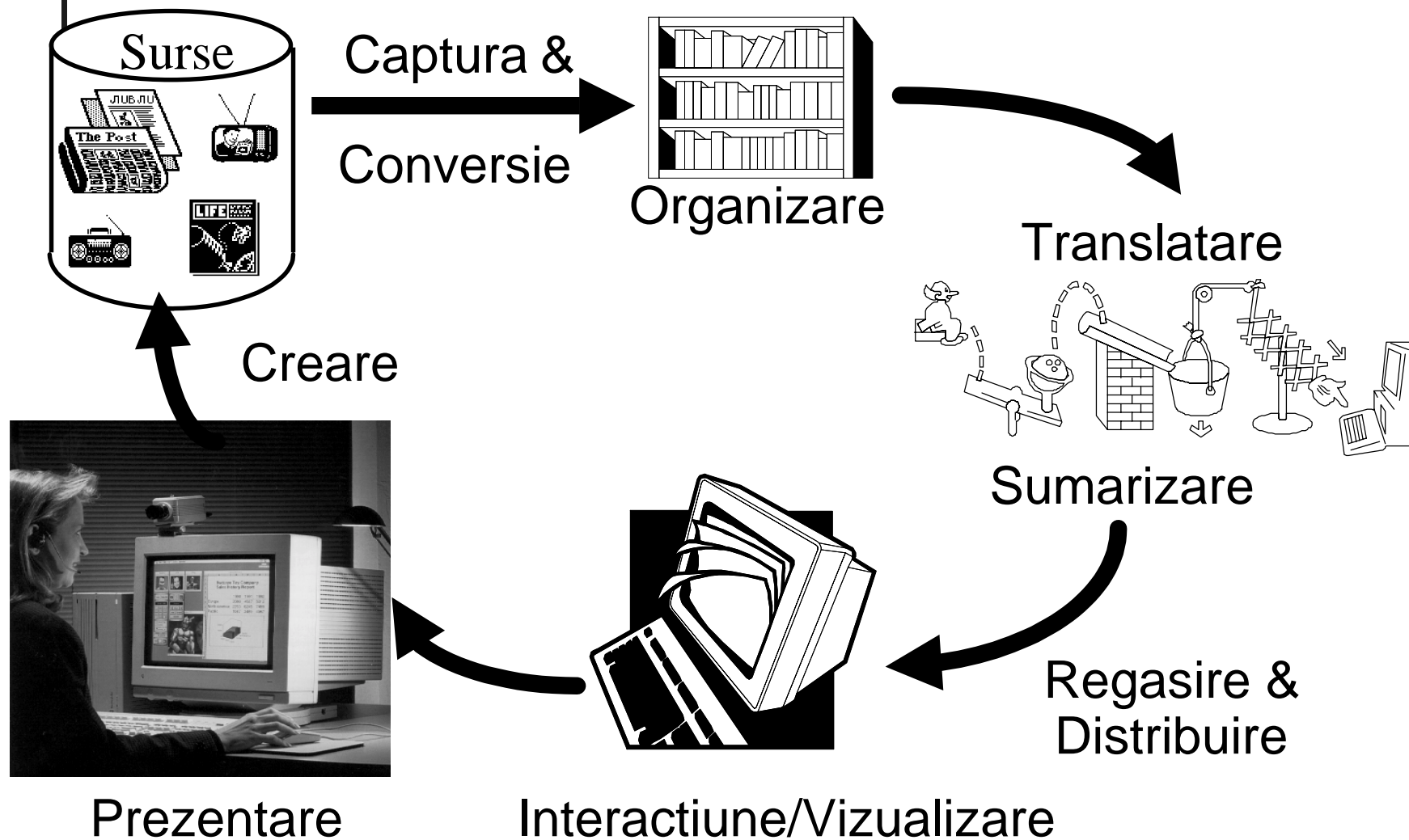
O F E R T A

- Convergenta tehnologiilor
- Servicii integrate
- Multimedia
- Usurinta utilizarii
- Independenta de platforma (sistem de operare, hardware)
- Flexibilitate

C O N T R A P R O

- Acces: viteza, limba (in special, engleza)
- Dezorientare (prea multe informatii, nestructurate)
- Superficialitate
- Interactivitate
- Colaborare
- Utilizari combinate

Circuitul informatiilor pe Web



Directii si probleme

- Integrarea de noi medii de comunicare (TV, realitatea virtuala)
- Modalitati de interactiune
- Accesarea informatiilor
- Societatea informationala mondiala (McLuhan: "satul global")
- Introducerea de tehnologii noi
- Suport acordat cercetatorilor din orice domeniu



Web - depozit informational

- Biblioteca virtuala distribuita la nivel mondial
- Articole si documentatii (din orice domeniu) disponibile pe baza de abonament/gratuit
- Publicatii electronice on-line (Elsevier, Springer-Verlag, ACM,...)
- Grupuri de stiri (news-groups), comunitati stiintifice virtuale - **sci.chemistry**
- Colaborare internationala via Web/Internet

Informatii pe Web

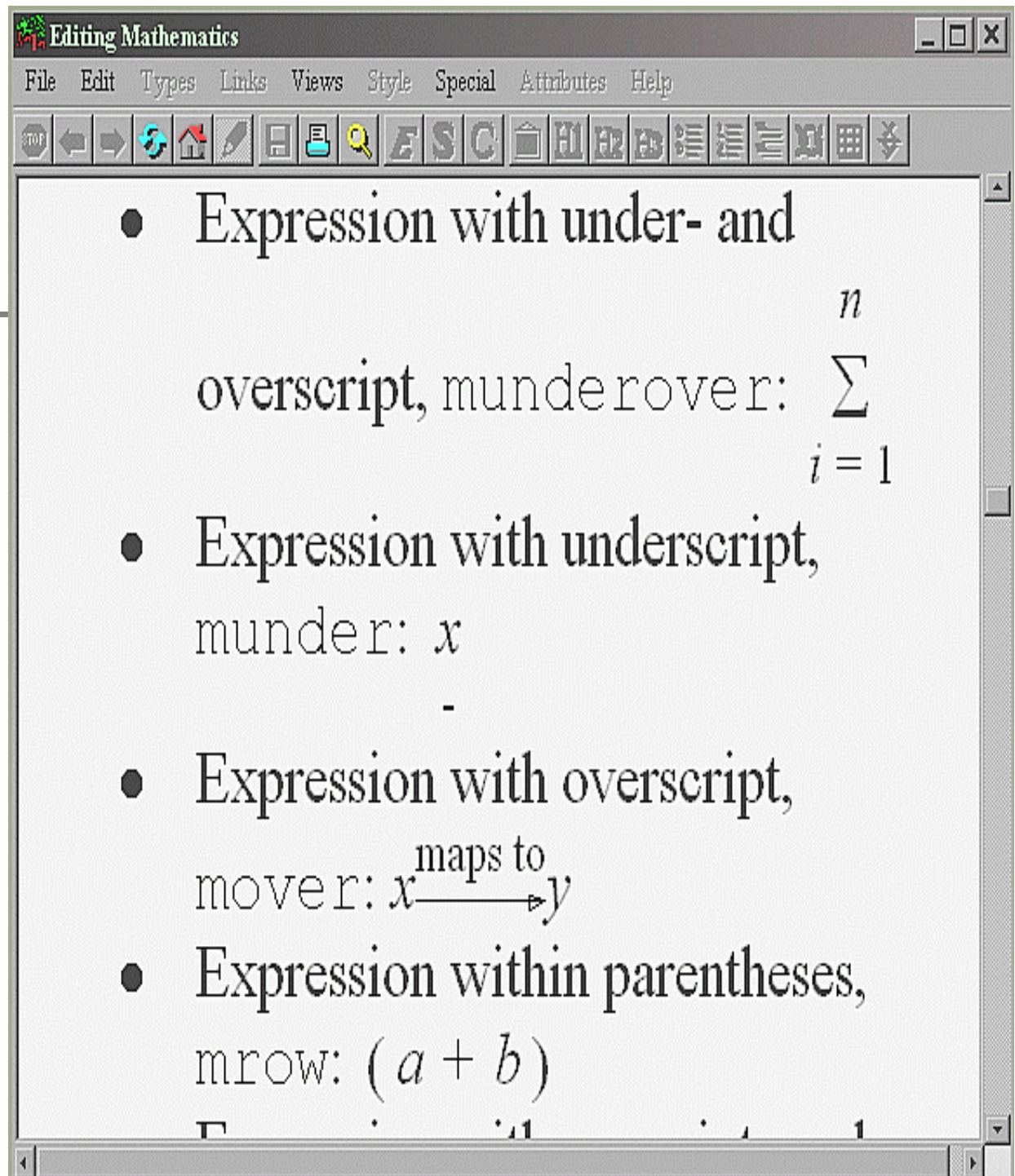
- HTML (HyperText Markup Language)
 - "Lingua franca" a Web-ului
 - Limbaj de adnotare (marcare) a hipertextului (1990-prezent)
 - Descendent al SGML (Standard Generalized Markup Language)
 - Nu poate descrie informatii structurale complexe (expresii matematice, formule chimice, structuri macromoleculare sau biologice etc.)

Alternative la HTML

- Limbaje specializate
 - **MathML** - modeleaza expresii matematice sofisticate (vizualizate cu Amaya)
 - **ChemML, CML** - descriu formule chimice oricit de complexe (vizualizate cu Jumbo)
 - **VRML** (Virtual Reality Modeling Language) - modeleaza in 3D compusii macromoleculari (vizualizate cu WorldView pentru Internet Explorer sau Netscape Communicator)

MathML

Vizualizare cu
Amaya

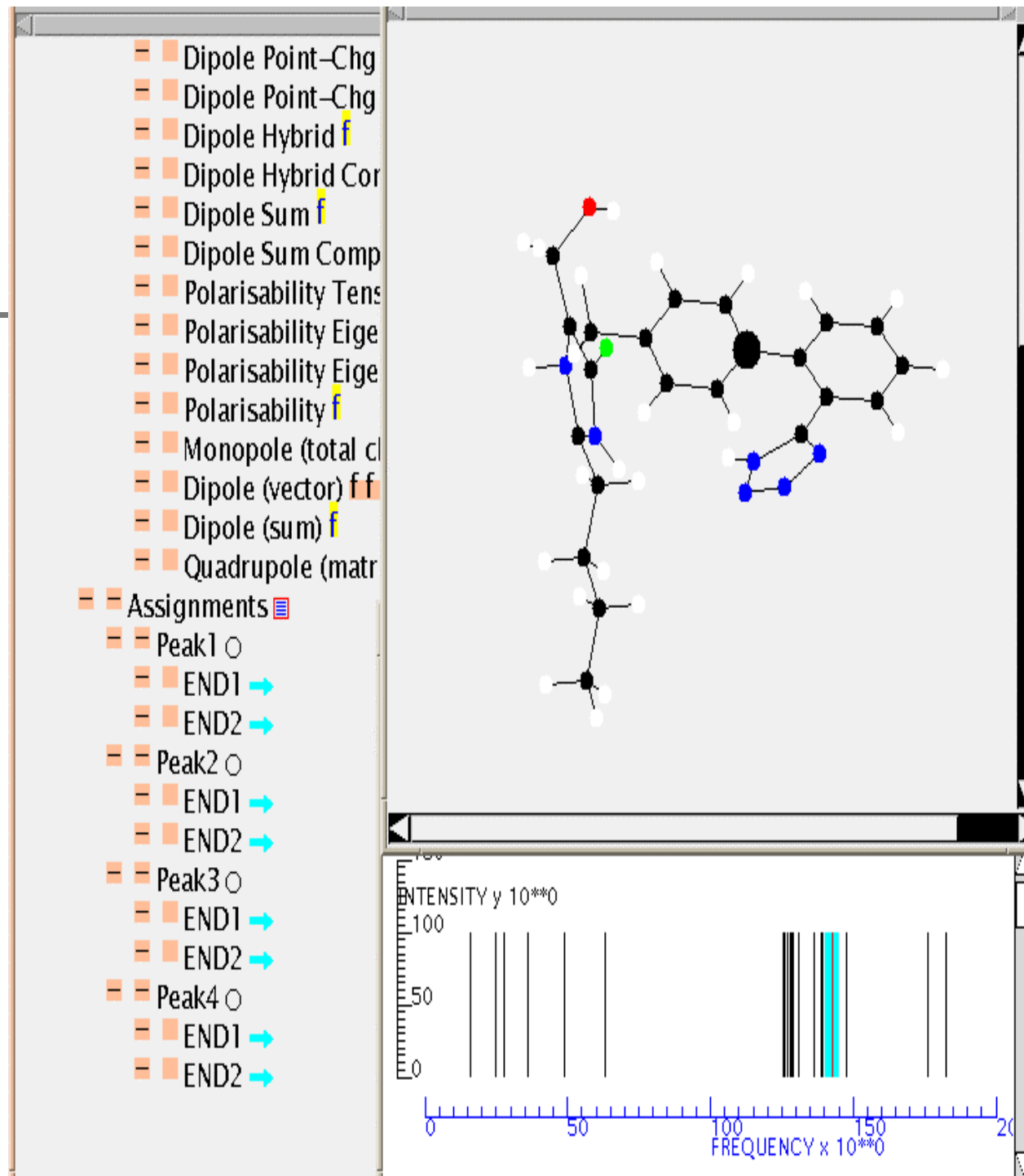


The screenshot shows a window titled "Editing Mathematics" with a menu bar (File, Edit, Types, Links, Views, Style, Special, Attributes, Help) and a toolbar with various icons. The main content area displays a list of bullet points, each describing a MathML expression and its visual output:

- Expression with under- and overscript, munderover: $\sum_{i=1}^n$
- Expression with underscript, munder: x
- Expression with overscript, mover: $x \xrightarrow{\text{maps to}} y$
- Expression within parentheses, mrow: $(a + b)$

ChemML

Vizualizare cu
Jumbo

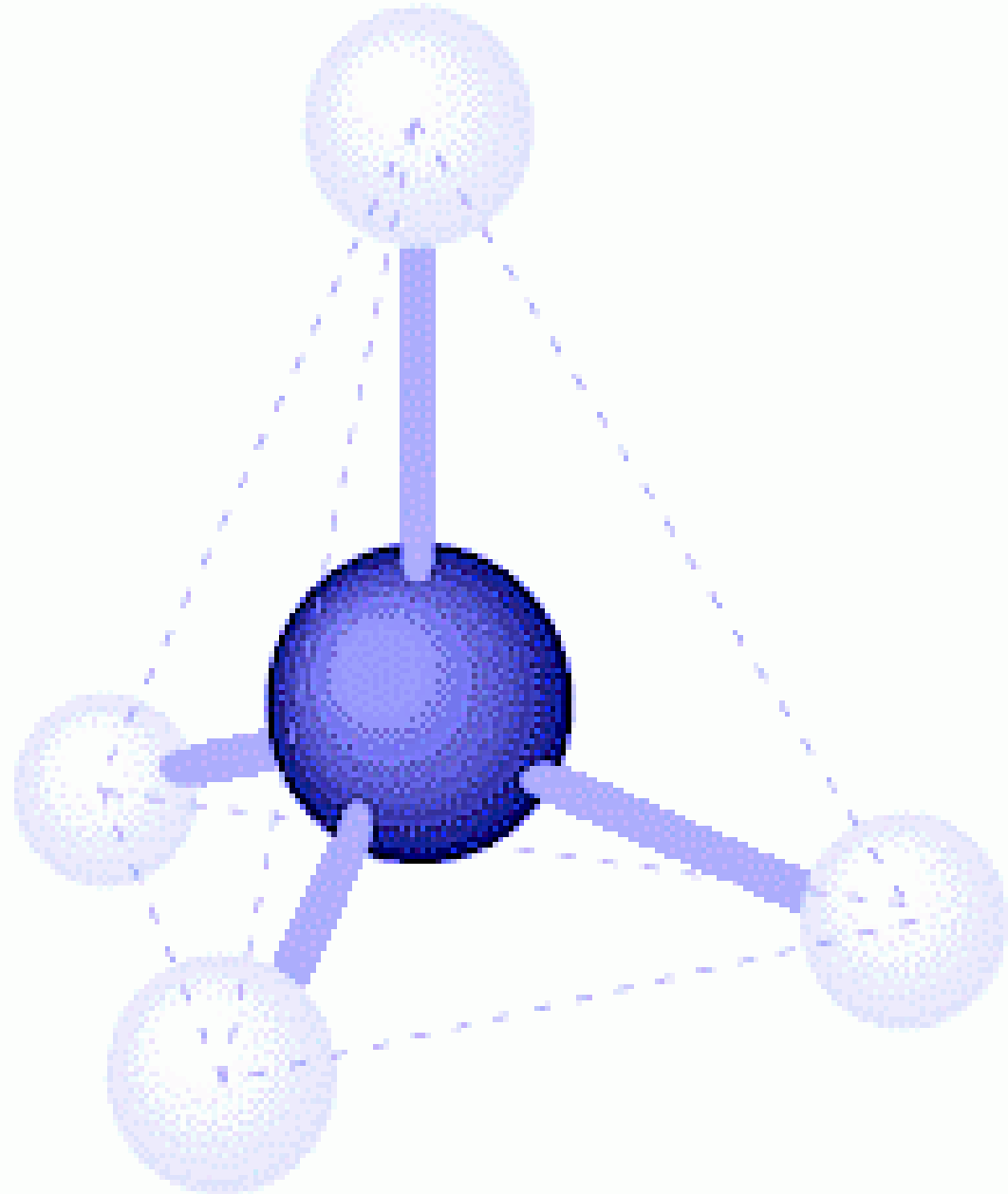


Aplicatii ale ChemML

- Cristalografie
- Molecule organice/anorganice
- Macromolecule: secvente proteinice
- Hiper-vocabulare moleculare: termeni si modelari grafice
- Specificatia limbajului:
<http://www.venus.co.uk/omf/cml/>

VRML

Vizualizare cu
WorldView
(IE/NS)

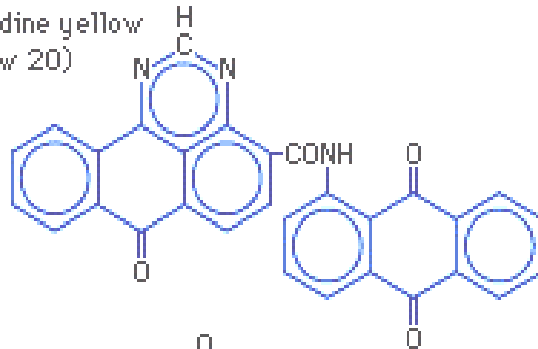
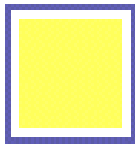


Suport pentru cercetare

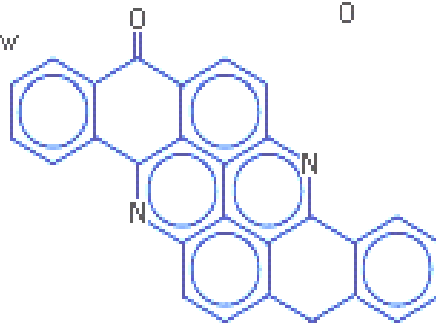
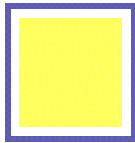
- Web = mediu distribuit computational
- Studiul in retea al proprietatilor & caracteristicilor compusilor macromoleculari
- Posibilitati avansate de cautare a informatiilor din domeniul chimiei
 - Motoare de cautare generale (Altavista, Google)
 - Tehnici specializate - limbaje de interogare
WQFL - Web Query Formulating Language
[S.C.Buraga, T.Rusu - 2000]

Suport pentru cercetare (Britannica Online - www.eb.com)

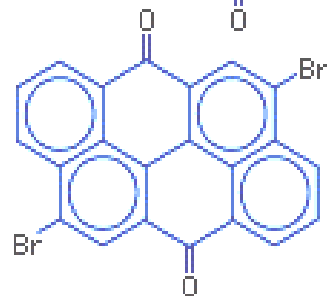
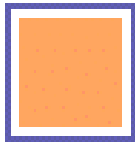
anthrapyrimidine yellow
(CI Vat Yellow 20)



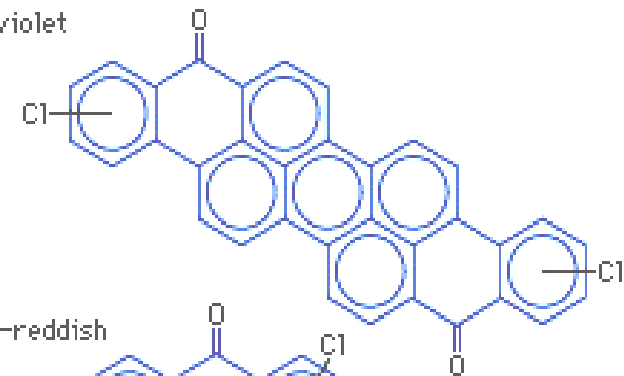
flavanthrone yellow
(CI Vat Yellow 1)



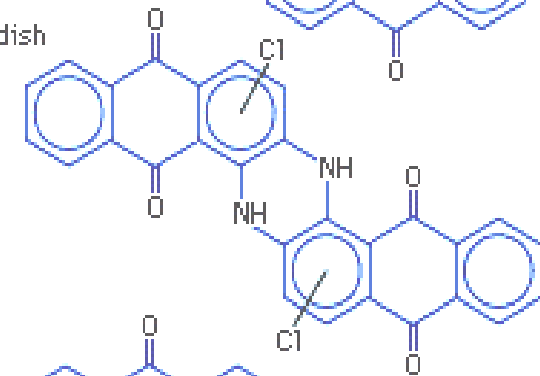
anthanthrone orange
(CI Vat Orange 3)



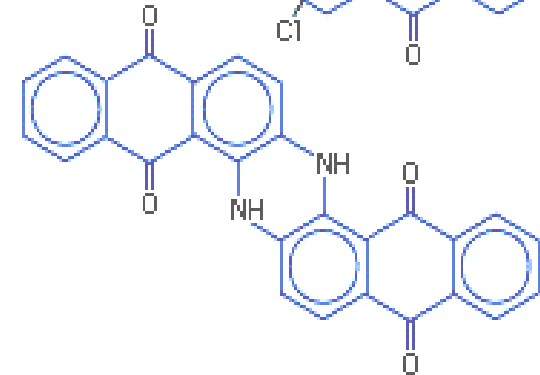
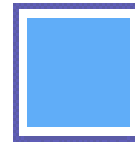
isoviolanthrone violet
(CI Vat Violet 1)



indanthrone blue-reddish
(CI Vat Blue 6)



indanthrone blue
(CI Vat Blue 4)



Viitor

- Universitati/institute virtuale
- Viteza mare de transfer
- Universalitate si coerenta
- "Web pentru toti"
- Servicii avansate facilitind cercetarea la nivel mondial: **medii stiintifice virtuale distribuite**
- Biblioteci digitale accesibile de catre oricine

Concluzii

- Spatiul WWW este in plina dezvoltare
- Existenta pe Web a unor mari depozite de date (din orice domeniu)
- Necesitatea unor limbaje specializate pentru modelarea/transferul informatiilor din chimie si pentru interogarea Web-ului
- Spre o societate informationala mondiala, la toate nivelele
- O alta mentalitate, a noului om

Posibilitati de cercetare in domeniul chimiei pe Web

Mulumiri pentru atentionia acordata!

Mai multe informatii
despre Web la adresa:
<http://www.infoiasi.ro/~busaco>

Intrebari?