The Impact of Informatics

Alan Hewat
ILL Grenoble

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...10110010100010010001000
0101001000010010000...0101
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0100101...00101100101010
010101001000100...110010
0011...00101001001001010...

- Number Crunching
  - Modelling
    - Neutron Instruments
    - Crystal Structures
    - Lattice Vibrations
    - Wave Functions
    - ... etc ... etc
  - Example
    - Genetic Algorithms for structure modelling

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- **Number Crunching**

  ... is still an important application of computers,

  but is no longer the most important...

  - **Most people already have enough power, even with their personal computer, to refine and display their data.**

- **So where is the future impact ?**

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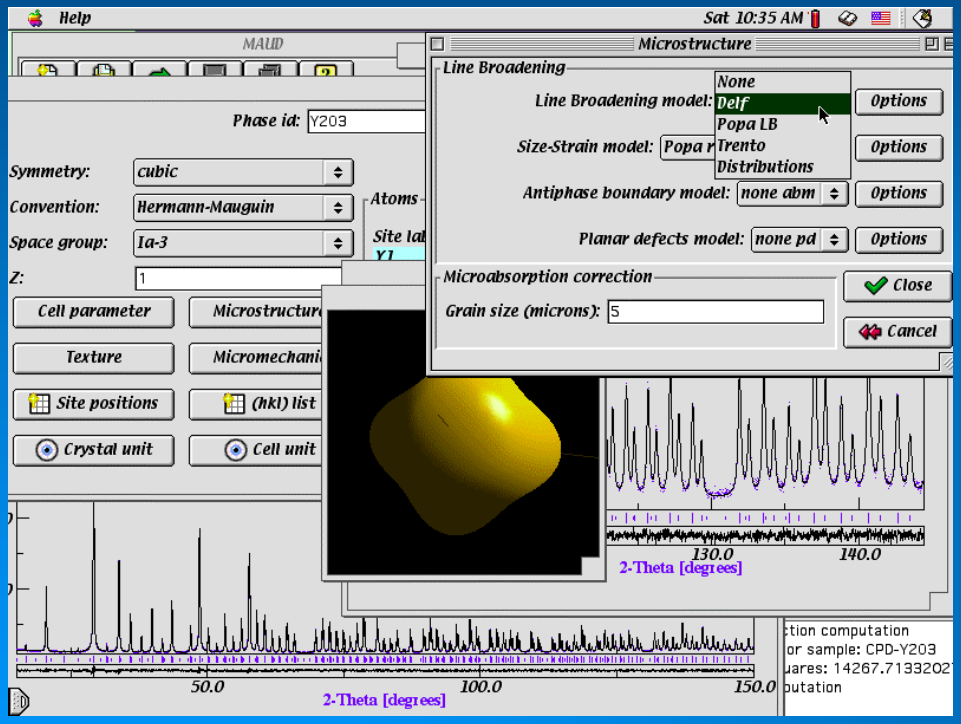

- **GUI User Interfaces**
  - **User survival in a more complex world**
    - **Macintosh GUI**
    - **Windows GUI**
    - **WWW GUI (html, perl)**
    - **Java, Tcl/Tk GUI's etc**
  - **Examples**
    - **BARNS Data analysis via the WWW**
    - **MAD-GUI Instrument control with Java**

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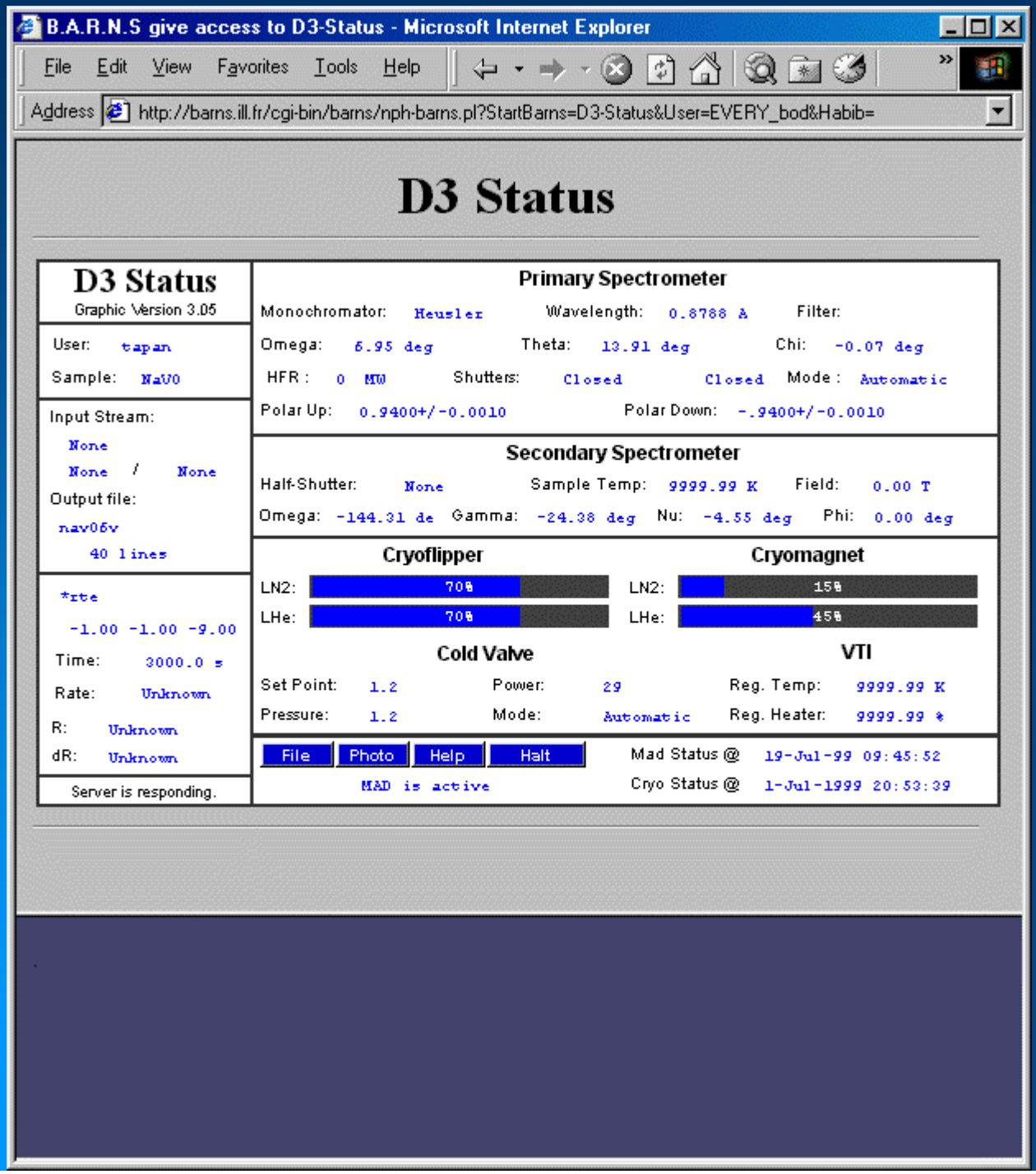
ILL BARNS Data Server



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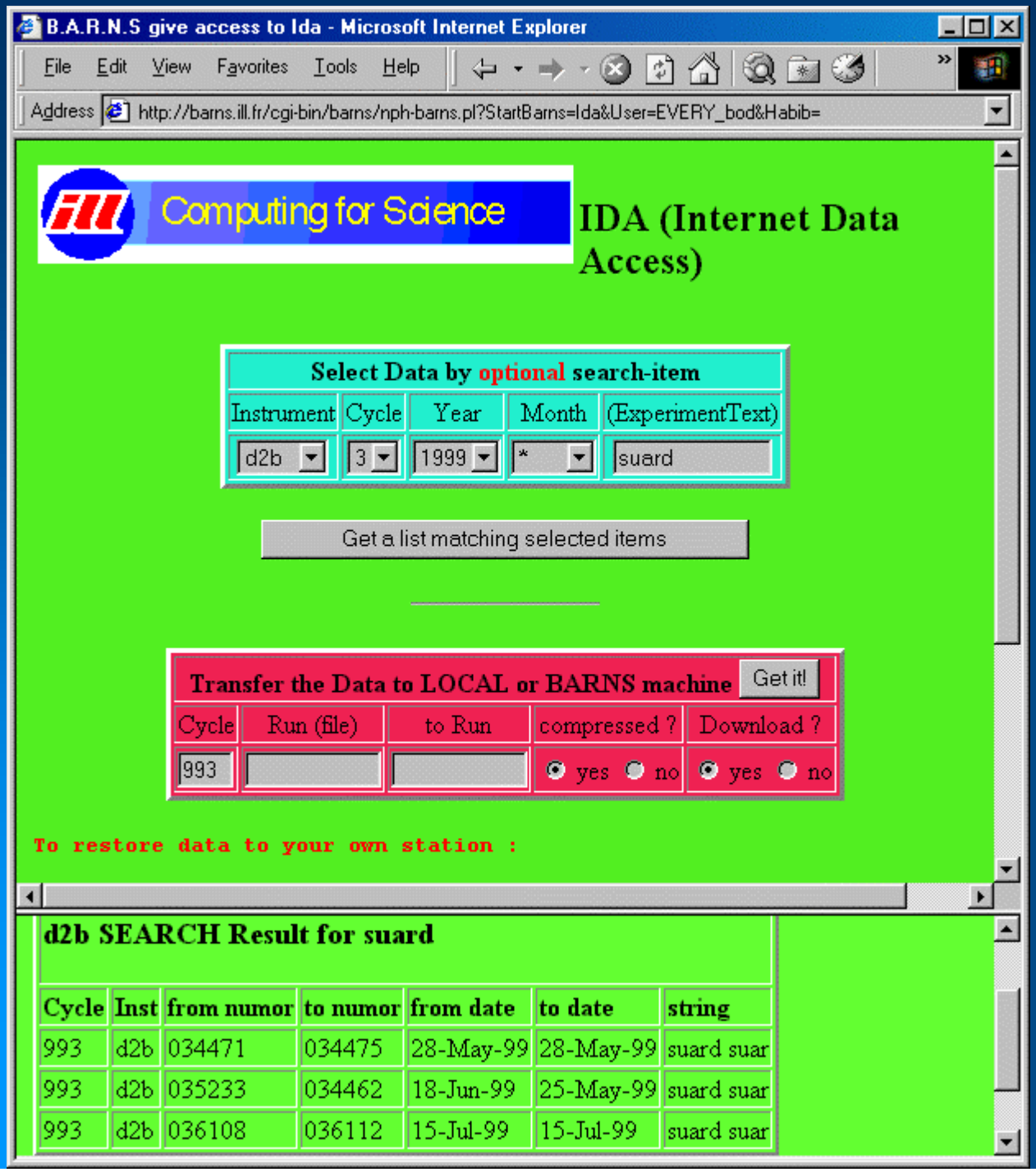
ILL BARNS Data Server



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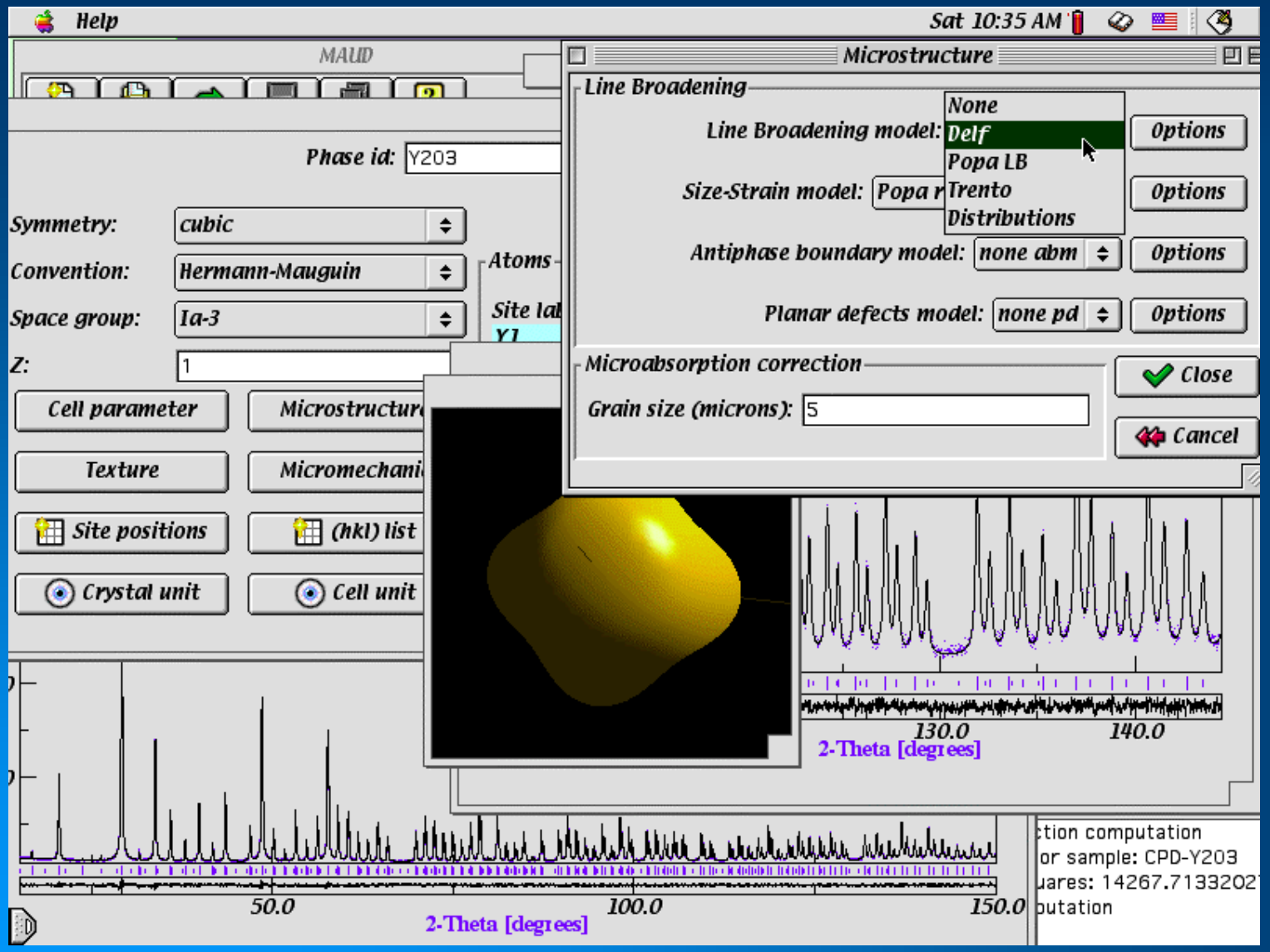

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MAUD Java GUI

MAUD. Java GUI "Material Analysis using Diffraction" Luca Lutterotti et al. Universita di Trento

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- Experiments without local contacts ?
  - … or even without a user manual … ?
  - Or at least greater independence for users…
  - …should result in better control of experiments and therefore better experiments…
- Ease of Use (Graphic User Interface's) may be more important in future than number crunching

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- What will have the greatest impact ?

INFORMATION !!

Knowledge is power ?

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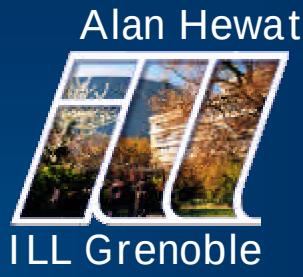
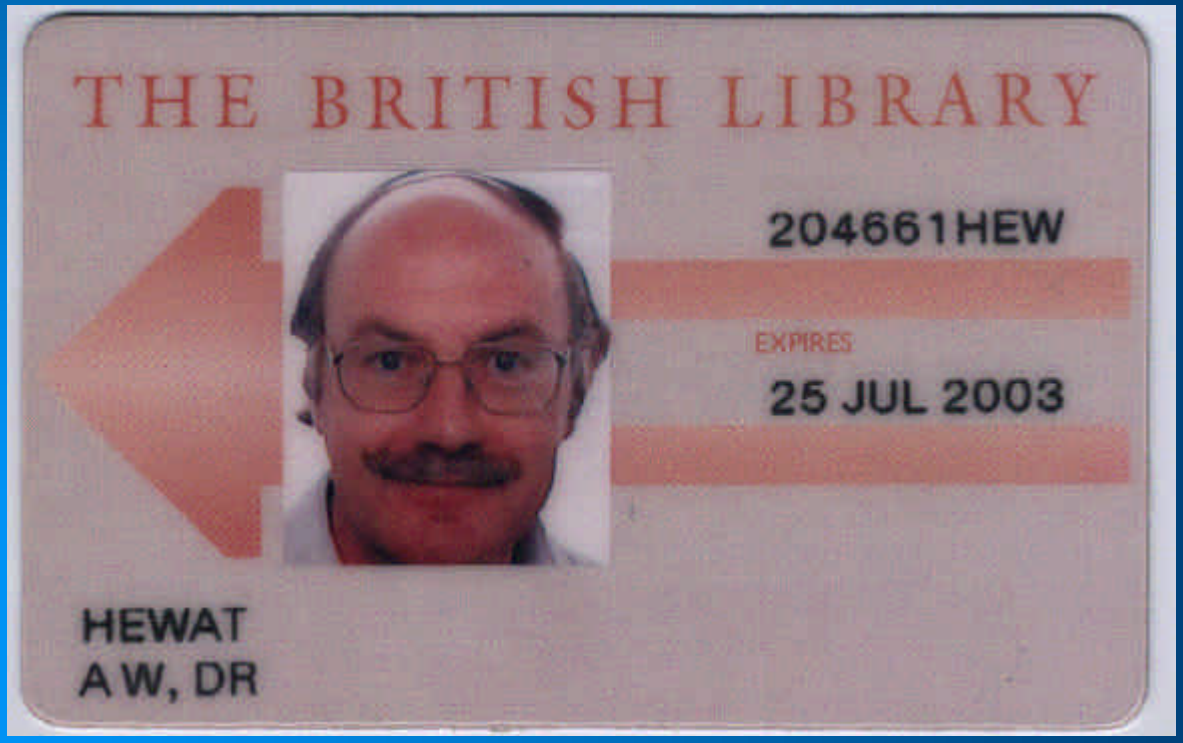


- **Informatics & The British Library**



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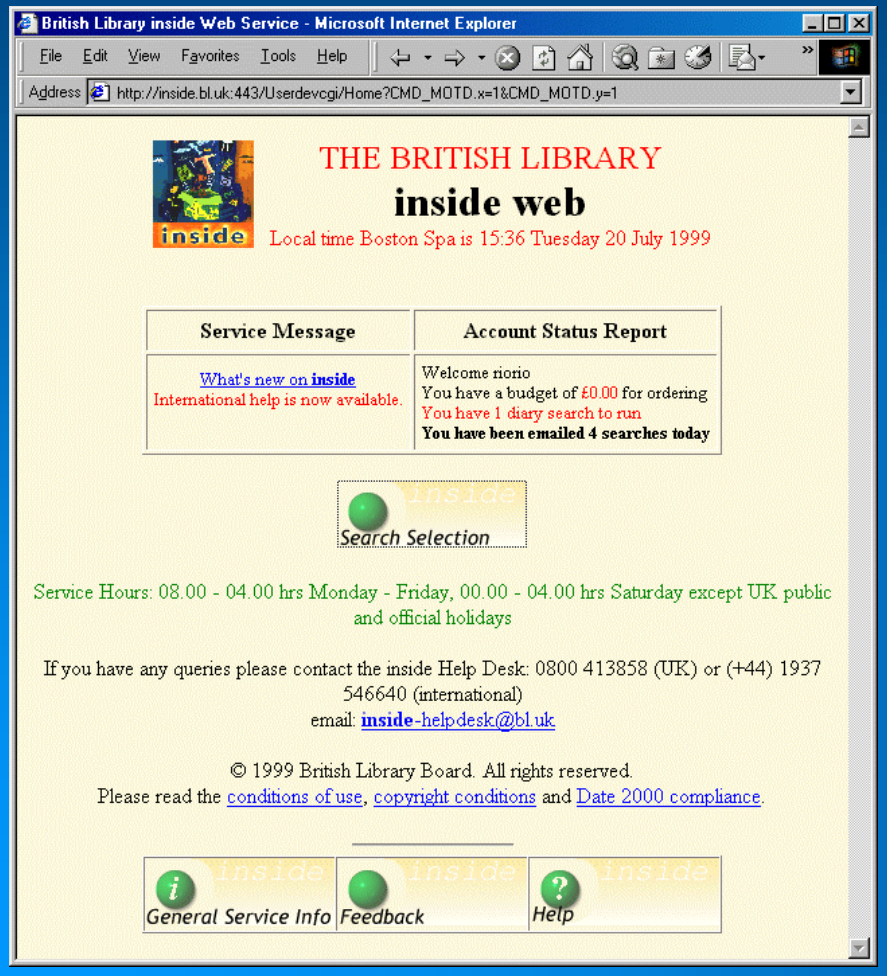
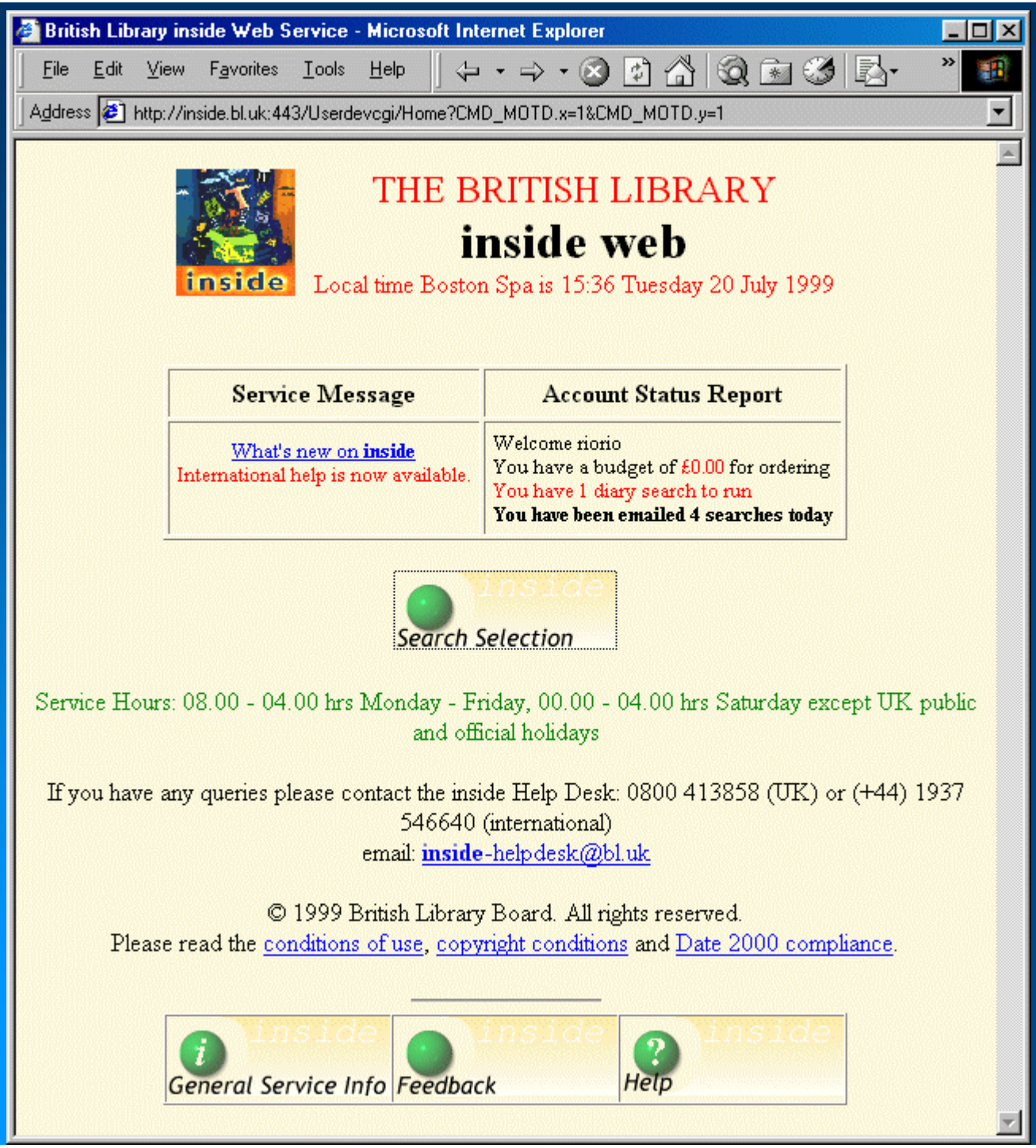


- **WWW Data Bases**
  - **Reference databases**
    - **British Library "Inside"**
    - **ILL/ESRF publications**



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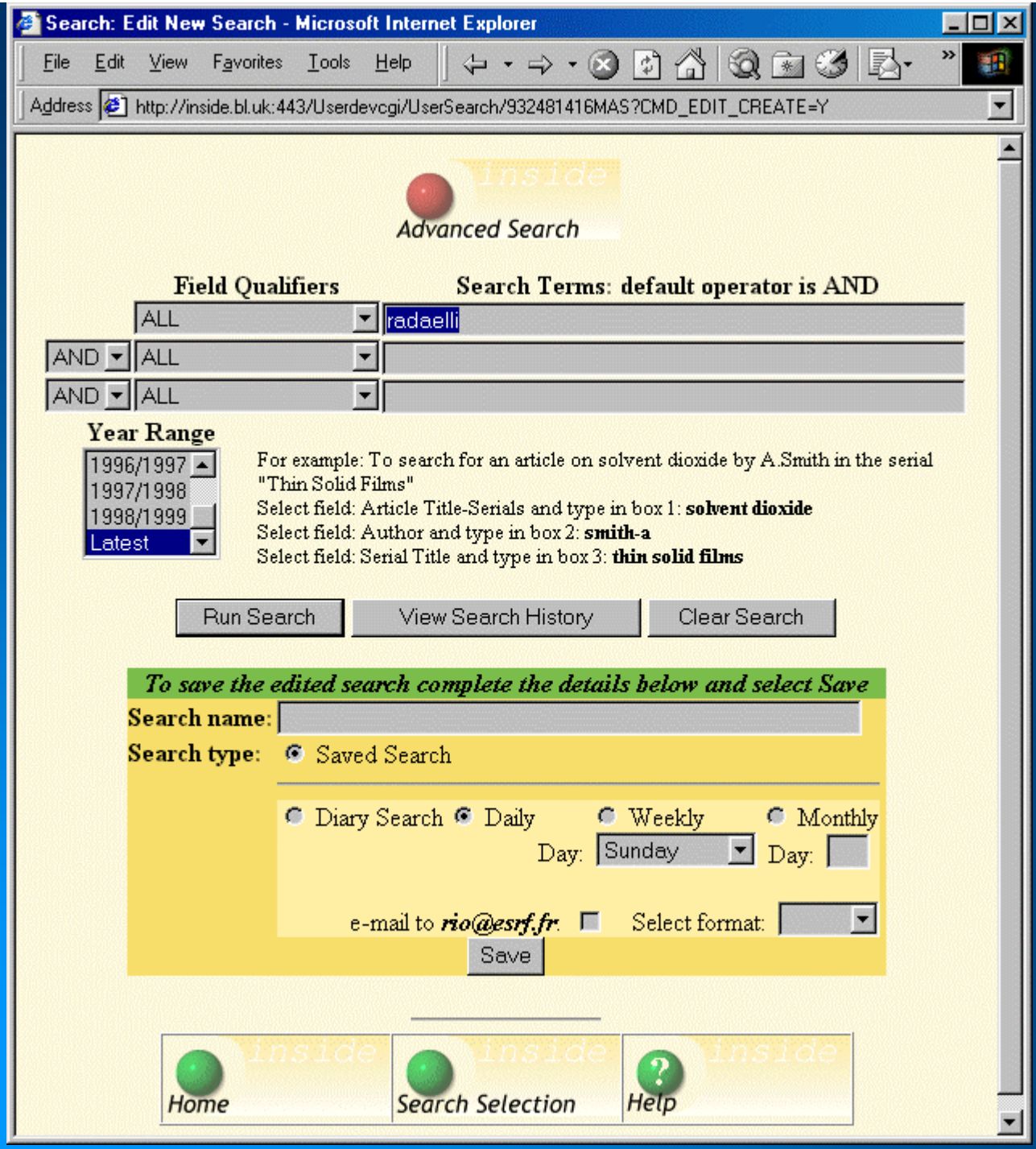
British Library "Inside Web"



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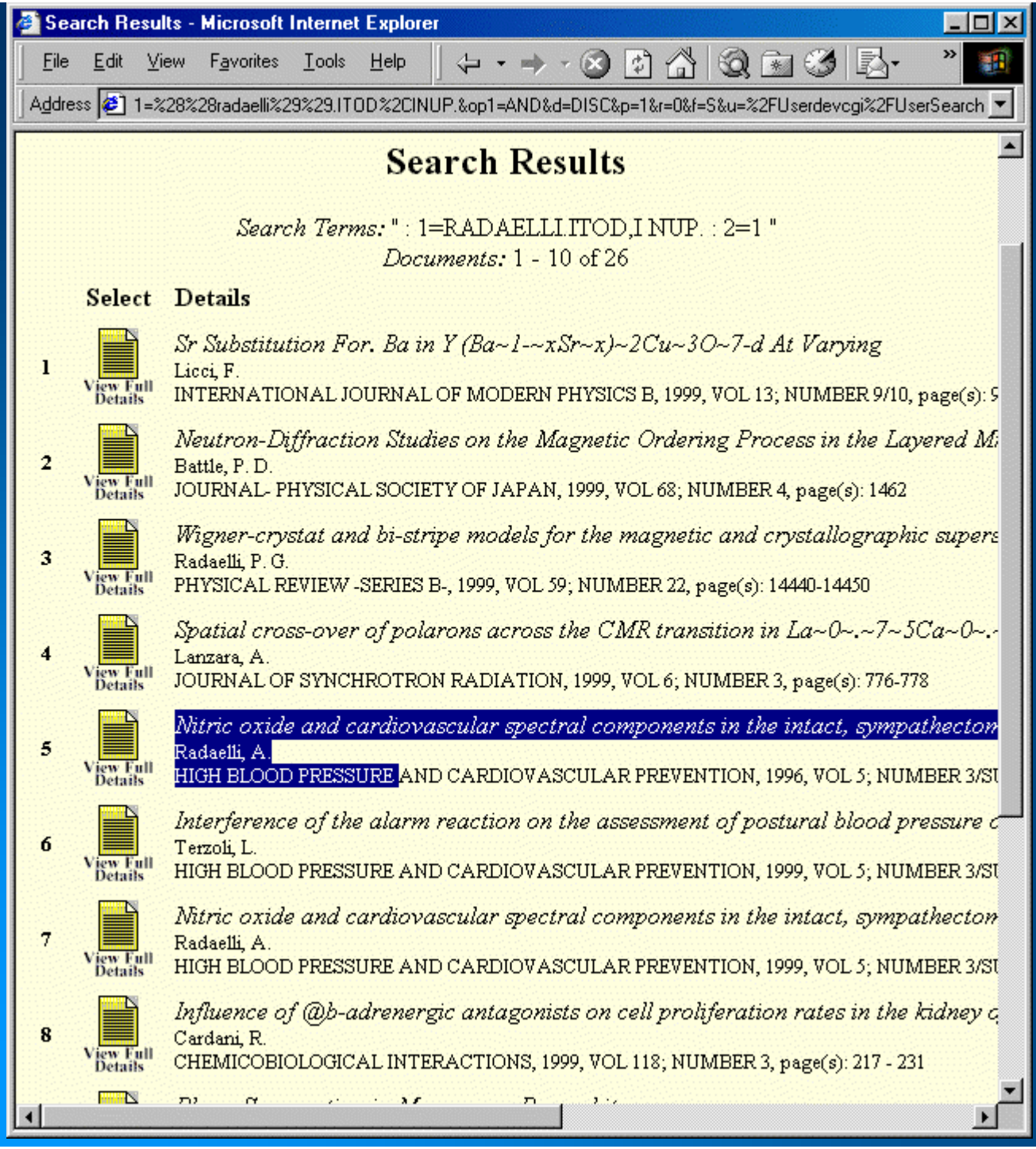
British Library "Inside Web"



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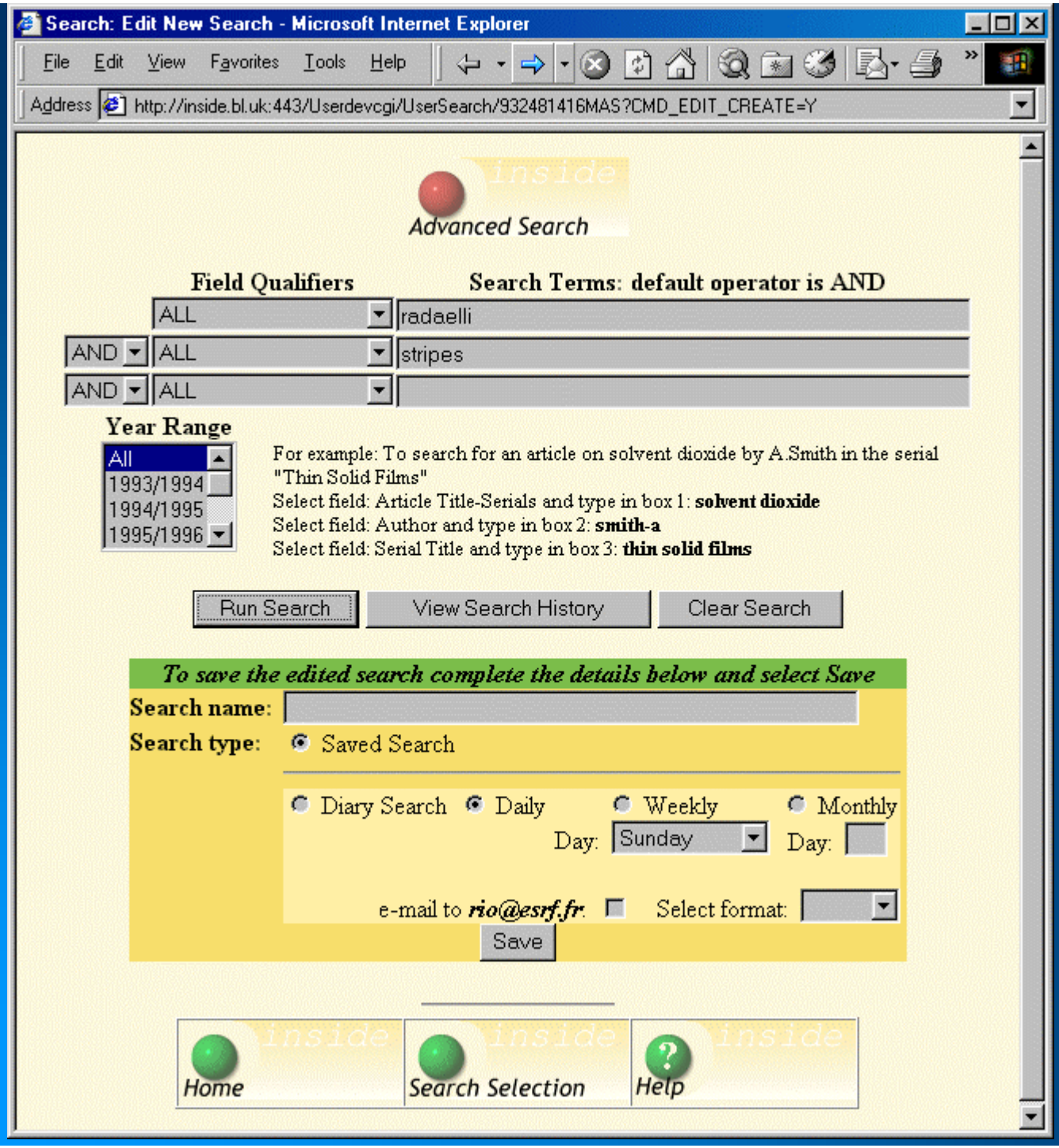

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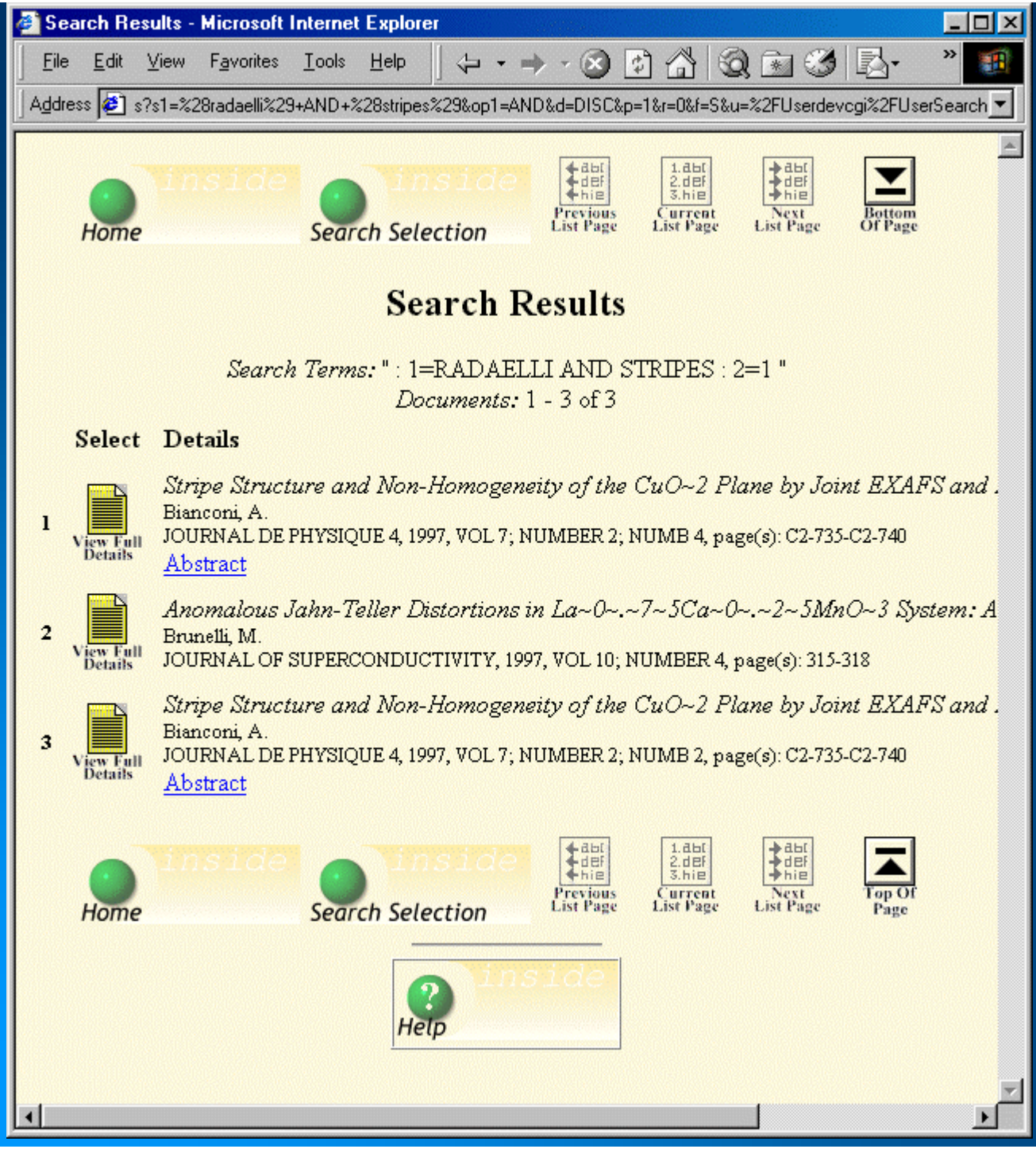

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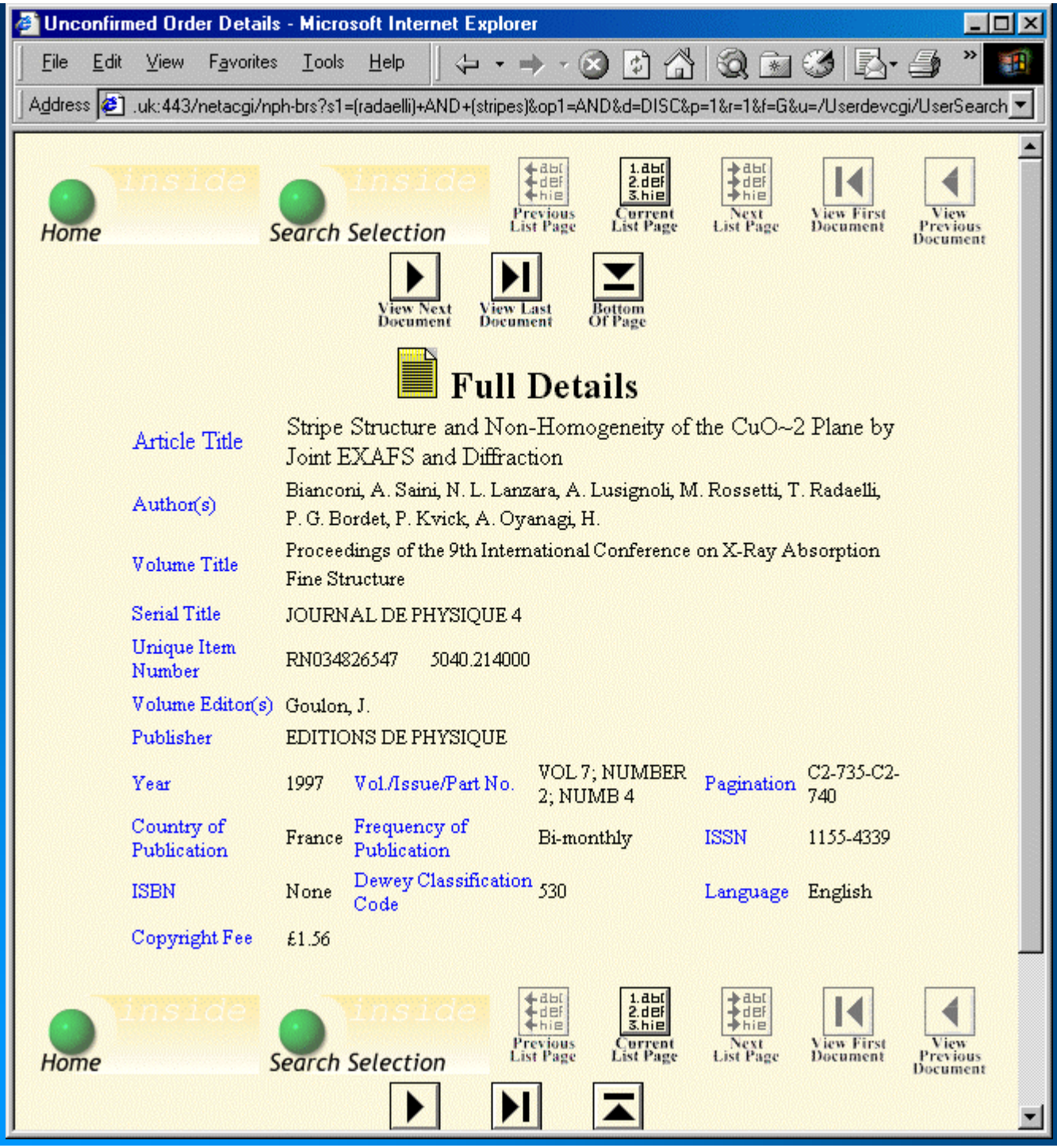
British Library "Inside Web"



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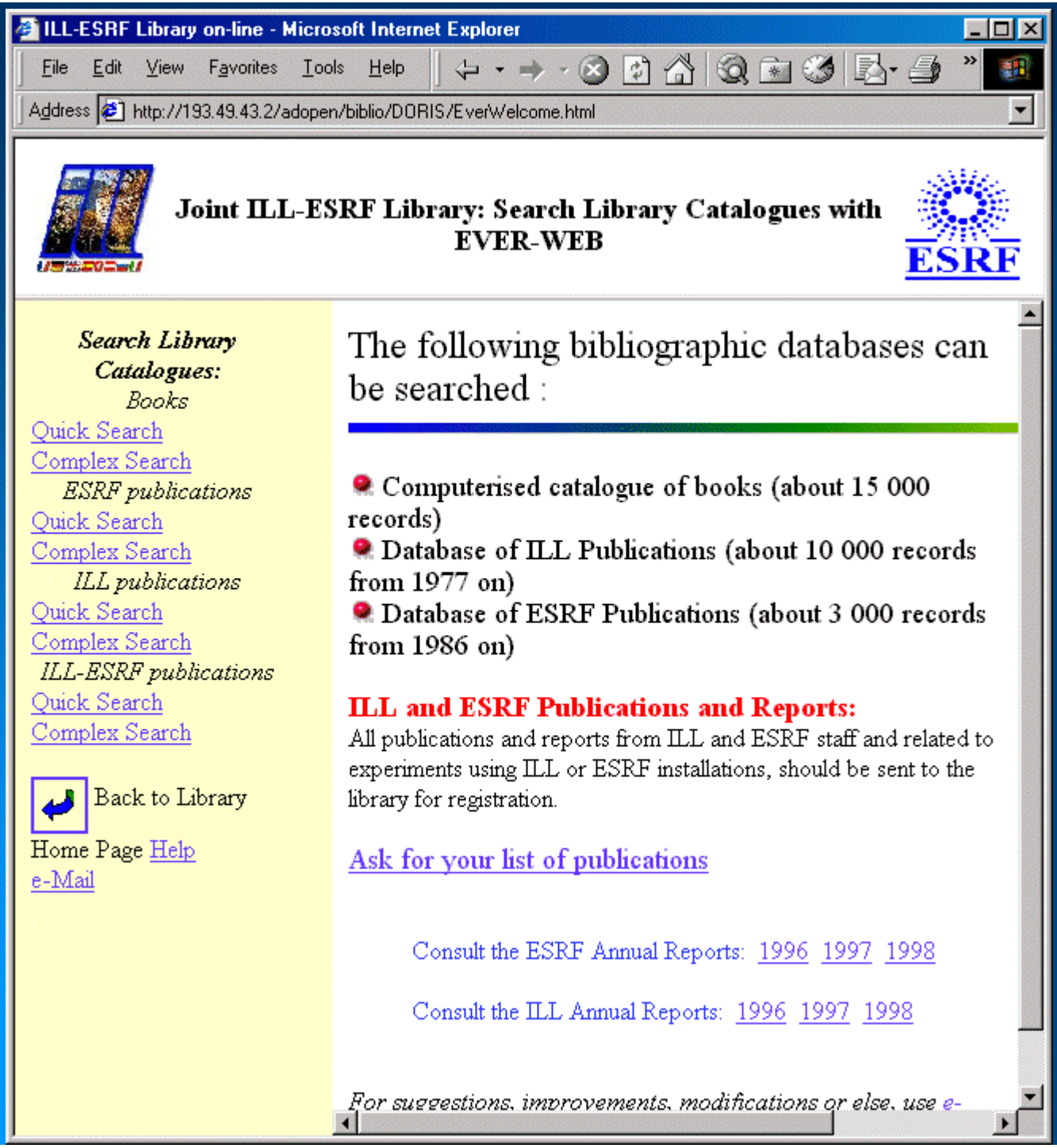
British Library "Inside Web"



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ILL Library 10,000 ILL Publications

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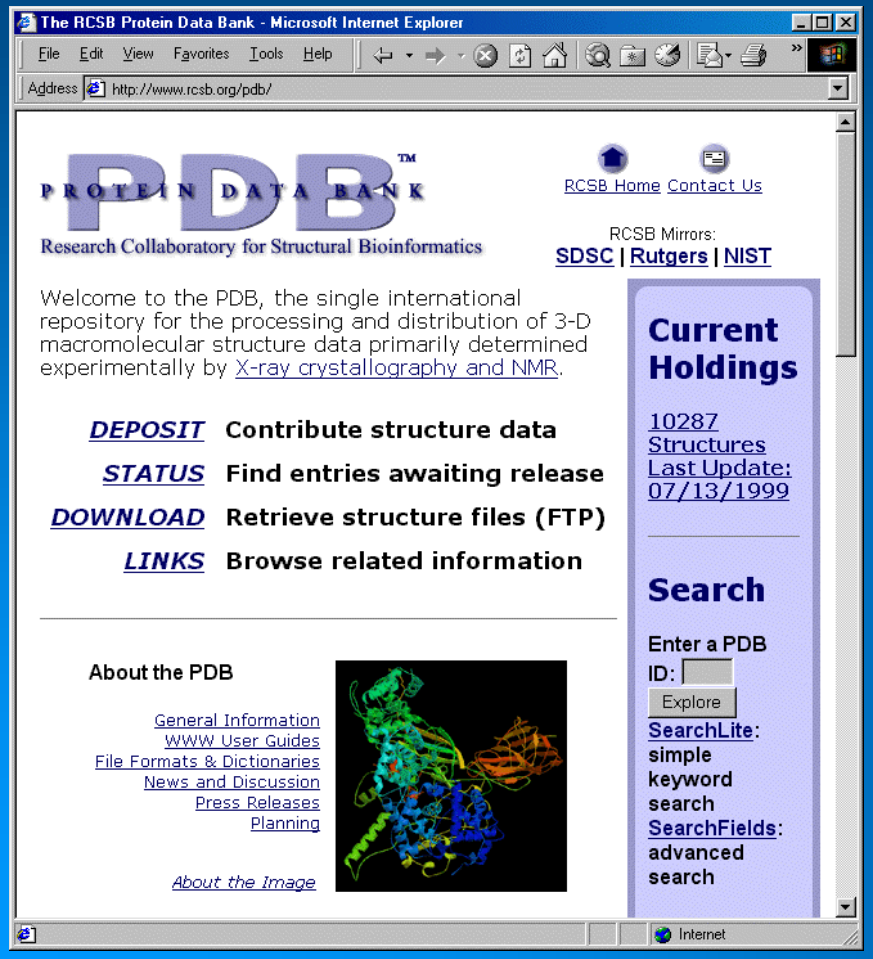
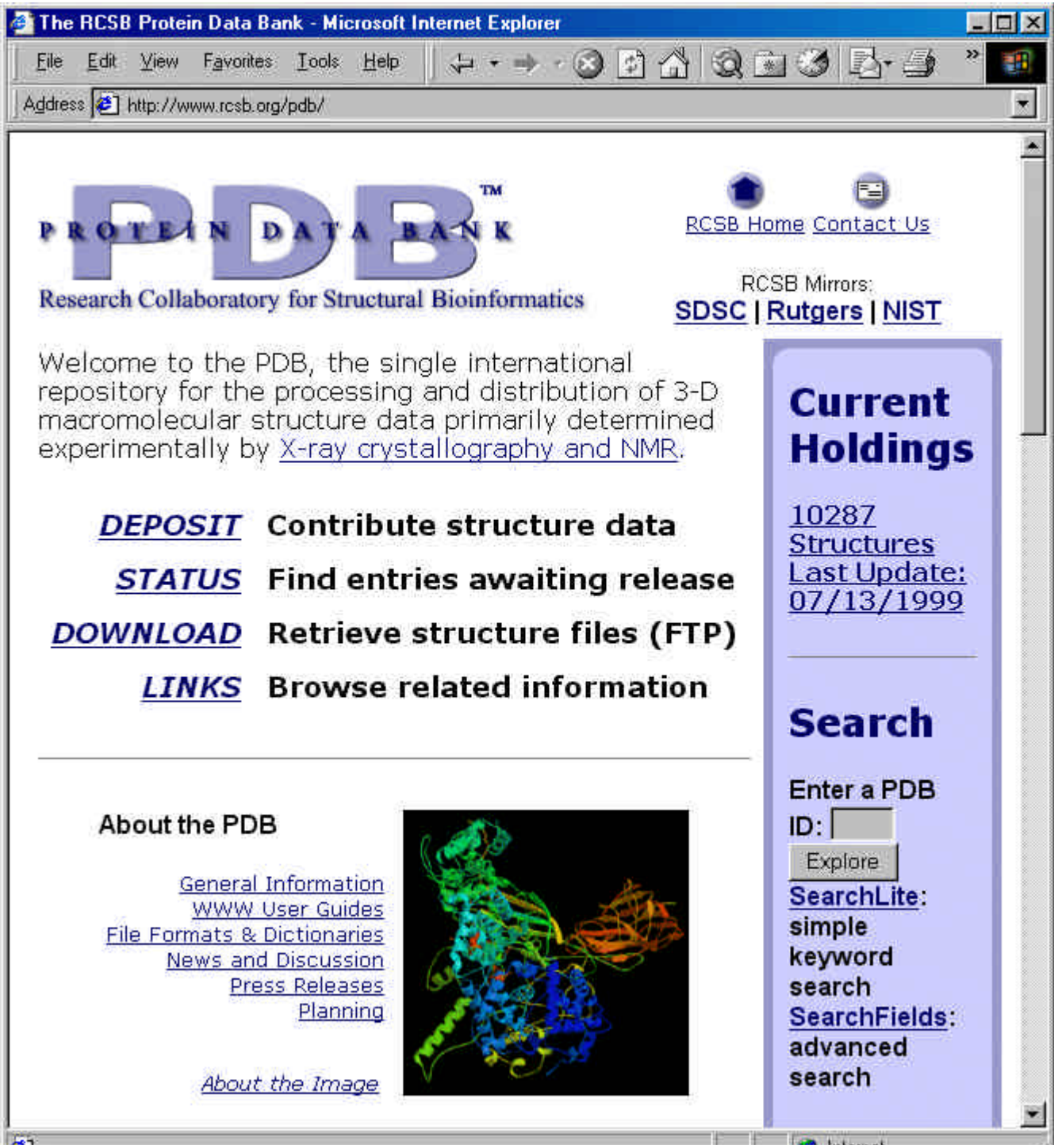


- **WWW Data Bases**
  - **Advantages**
    - **Everyone has access (even non-experts)**
    - **Standard WWW interface (familiar to all)**
    - **Centrally maintained (data is up to date)**
    - **New software versions installed 'automatically'**
  - **Example**
    - **New Protein Data Bank**
      US National Science Foundation



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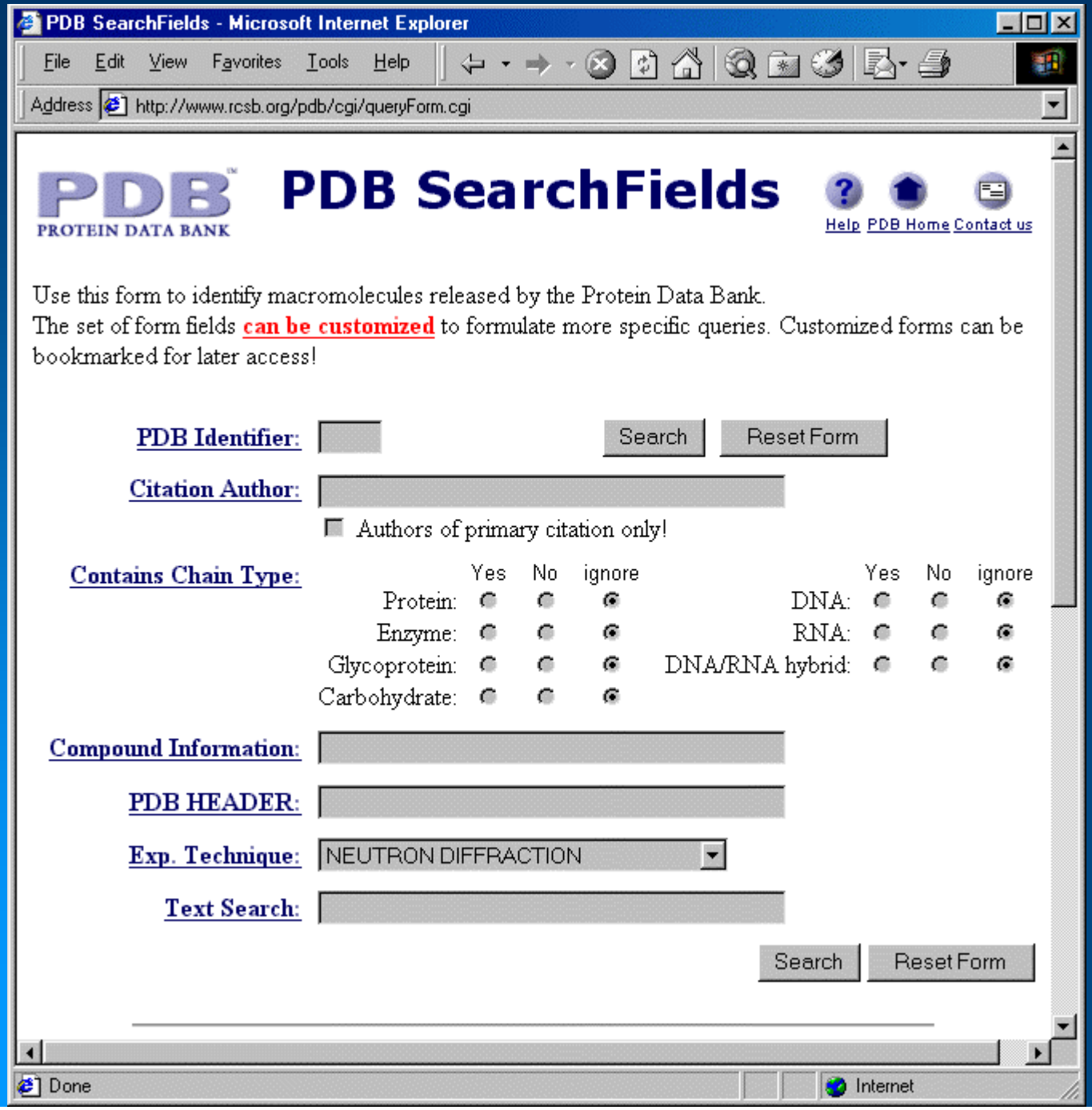
PDB Protein Data Bank



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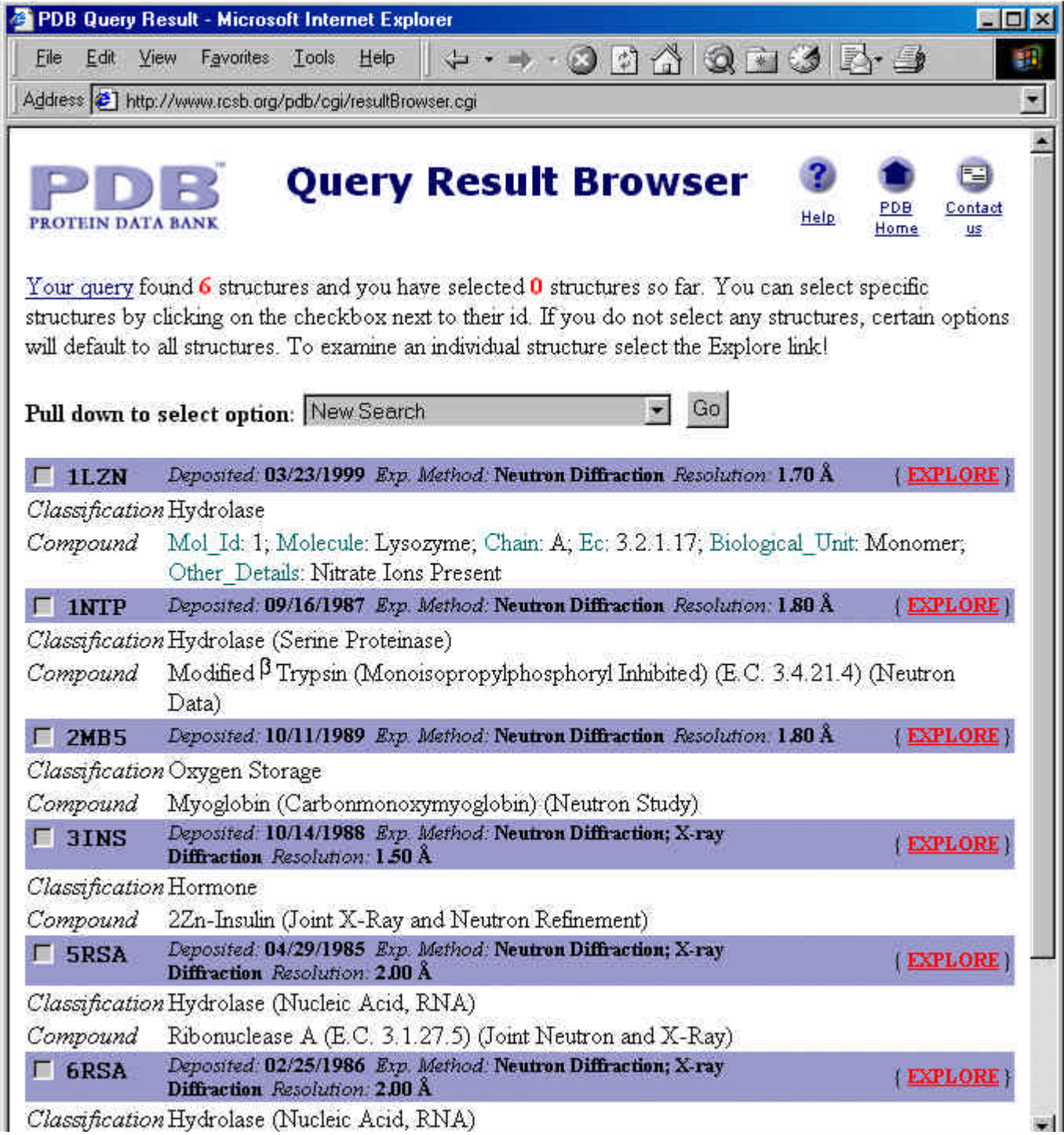
PDB Protein Data Bank



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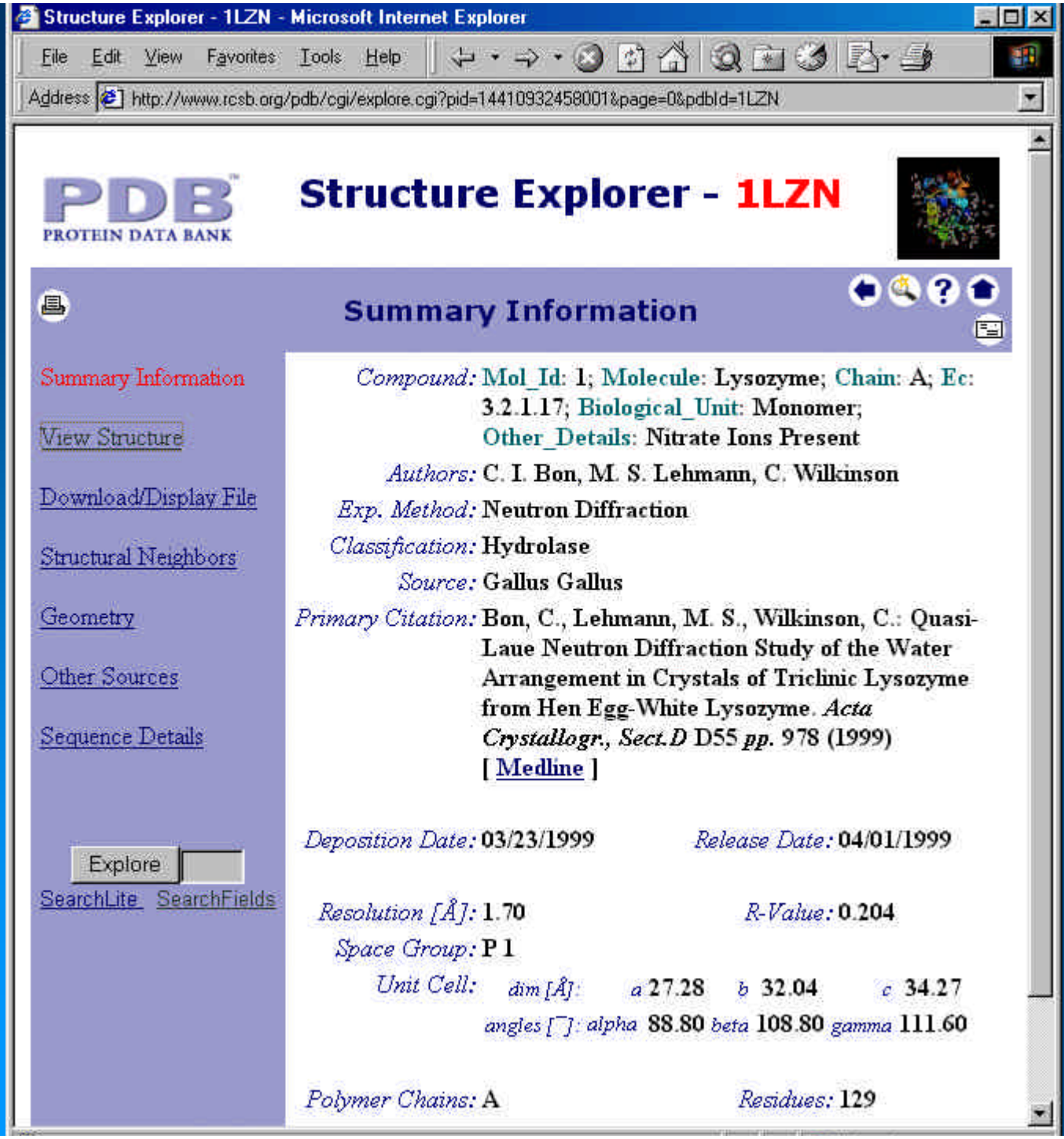
PDB Protein Data Bank



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PDB Protein Data Bank

Structure Explorer - 1LZN - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address http://www.rcsb.org/pdb/cgi/explore.cgi?job=graphics&pdbId=1LZN&page=0&pid=14410932458001

PDB PROTEIN DATA BANK

Structure Explorer - 1LZN

Classification **Hydrolase**
Compound **Mol_Id: 1; Molecule: Lysozyme; Chain: A; Ec: 3.2.1.17; Biological_Unit: Monomer; Other_Details: Nitrate Ions Present**
Exp. Method **Neutron Diffraction**

View Structure

Summary Information
View Structure
Download/Display File
Structural Neighbors
Geometry
Other Sources
Sequence Details

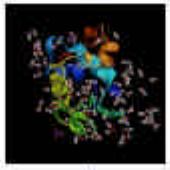
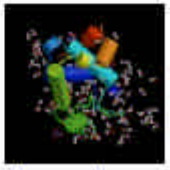
Explore
SearchLite SearchFields

Interactive 3D Display:

Choose from the following display options:

- VRML (default options): Interactive immersive ribbon diagram
- VRML (custom options, full screen display): Interactive immersive ribbon or cylinder diagram with ligands
- Rasmol
- Chime
- Java (simple interactive sequence/structure/property backbone diagram): QuickPDB

Still Images:

Ribbons (250x250) Cylinders (250x250)

Ribbons (500x500) Cylinders (500x500)

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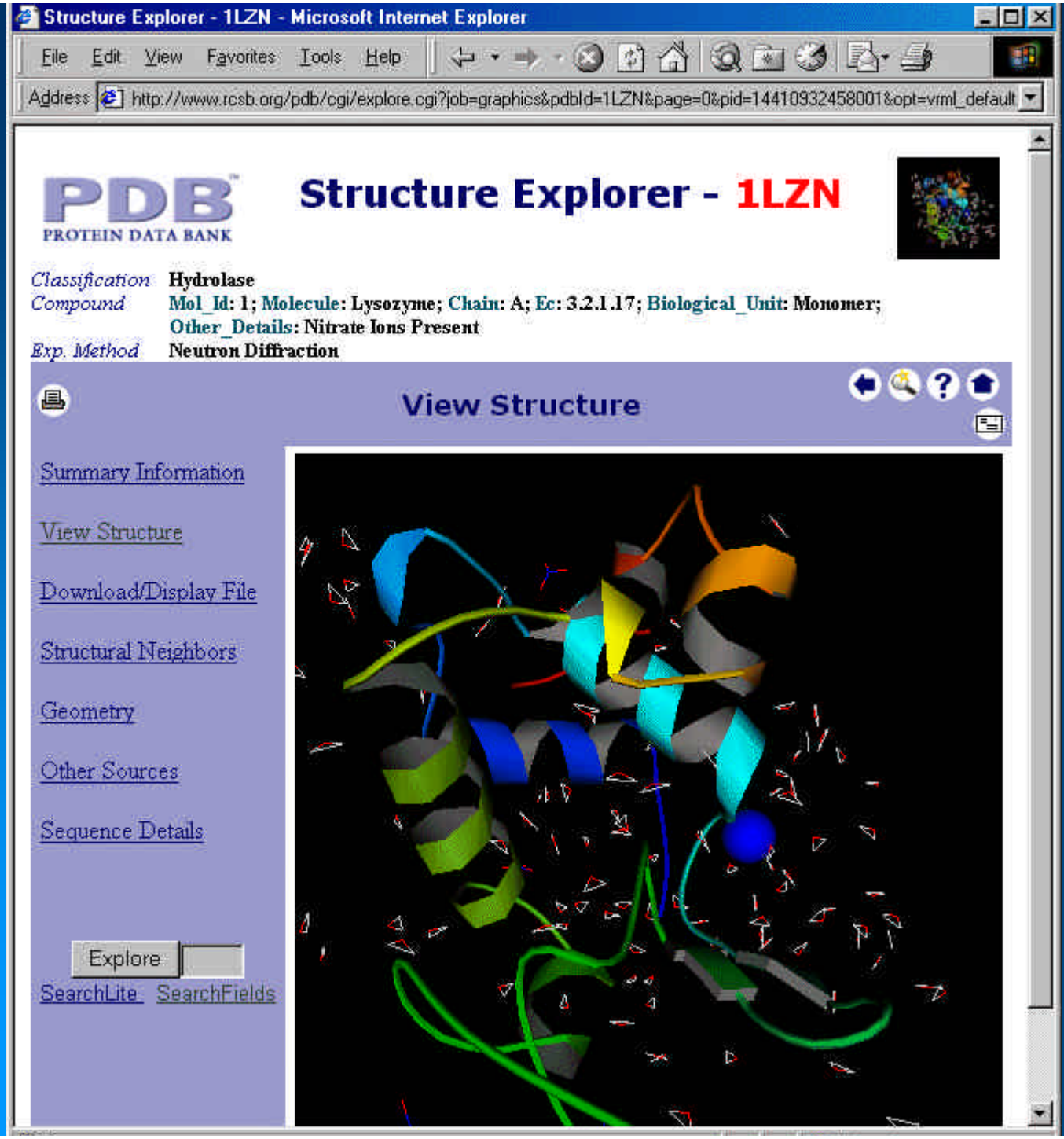
PDB Protein Data Bank



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PDB Protein Data Bank

Display Options

- VRML
- RASMOL
- CHIME
- JAVA

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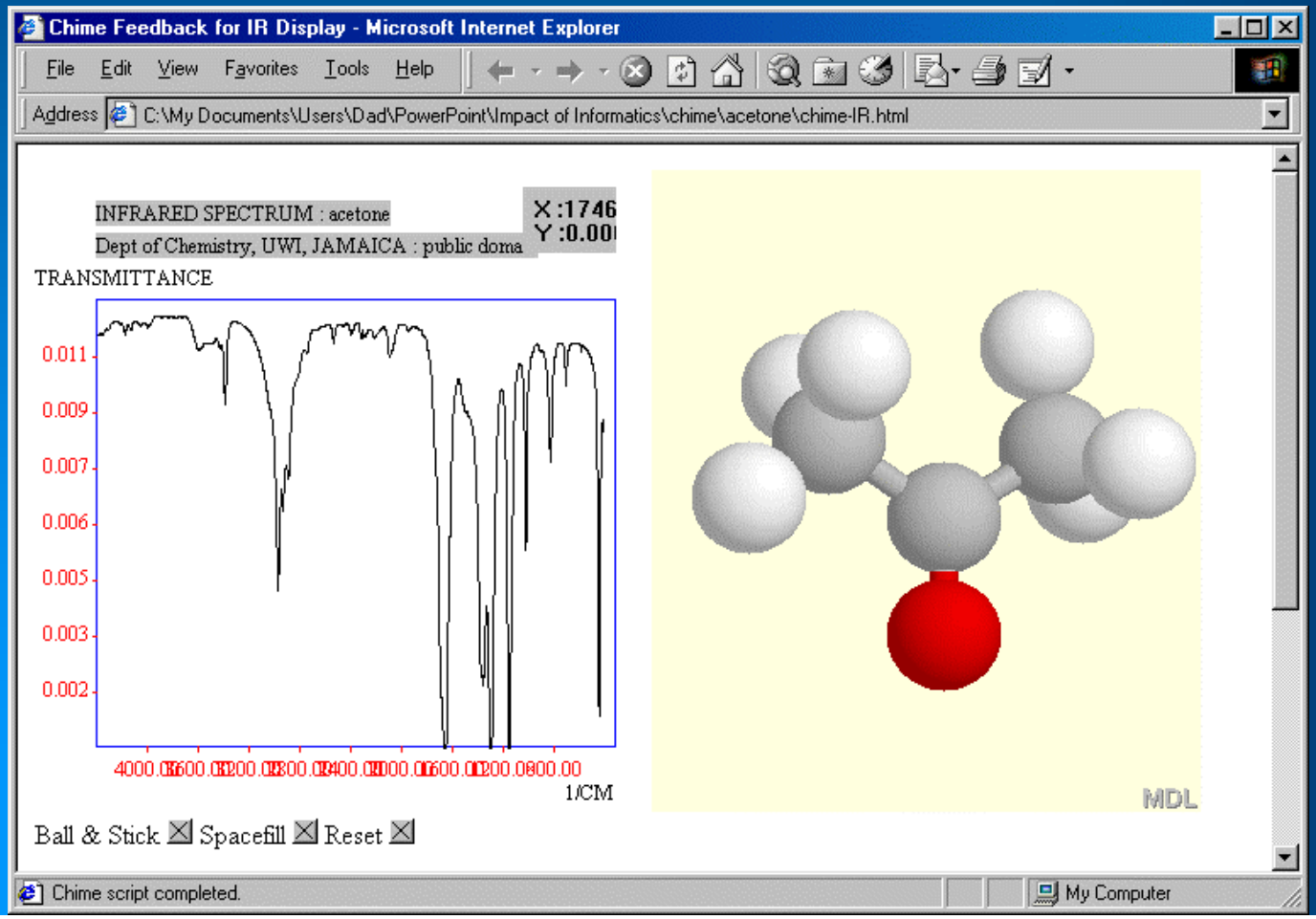
WWW Data Bases - Inelastic spectra



RasMol

Chime

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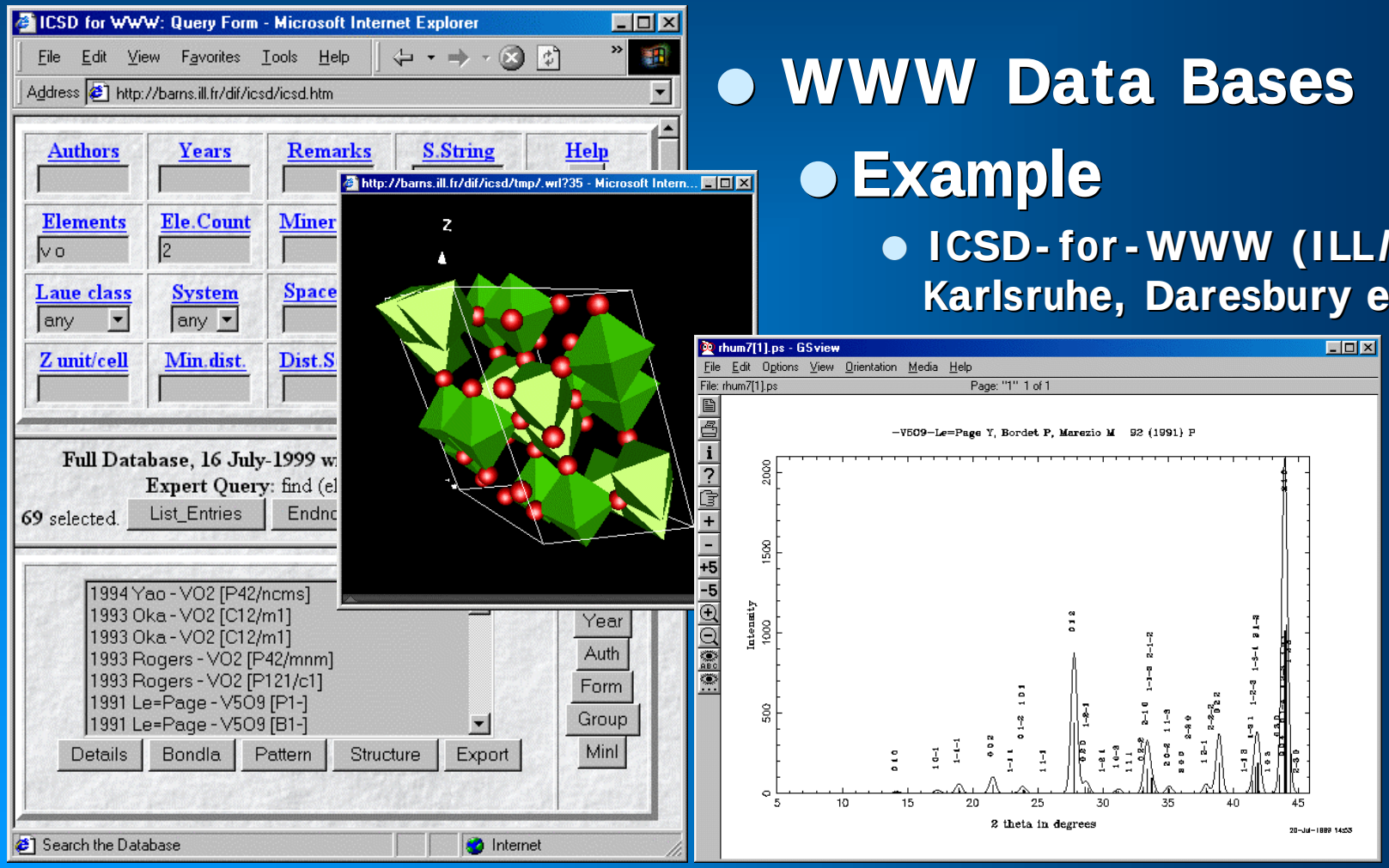
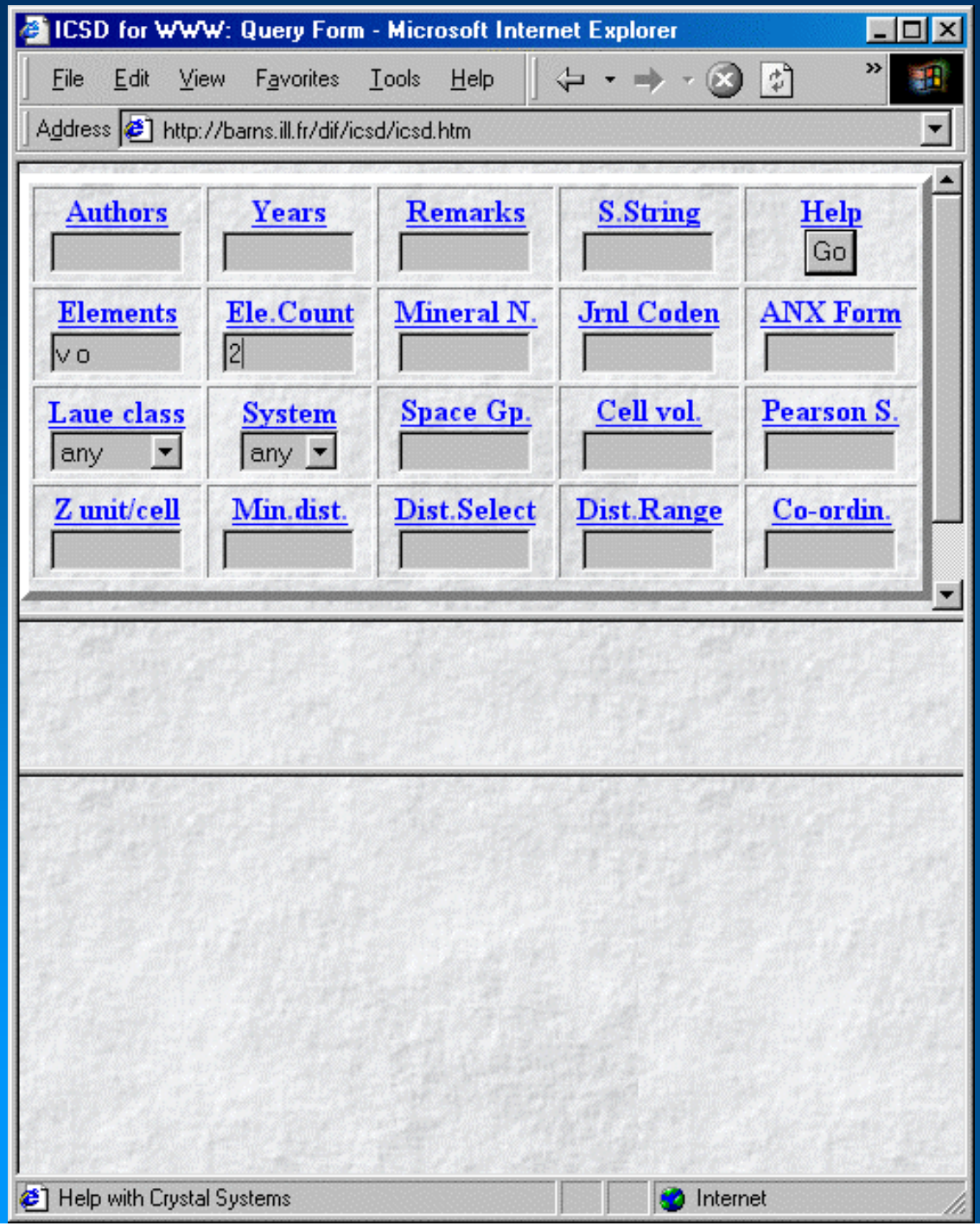


- WWW Data Bases
  - Example
    - ICSD-for-WWW (ILL/ESRF Karlsruhe, Daresbury etc)



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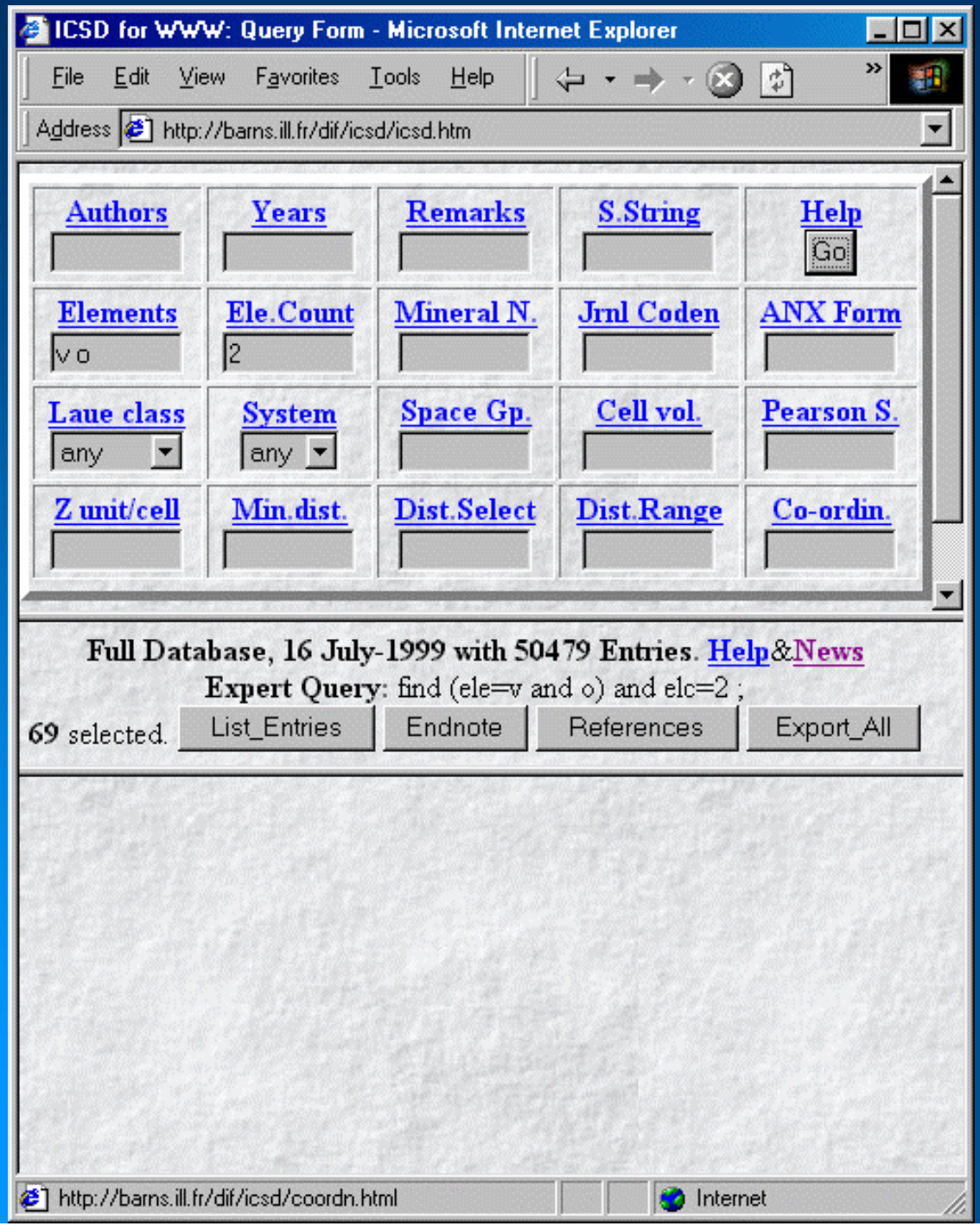
ICSD-for-WWW ILL - Karlsruhe crystal structures



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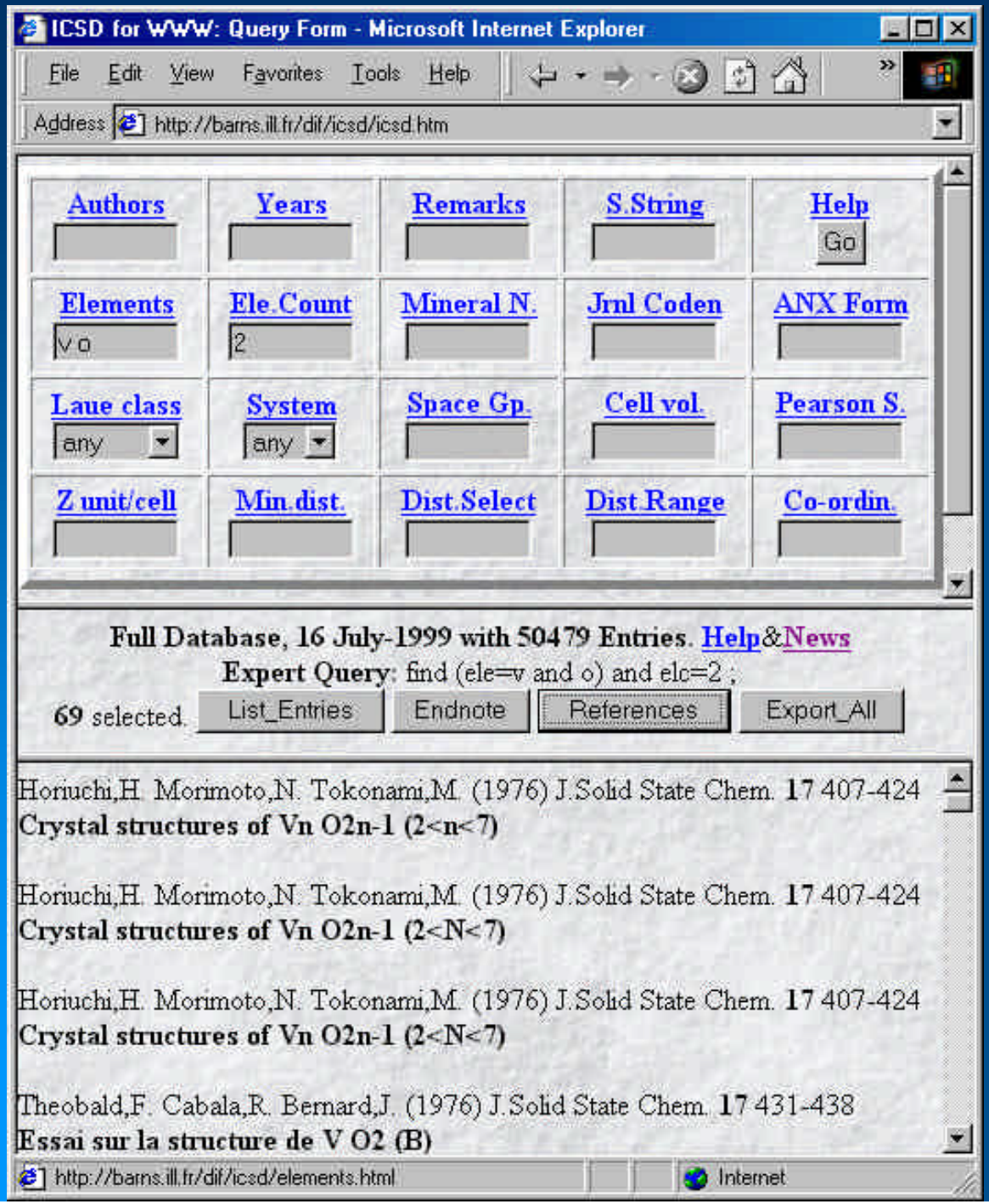
ICSD-for-WWW
ILL - Karlsruhe
inorg. crystal
structures



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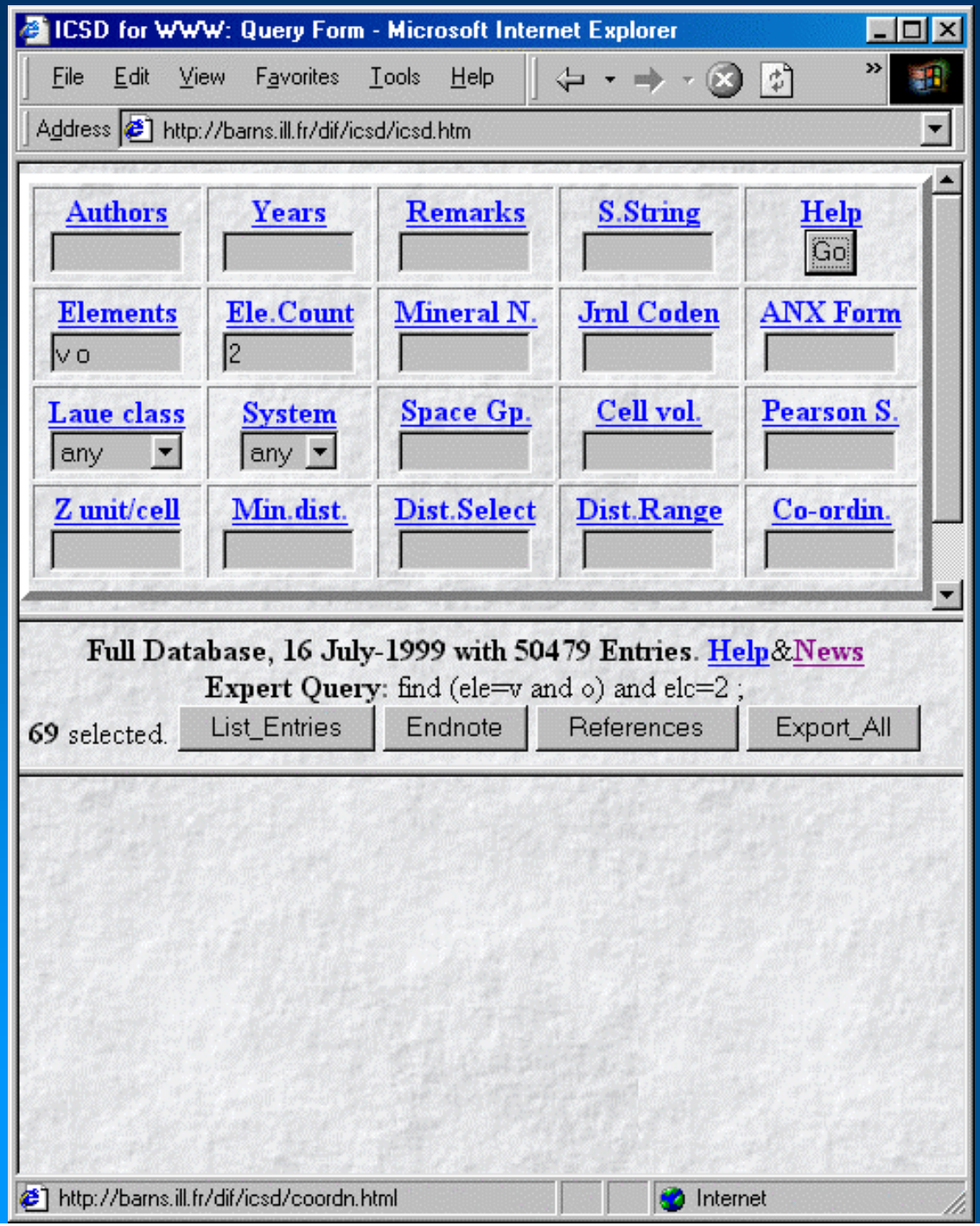

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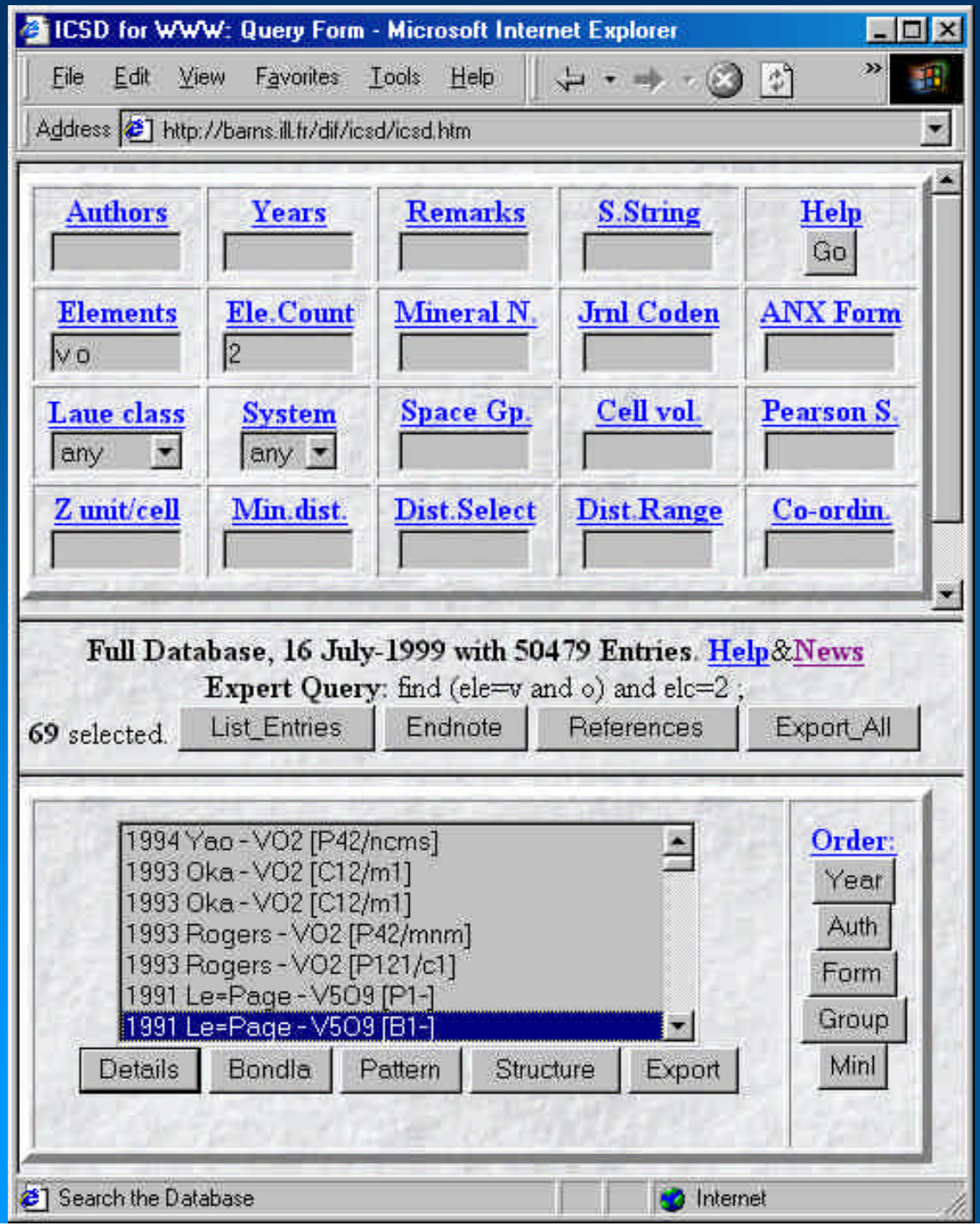

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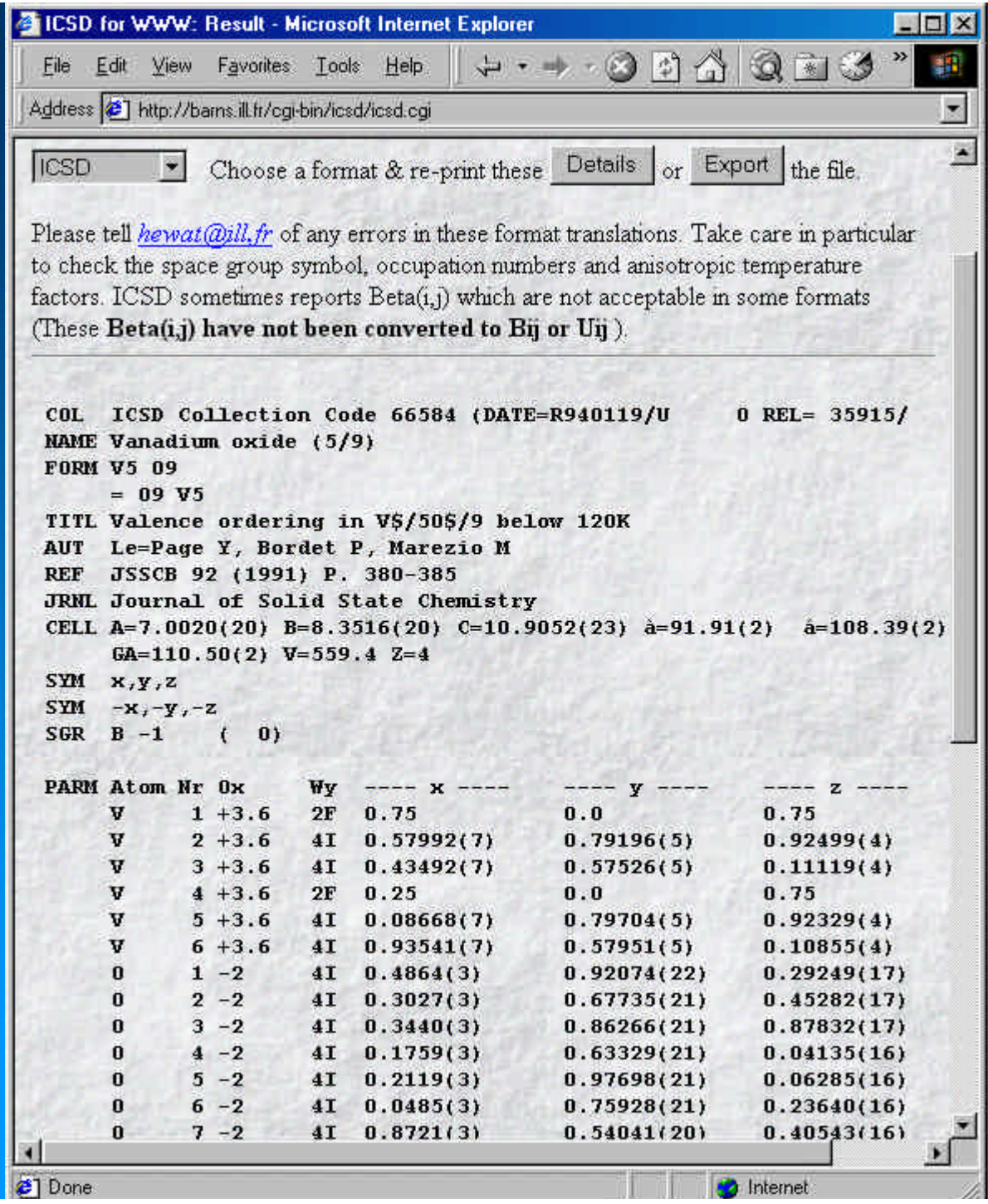

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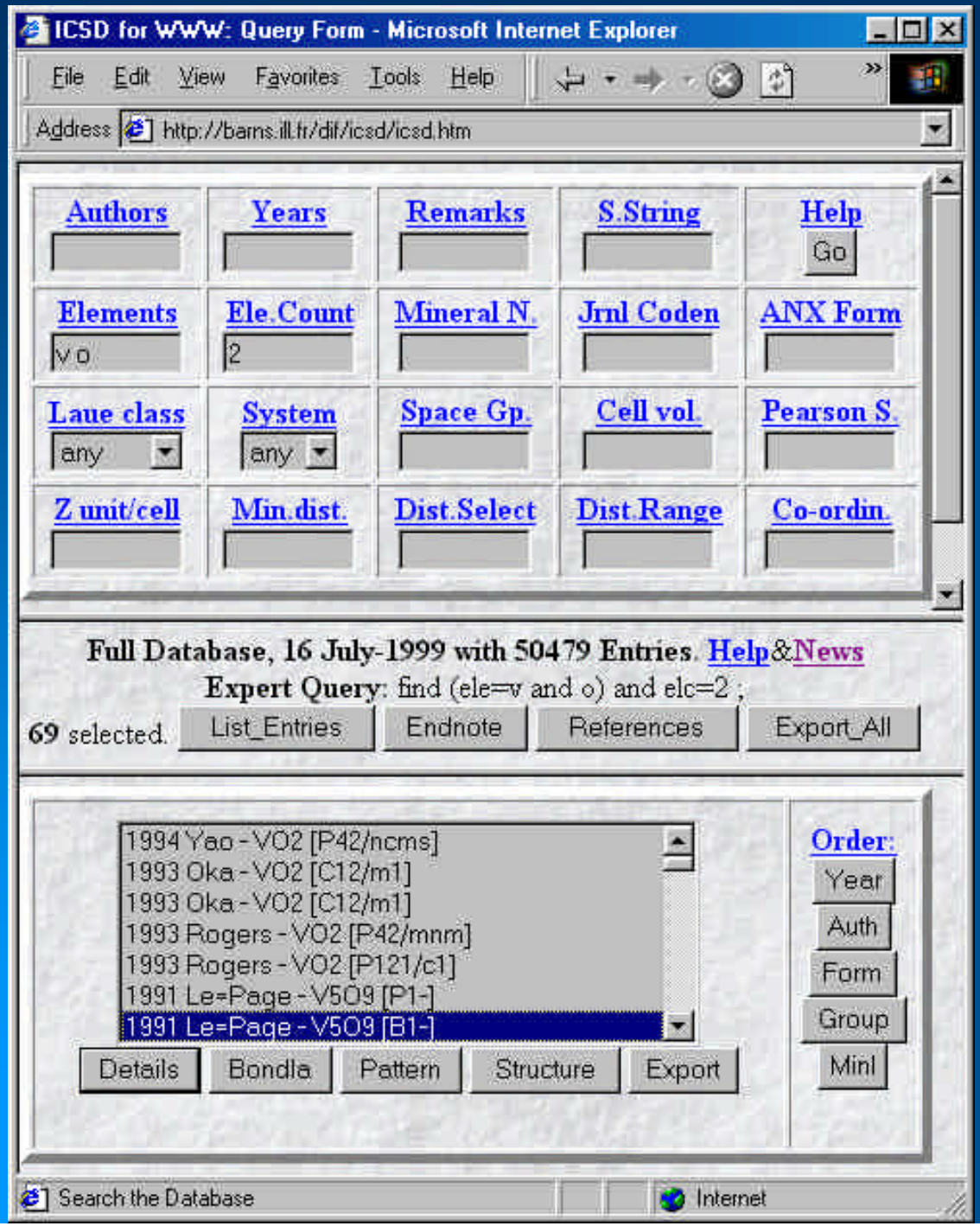

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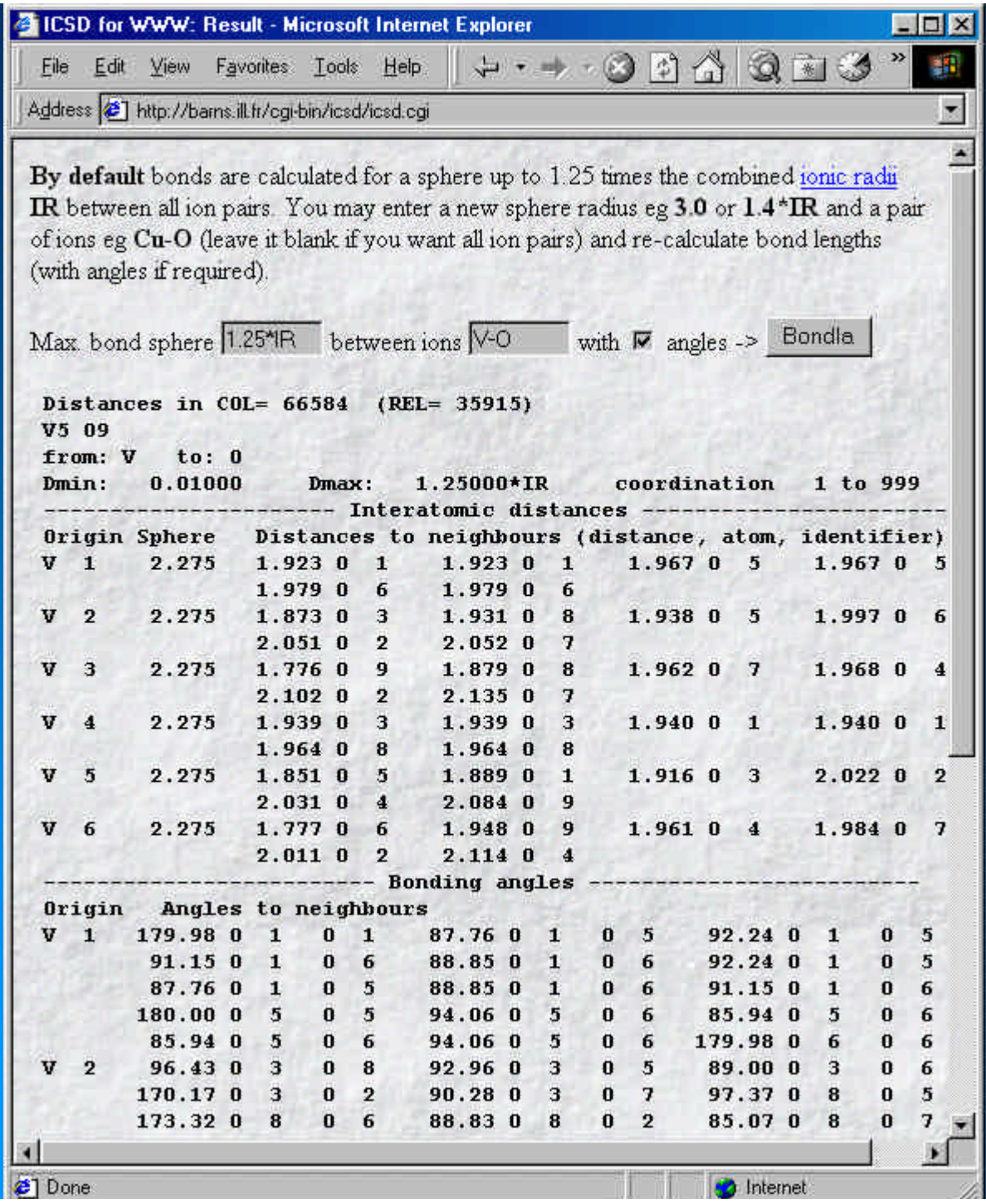

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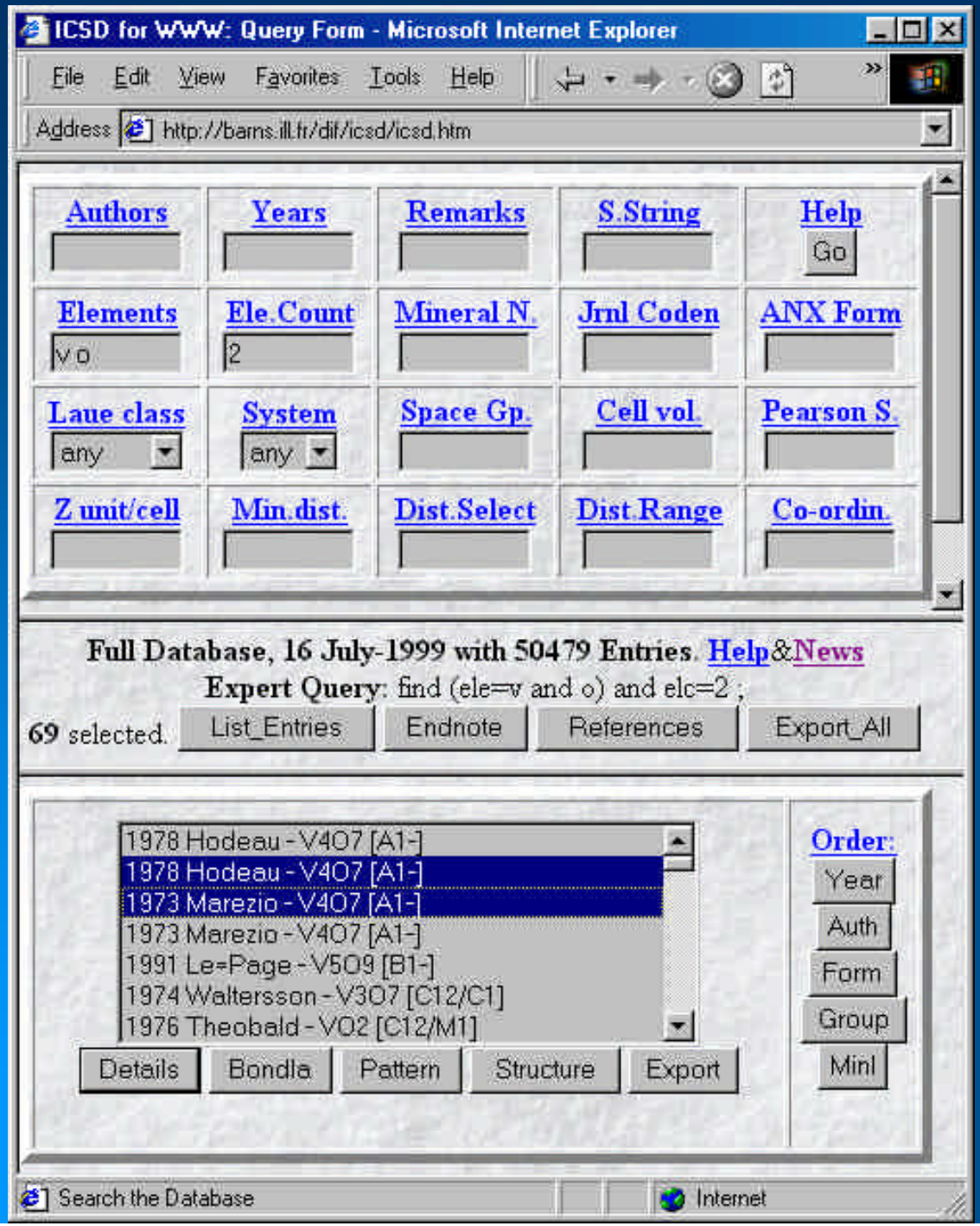

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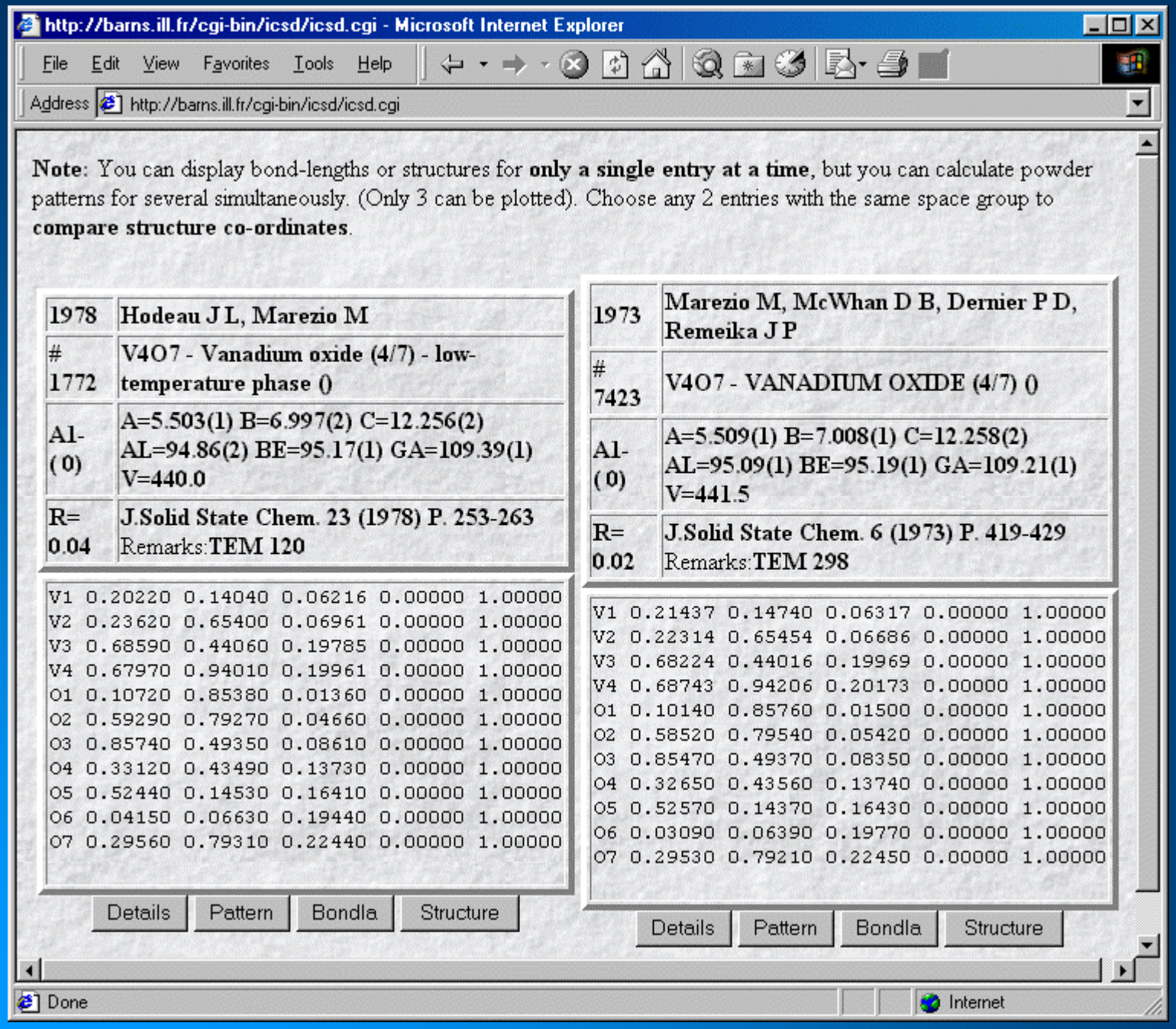

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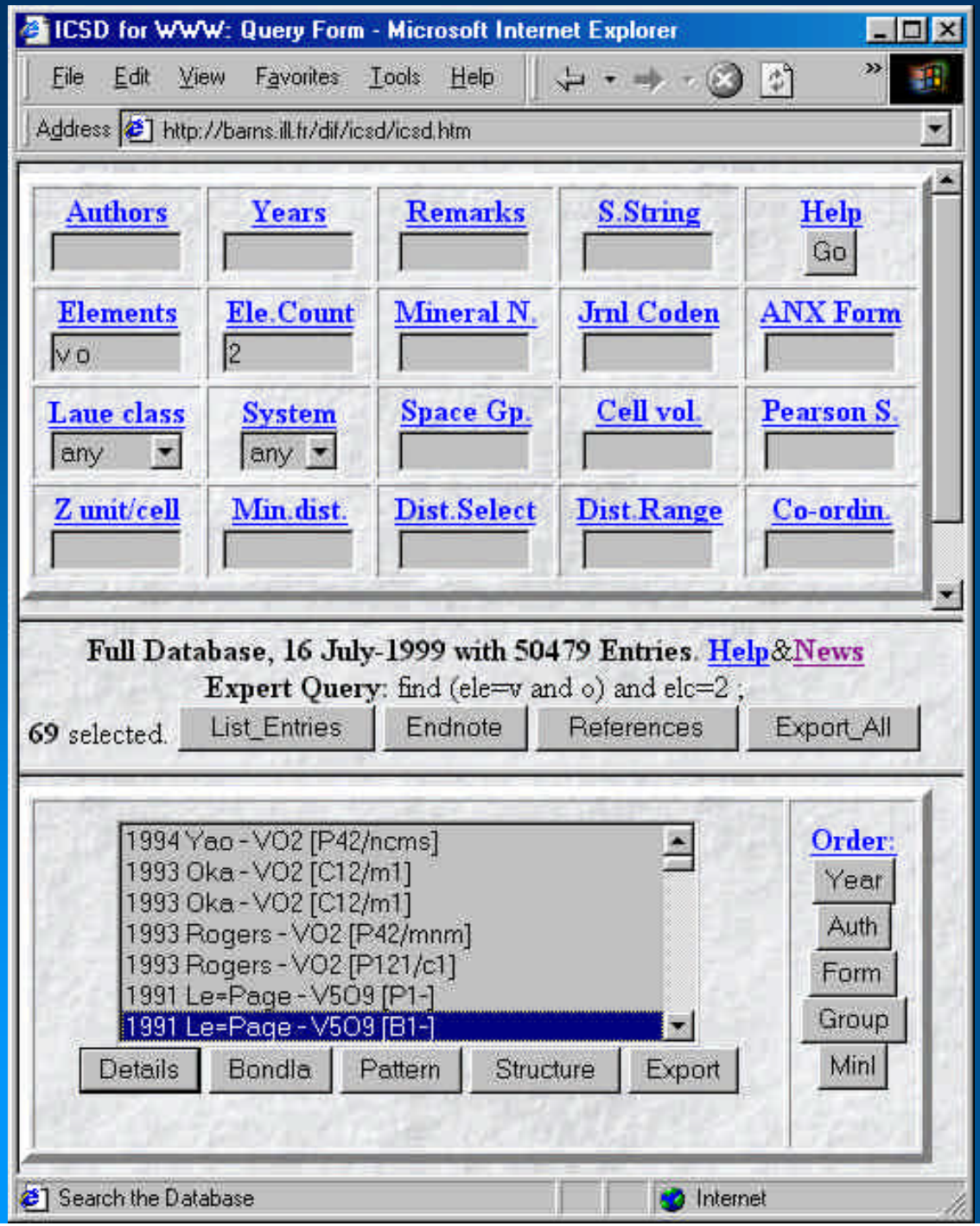

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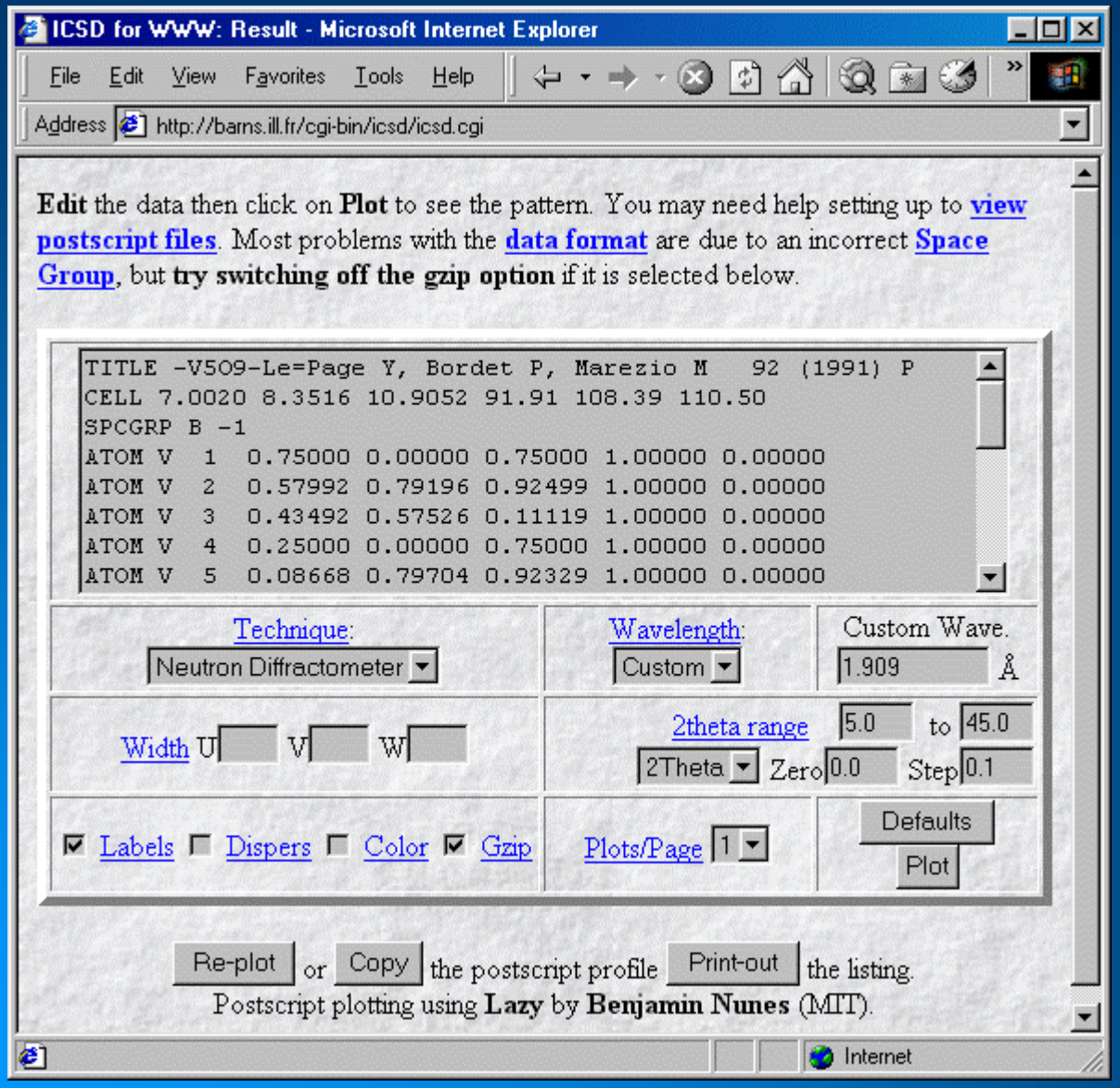

ICSD-for-WWW
ILL - Karlsruhe
inorg. crystal
structures

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ICSD for WWW: Result - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address http://barns.ill.fr/cgi-bin/icsd/icsd.cgi

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Labels

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File Edit Options View Orientation Media Help

File: rhum7[1].ps Page: "1" 1 of 1

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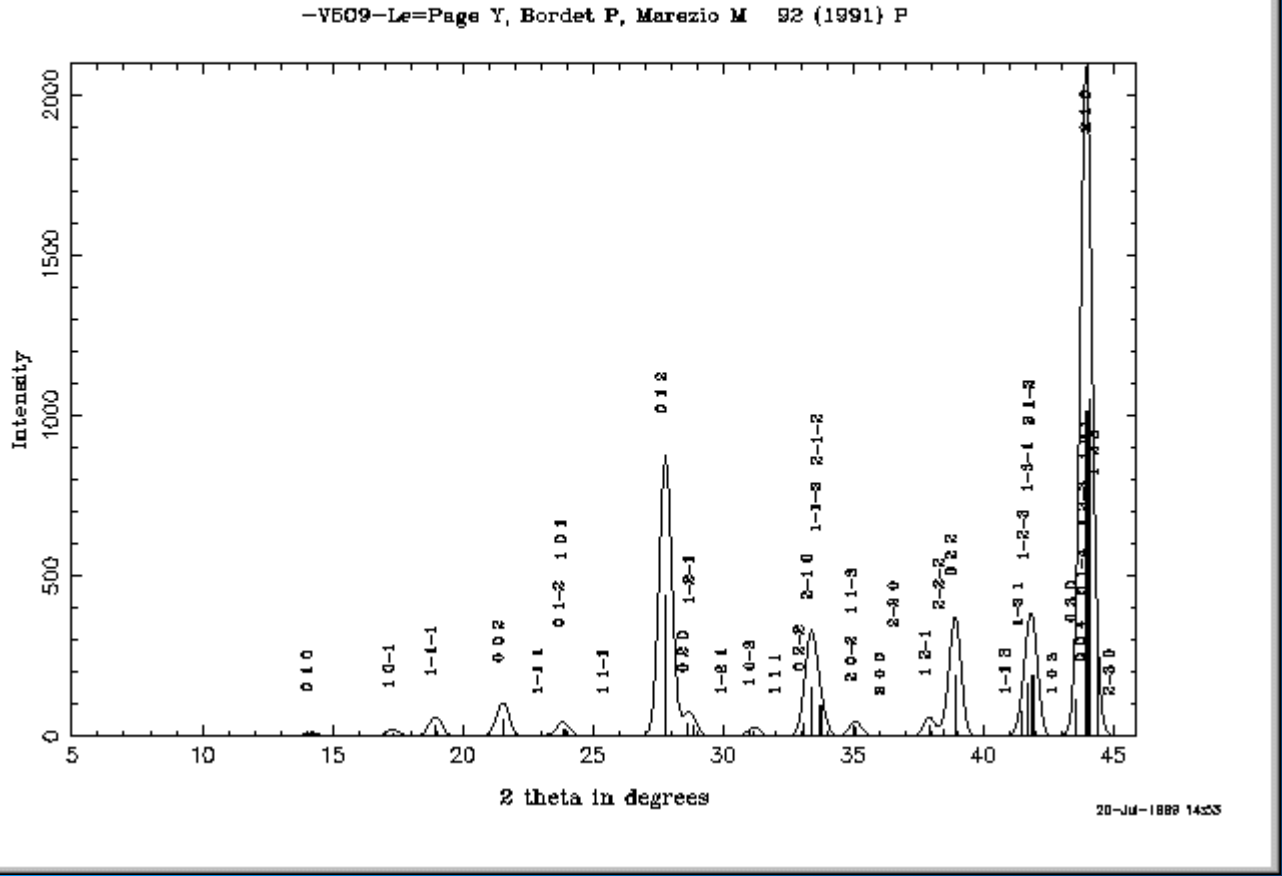

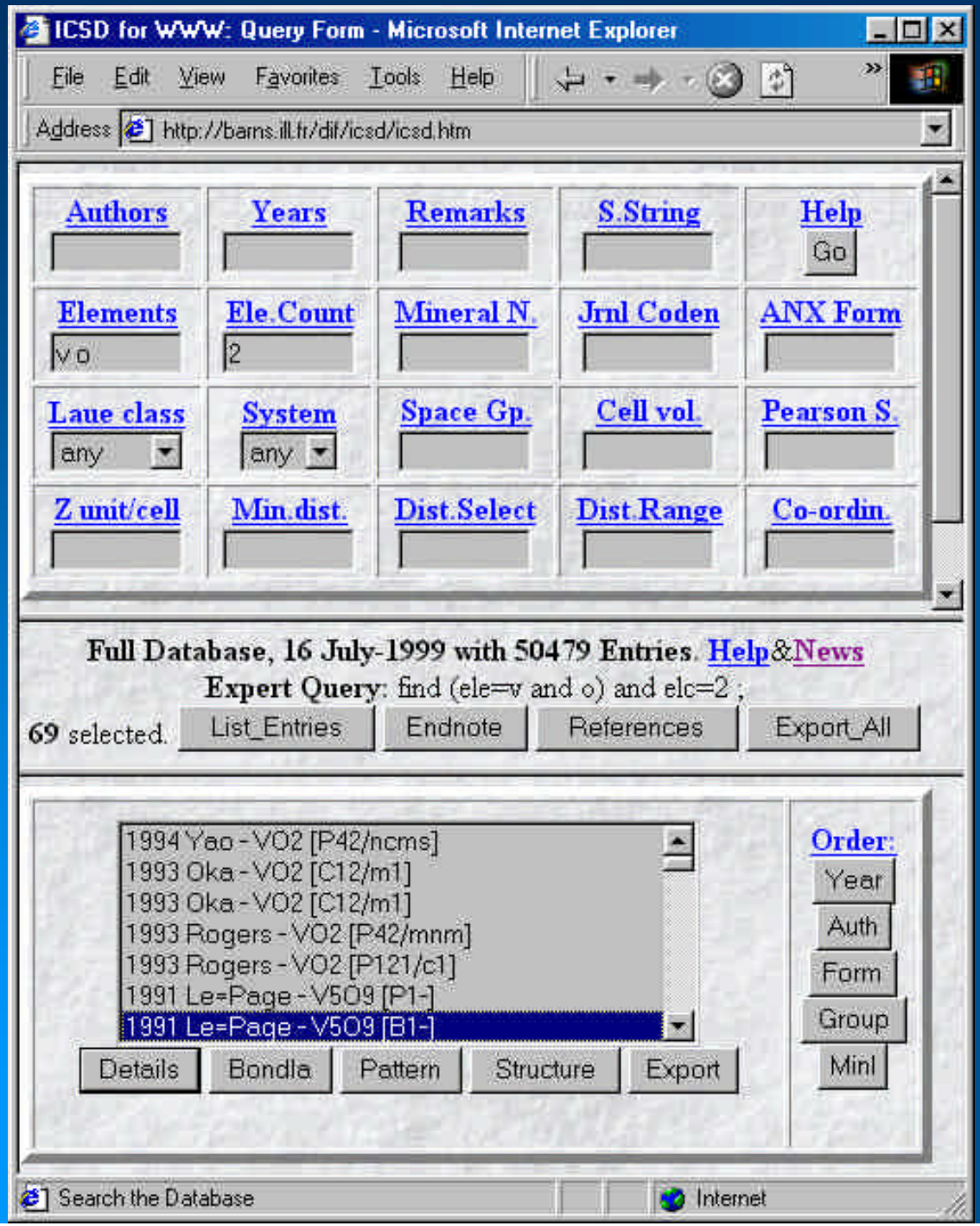

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ICSD-for-WWW
ILL - Karlsruhe
inorganic crystal
structures

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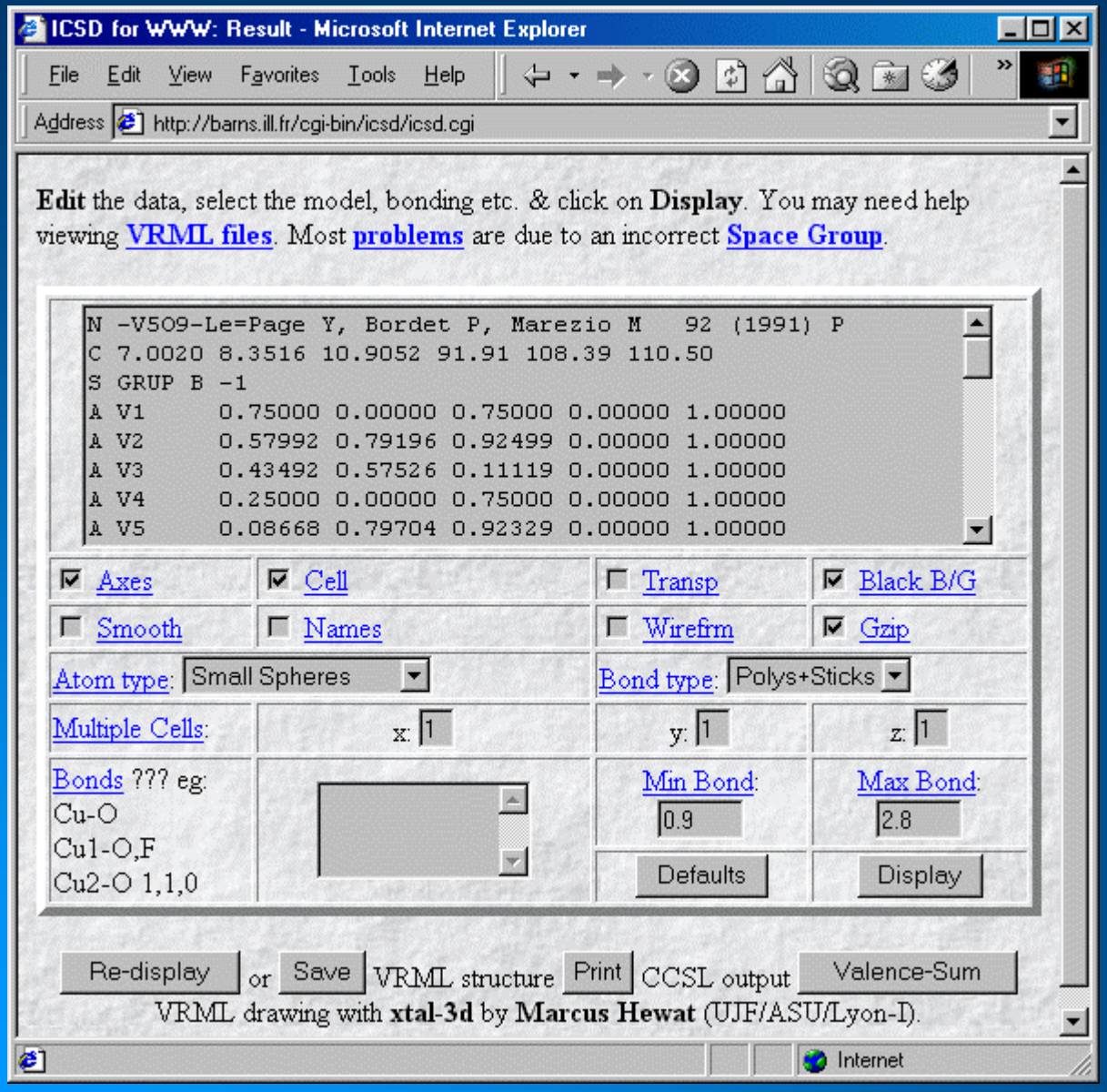
ICSD-for-WWW ILL - Karlsruhe inorganic crystal structures



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ICSD-for-WWW ILL - Karlsruhe inorganic crystal structures

ICSD for WWW: Result - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address http://barns.ill.fr/cgi-bin/icsd/icsd.cgi

Edit the data, select the model, bonding etc. & click on **Display**. You may need help viewing VRML files. Most problems are due to an incorrect Space Group.

```
N -V509-Le=Page Y, Bordet P, Marezio M   92 (1991) P
C 7.0020 8.3516 10.9052 91.91 108.39 110.50
S GRUP B -1
A V1      0.75000 0.00000 0.75000 0.00000 1.00000
A V2      0.57992 0.79196 0.92499 0.00000 1.00000
A V3      0.43492 0.57526 0.11119 0.00000 1.00000
A V4      0.25000 0.00000 0.75000 0.00000 1.00000
A V5      0.08668 0.79704 0.92329 0.00000 1.00000
```

Axes | Cell | Transp | Black

Smooth | Names | Wirefrm | Gzip

Atom type: Small Spheres | Bond type: Polys+Sticks

Multiple Cells: x: 1 y: 1 z:

Bonds ??? eg:
Cu-O
Cu1-O,F
Cu2-O 1,1,0

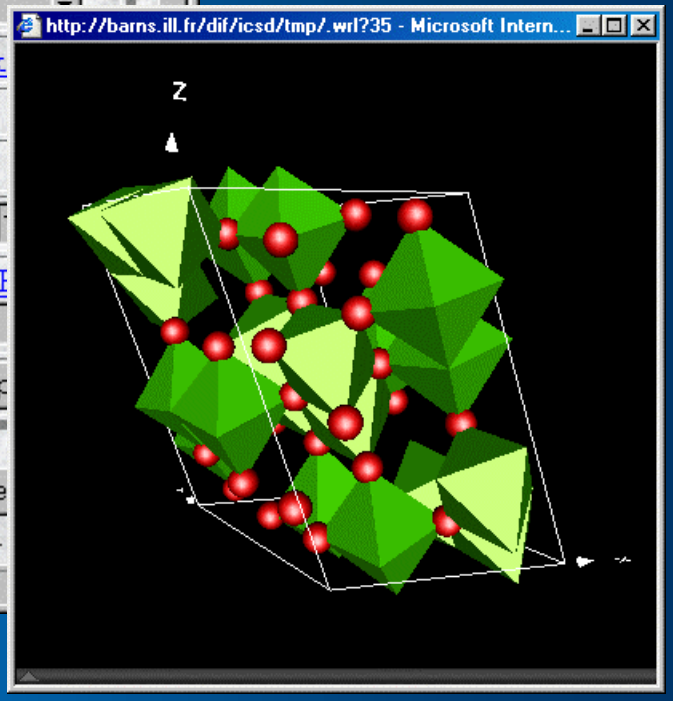
Min Bond: 0.9 | Max B: 2.8

Defaults | Disp

Re-display or Save VRML structure | Print CCSL output | Valence

VRML drawing with **xtal-3d** by **Marcus Hewat** (UJF/ASU/Lyon-I).

Internet



Alan Hewat

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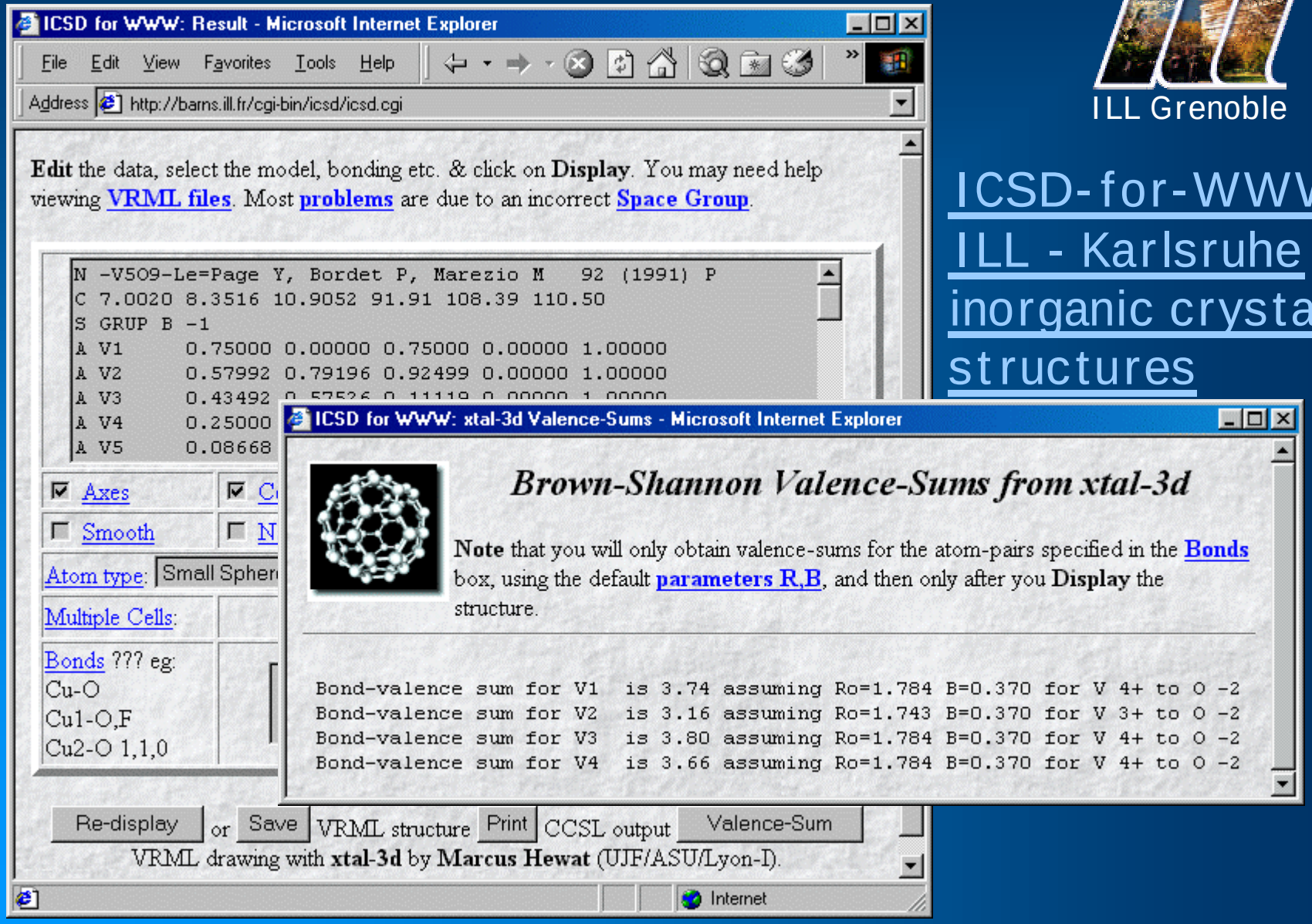
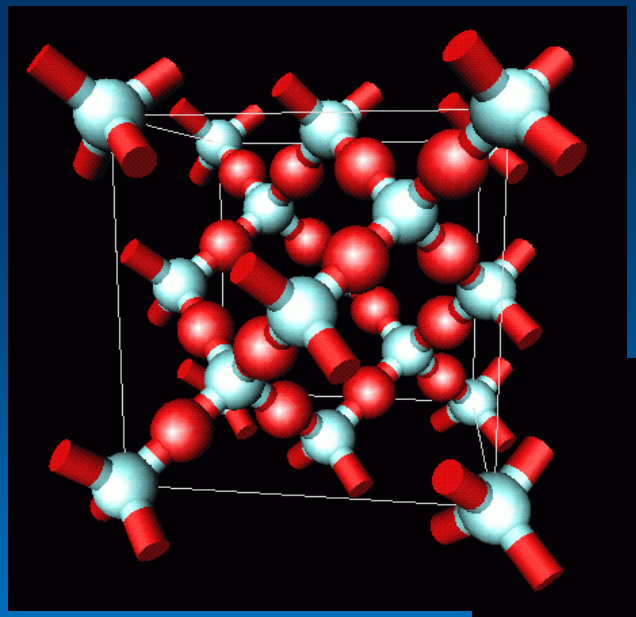
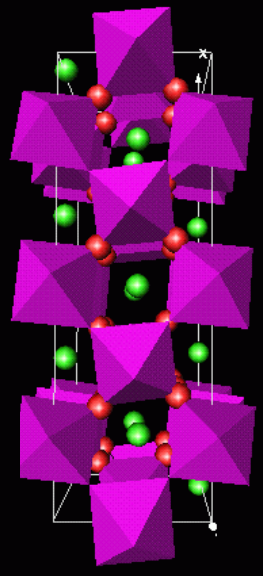
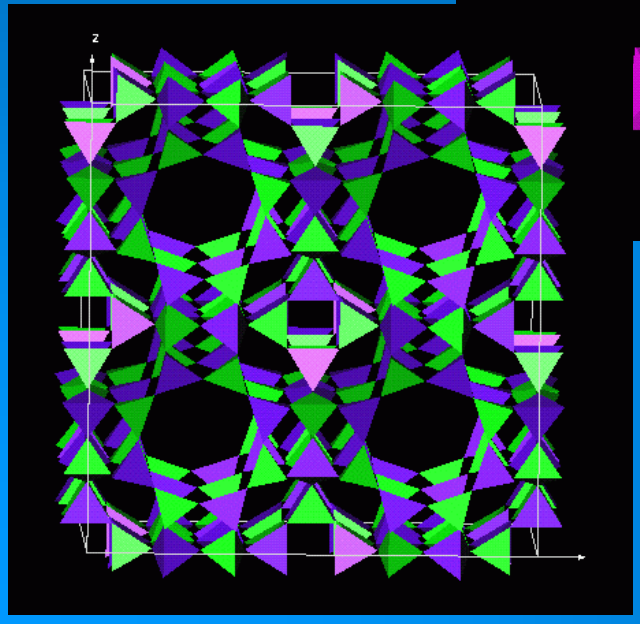
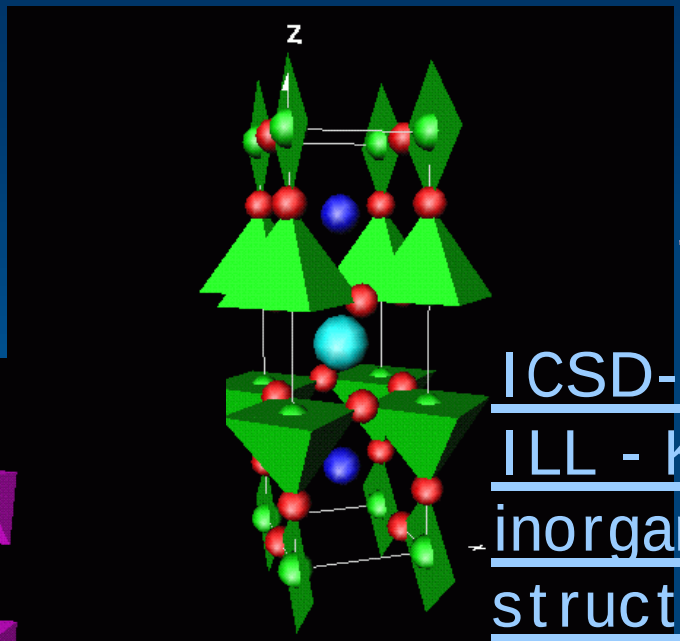
ICSD-for-WWW ILL - Karlsruhe inorganic crystal structures

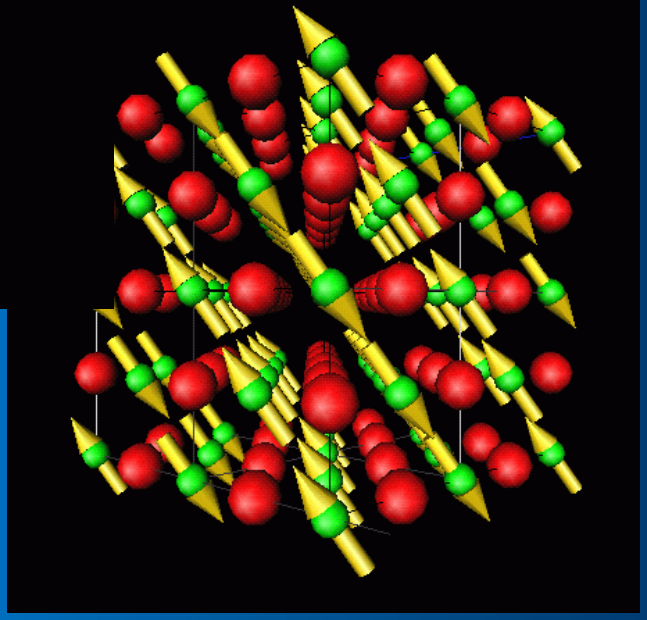












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ILL - Karlsruhe inorganic crystal structures

The Impact of Informatics

Alan Hewat, Diffraction Group, ILL Grenoble

Alan Hewat

ILL Grenoble

Science 12 March 1999

COOL IMAGES

Material World

What do buckeyballs, superconductors and talc have in common? They're all inorganic materials, and they all come under scrutiny at Making Matter,* a Web gallery at the Institute Laue-Langevin in Grenoble, France. The institute houses a neutron source used to decipher atomic structures, and researcher Alan Hewat has created a tutorial using dozens of images computer generated with data from the institute's archive. The colorful images—manipulable in 3D—demonstrate how atoms pack in metals and rock salt, how sliding layers give talc its slipperiness, how holes in zeolites make the structures useful, and how a "charge reservoir" lets superconductors do their thing. In the rendering above of manganese oxide, an antiferromagnet, arrows show the moments of green manganese atoms that cancel each other out.

*www.ill.fr/dif/3D-crystals/index.html

ICSD-for-WWW
ILL - Karlsruhe
inorganic crystal
structures

The Impact of Informatics

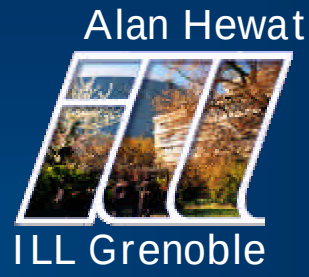
Alan Hewat, Diffraction Group, ILL Grenoble

Laboratories running ICSD-for-WWW

- ILL/ESRF
- CDS UK (UK academic community)
- CCP14 Daresbury UK
- CICS Spain (Spanish Scientific Research Council)
- ORNL (Oak Ridge National Laboratory, USA)
- NIST Washington USA
- CAOS/CAMM Netherlands
- Nagoya University, Japan
- NCHC Taiwan (Taiwan national database)

The Impact of Informatics

Alan Hewat, Diffraction Group, ILL Grenoble



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- WWW Data Bases
  - Disadvantage
  - Who pays ?
    - Cost of collecting data
    - Cost of updating software
    - Cost of running servers
  - Computer applications are paid for by selling cardboard boxes...

The Impact of Informatics

Alan Hewat, Diffraction Group, ILL Grenoble

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- Who Pays ?
  - National Labs.
    -As part of their service
  - National Grants eg
    -EPSRC Daresbury
    -New US PDB lab.
  - WWW data collection
    -Individual scientists enter new data
    -Automatic checking