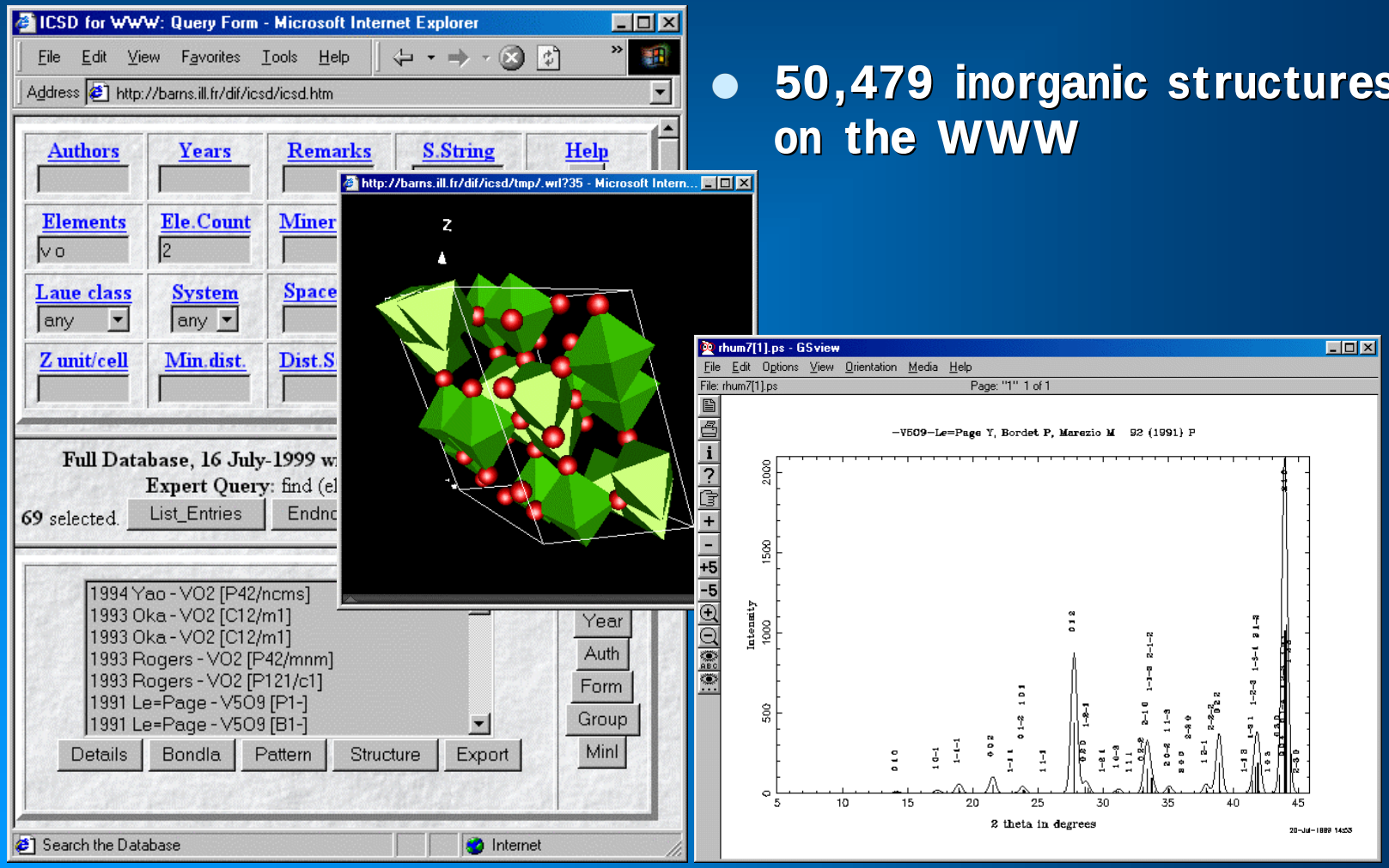
What's New with ICSD-for-WWW

WWW Inorganic Crystal Structure Database - ILL/FIZ

Alan Hewat
ILL Grenoble



- **50,479 inorganic structures on the WWW**

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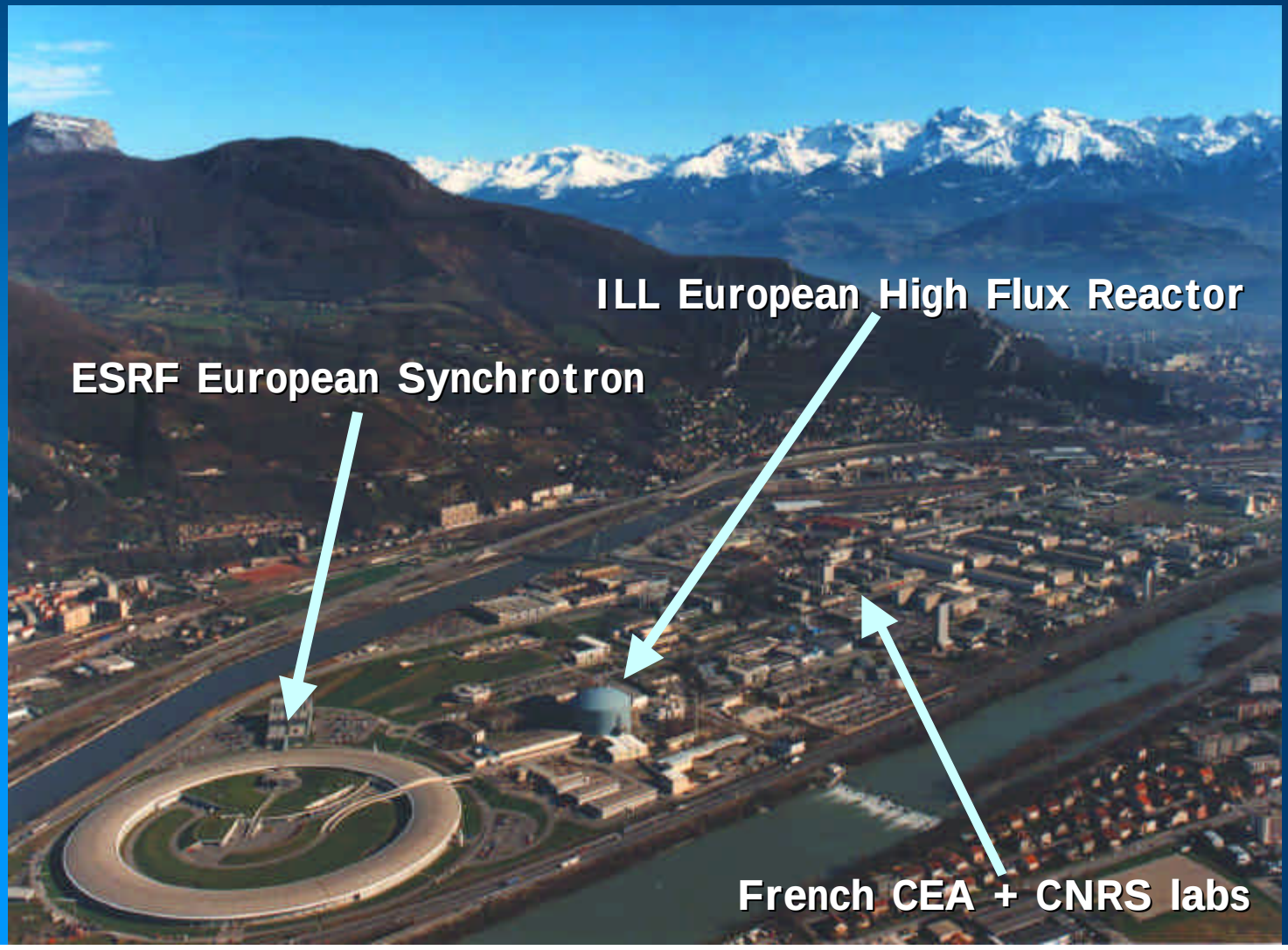

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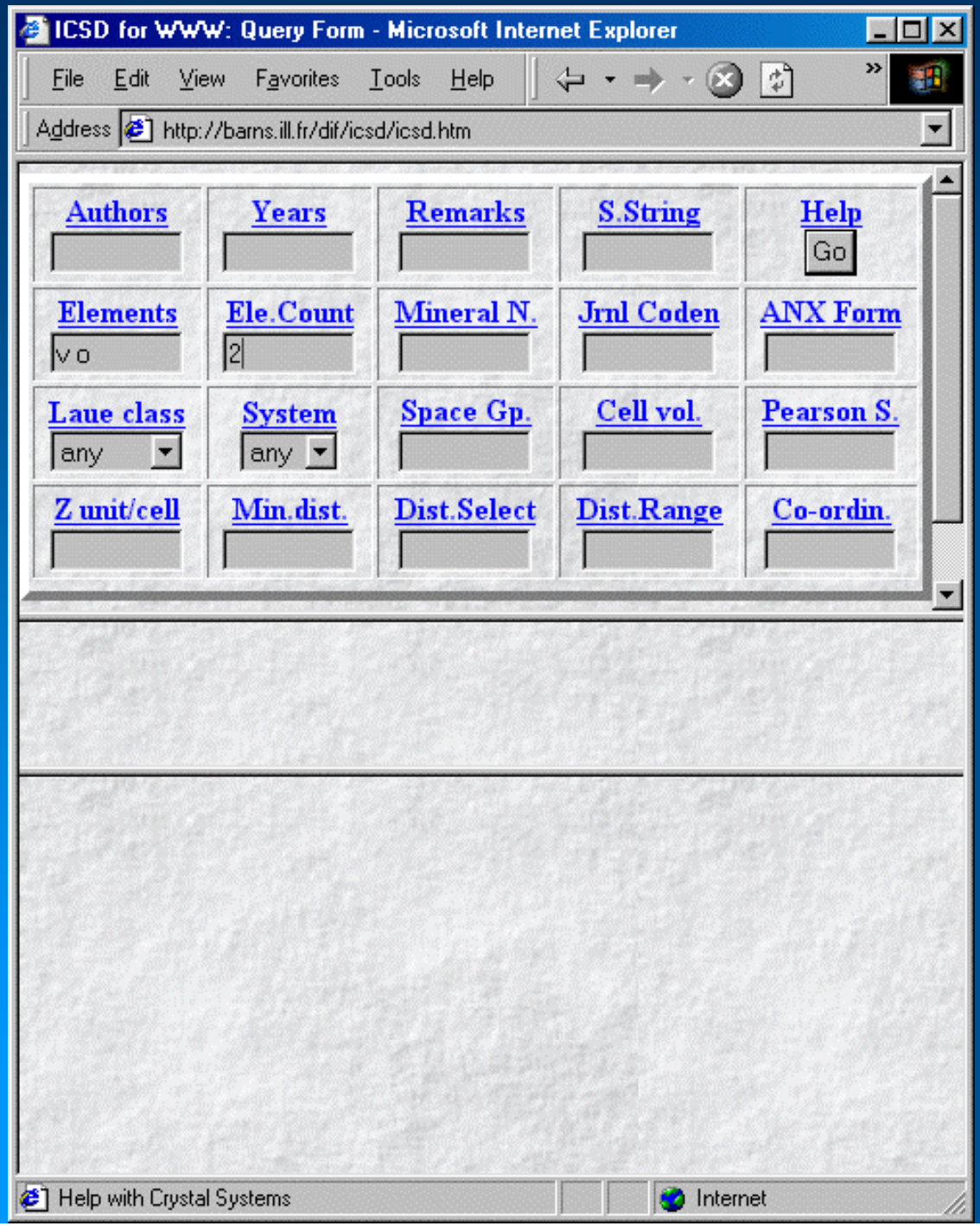
WWW Inorganic Crystal Structure Database - ILL/FIZ

- **Advantages of the WWW format**
  - Available immediately, on any computer, nothing to install
  - Available to everyone, within a laboratory, or whole country
  - Centrally maintained and always up-to-date
  - Familiar WWW graphic user interface, little new to learn
  - Uses latest software developed by Microsoft, Netscape etc

- **Disadvantages of the WWW format**
  - How is data entered into the database and checked ?
  - Who pays for maintaining the database with a "virtual" product ?



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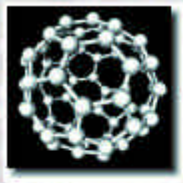
Search for vanadates

Elements = V O
Number elements= 2

File Edit View Favorites Tools Help



The ELE (Elements) descriptor class

This is one of the most useful search criteria. Entering eg **Al O** specifies *all* compounds containing **Al and O**. If you want just Al2O3, you should as well specify an element count of **2**, or perhaps elements **Al2 O3** (note the seperating space!)

- keyword = [element symbol]. Examples: **Fe, I**

- keyword = [symbol for a group of elements] Examples: **HAL** or **ALK** or **HAL not F** ACT in the **Elements** box produces a **list of all element groups** and the number of their references.

- keyword = [element symbol][+ or -][oxidation state] Chemical element in a specified oxidation state. The sign (+ or -) must never be omitted. To find elements with non-integer oxidation states ranges should be used. Examples: **As+3** or **S-2** or **Ni+0** or **Fe+2 to Fe+2.5** See notes 2 and 3.

- keyword = [element symbol][stoichiometric coefficient] Coefficients of the empirical formula should be used. Ranges may be meaningful. Examples: **Cl2** or **S2.2 to S2.8**

Examples:

Elements: **Cu1 Cl2** Ele.Count: **2**
Elements: **Y Ba Cu O** Ele.Count: **4-5**
Elements: **Y1 Ba2 Cu3 O** Ele.Count: **4**
Elements: **Y1 Ba2 Cu3 O6 to O7** Years: **86-88** (early HiTc papers)
Elements: **Cd (S or Se not O)**
Elements: **hal (alk not li)** (Neither **hal alk not li** nor **(alk not li) hal** will work).

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Help with any field
(Click on its title)

- Help with Elements

File Edit View Favorites Tools Help

The ELC (Element Count) descriptor class

The Ele.Count is the number of different chemical elements present in a compound without regard to their stoichiometry, oxidation state or bonding. A range can be specified so that **1 to 3** or **1-3** represents compounds with at most 3 different chemical elements.

Note: Ele.Count includes elements that are not on crystallographic sites, including trace elements in the FOrmula. It is recommended to specify ranges such as 2-3 to mean from 2 to 3 different elements.

ELC can be used to exclude complex structures, for example, Elements **MET O** and the Element Count **2** selects only binary metal oxides.

Examples:

Elements: **met O** Ele.Count: **2**
Elements: **Cu1 Cl2** Ele.Count: **2**
Elements: **Y Ba Cu O** Ele.Count: **4-5**
Elements: **Y1 Ba2 Cu3 O** Ele.Count: **4**

Help file adapted from the CRYSTIN search program (copyright R. Hundt & R. Sievers)
Please report any problems with **ICSD for WWW** to hewat@ill.fr (Alan Hewat).

Alan Hewat
ILL Grenoble

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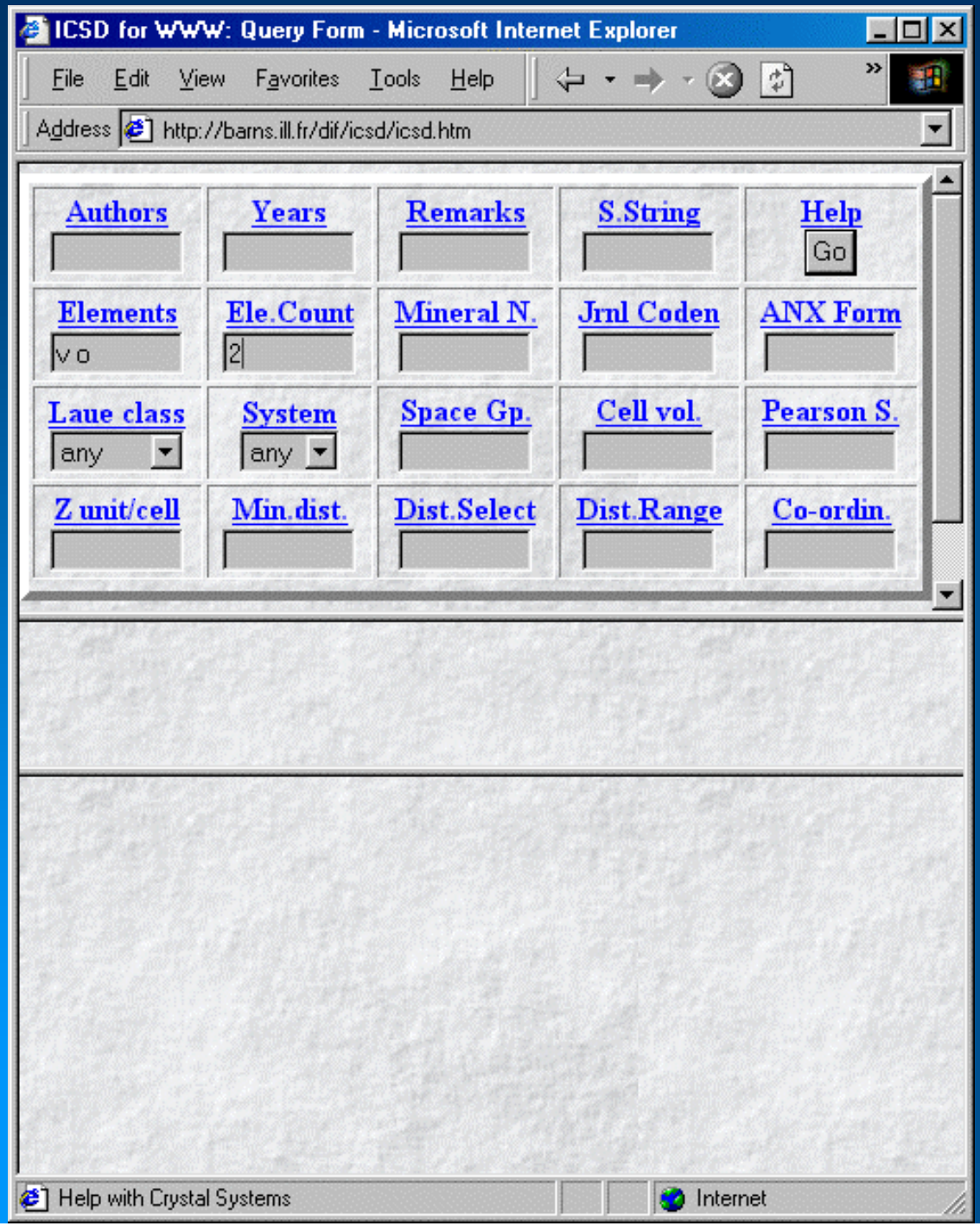
Help with any field
(Click on its title)

- Help with Elements
- Help with Nº Elements



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Search for vanadates

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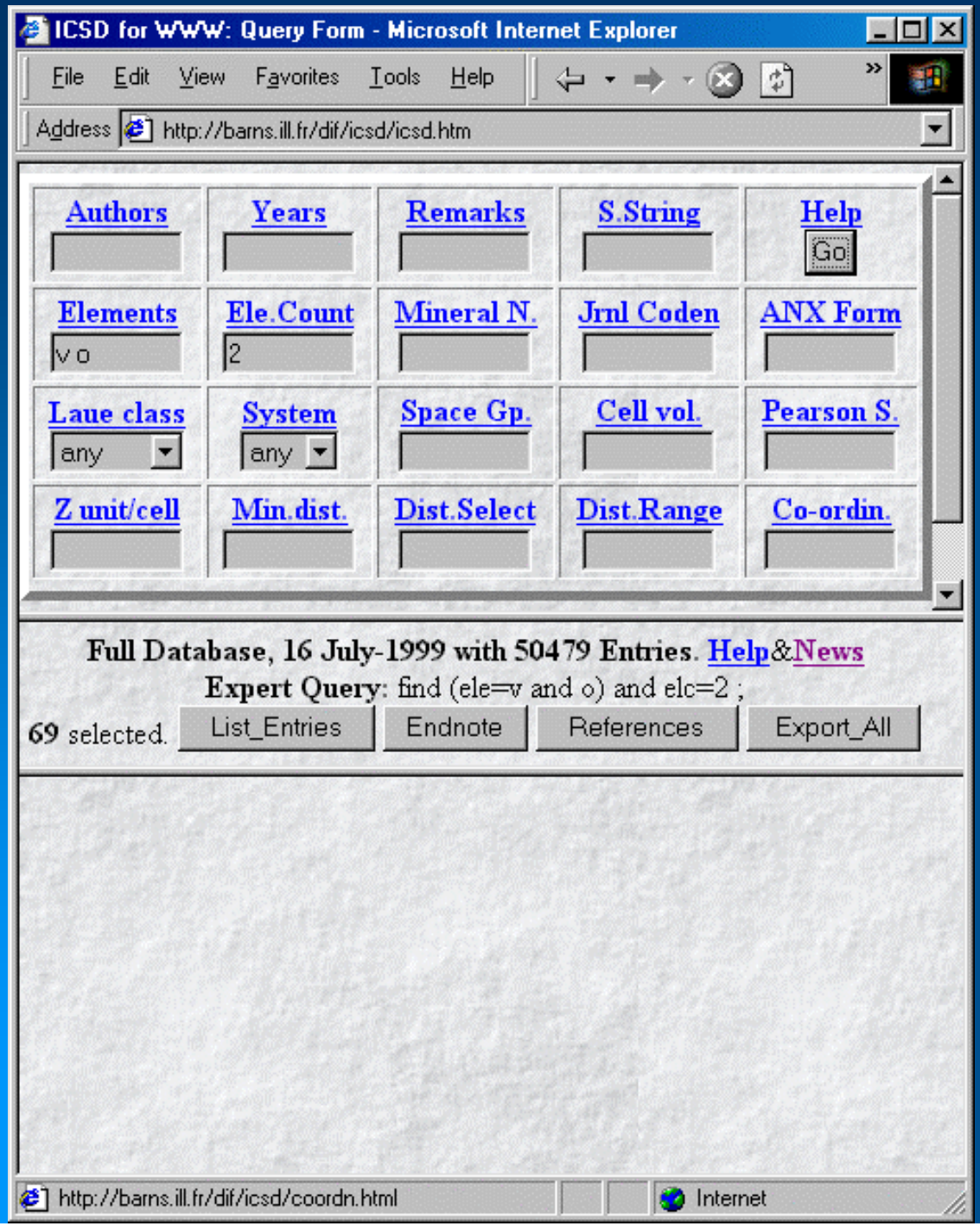
Number elements= 2



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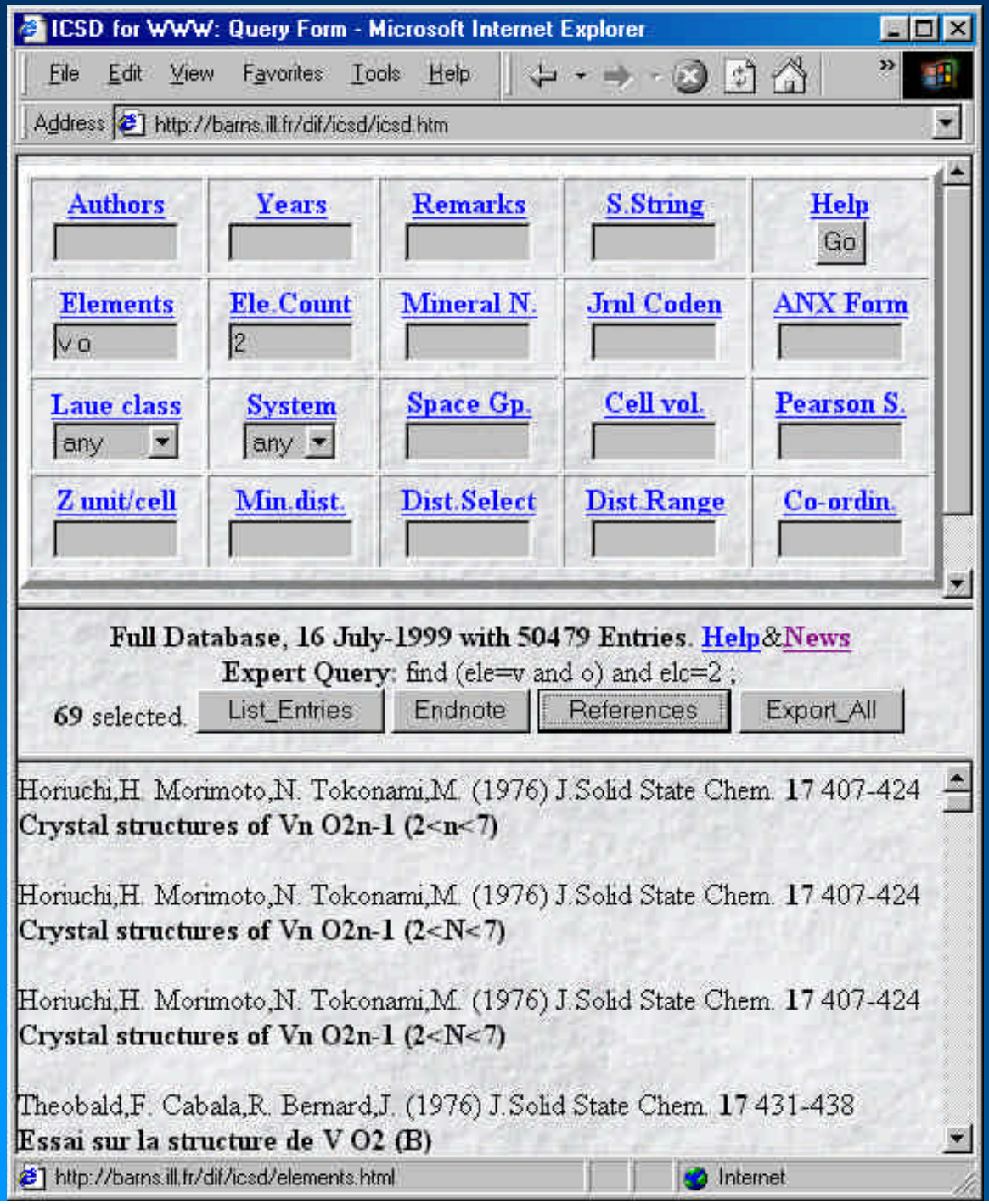

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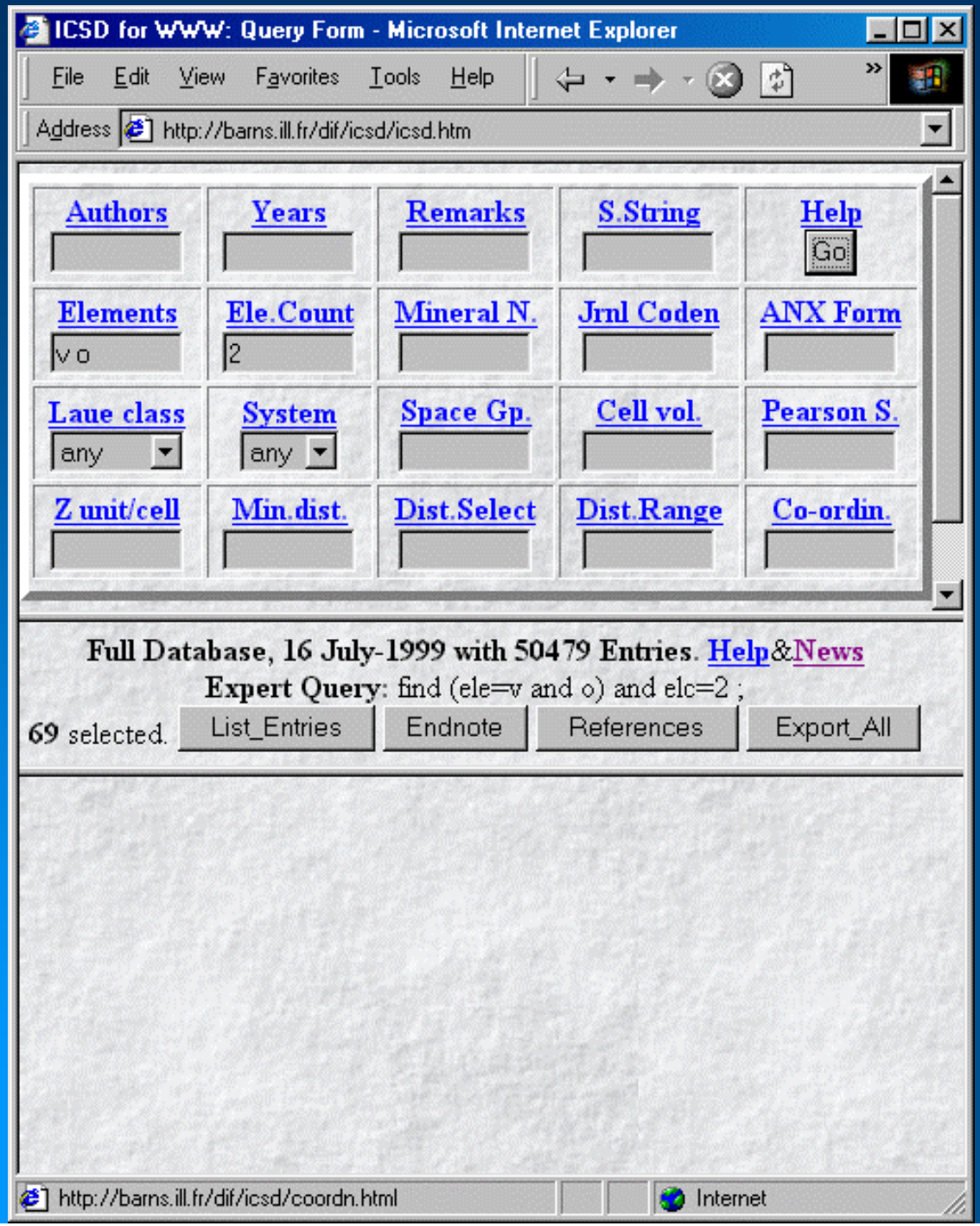
List References



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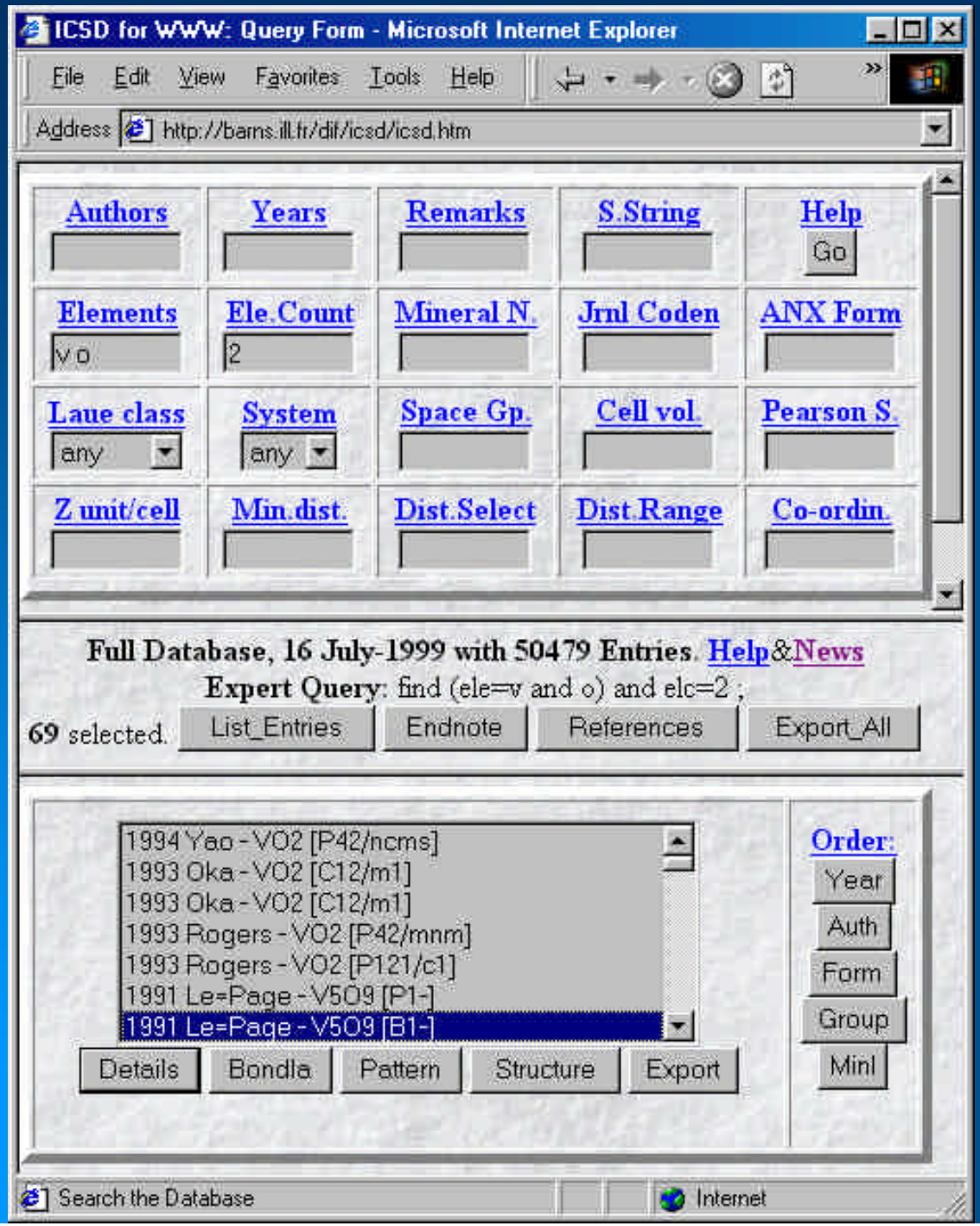

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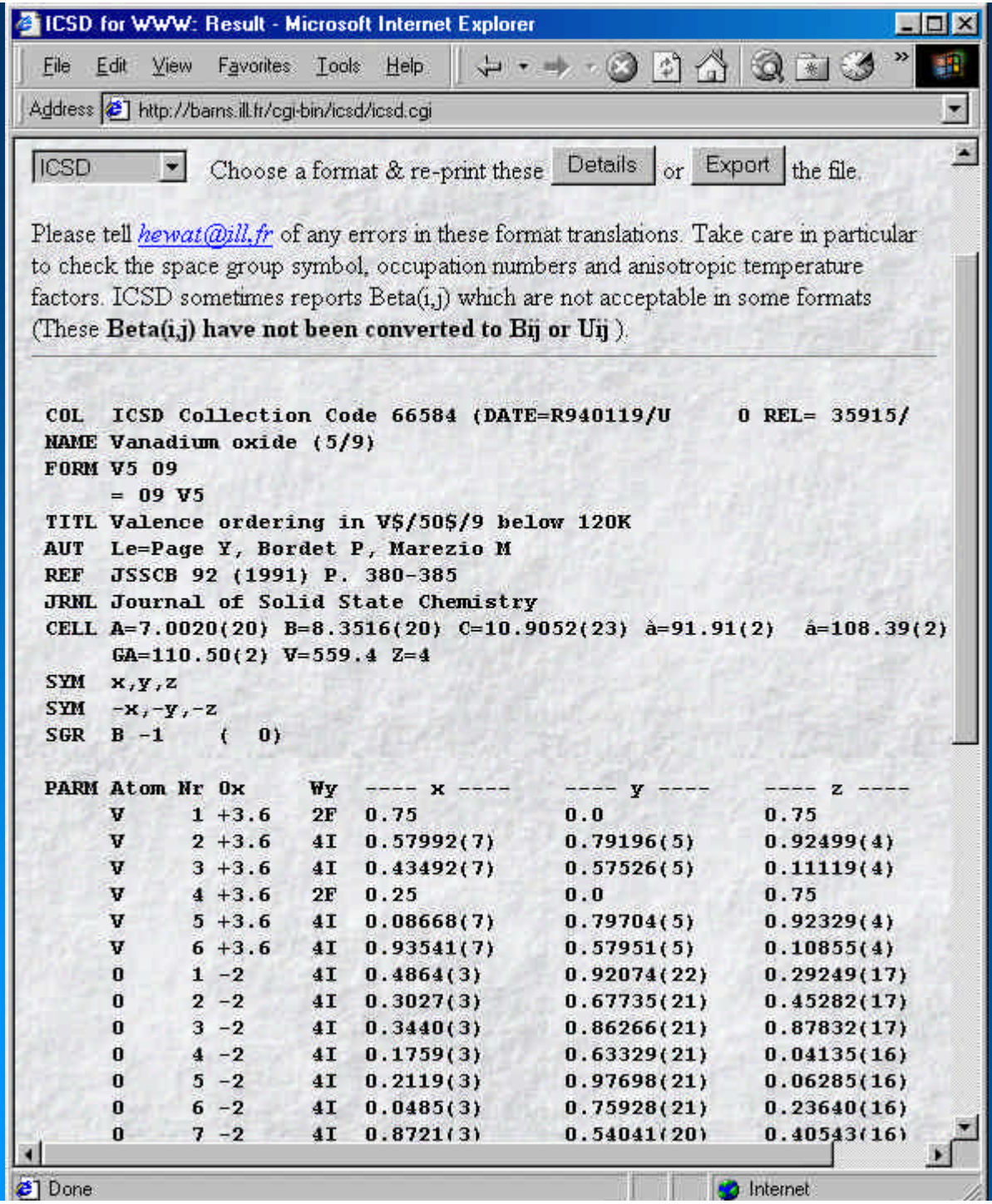
List Entries

Entries can be sorted

- Year
- Author
- Formula
- Space Group
- Mineral Name



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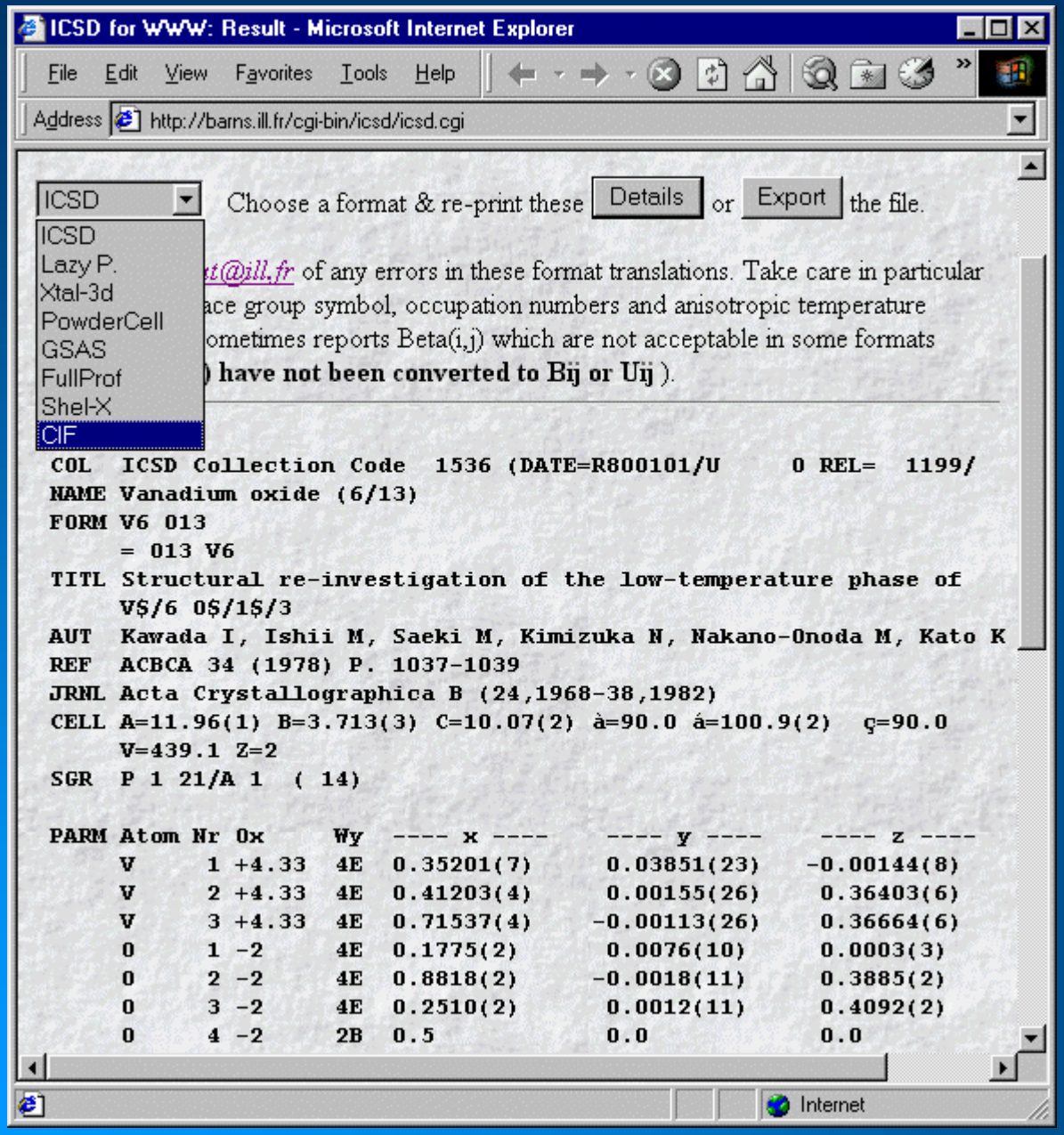
List Details of Entry



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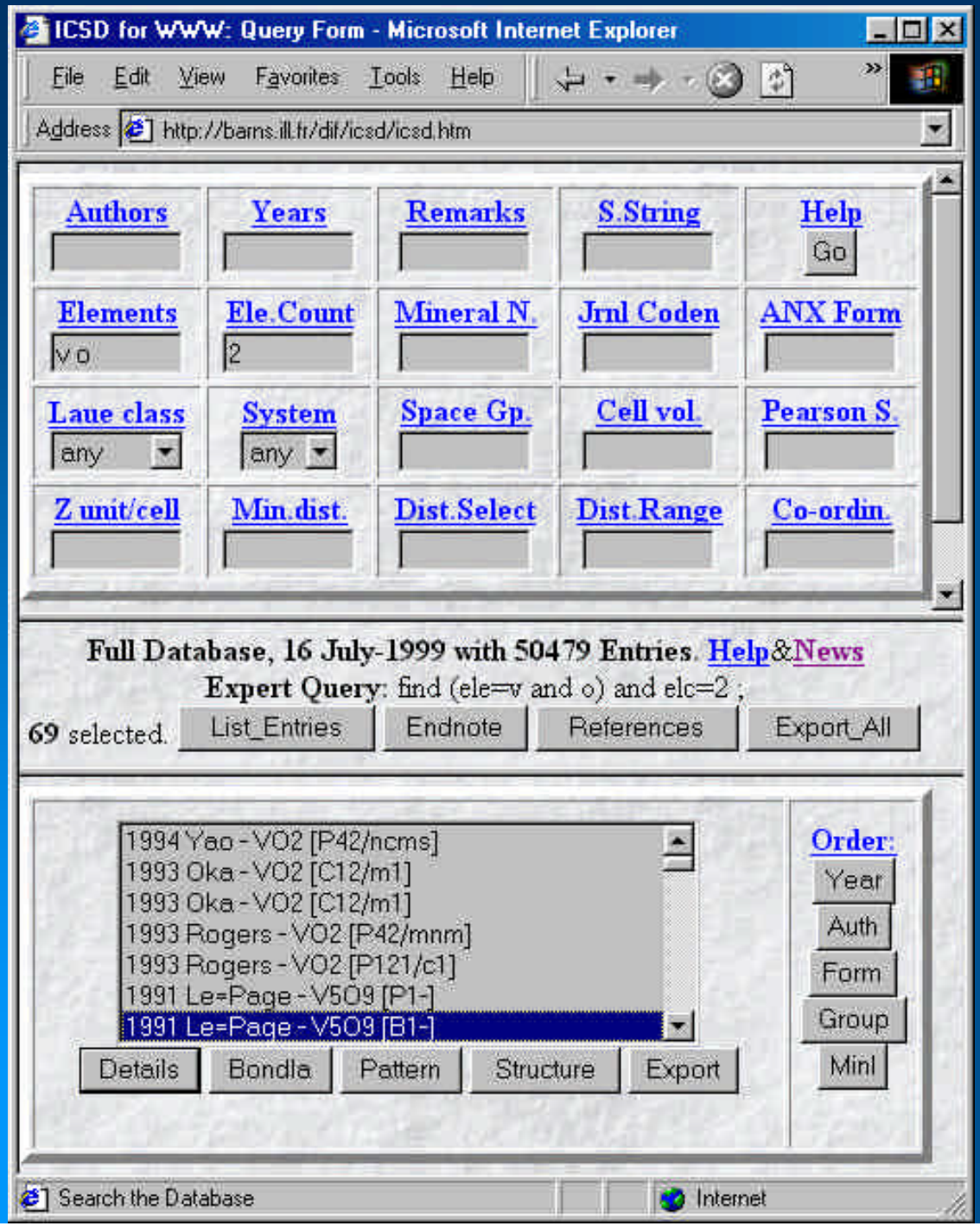
List or Export Details in many formats

- ICSD
- Lazy Pulverix
- CCSL
- PowderCell
- GSAS
- FullProf
- Shel-X
- CIF



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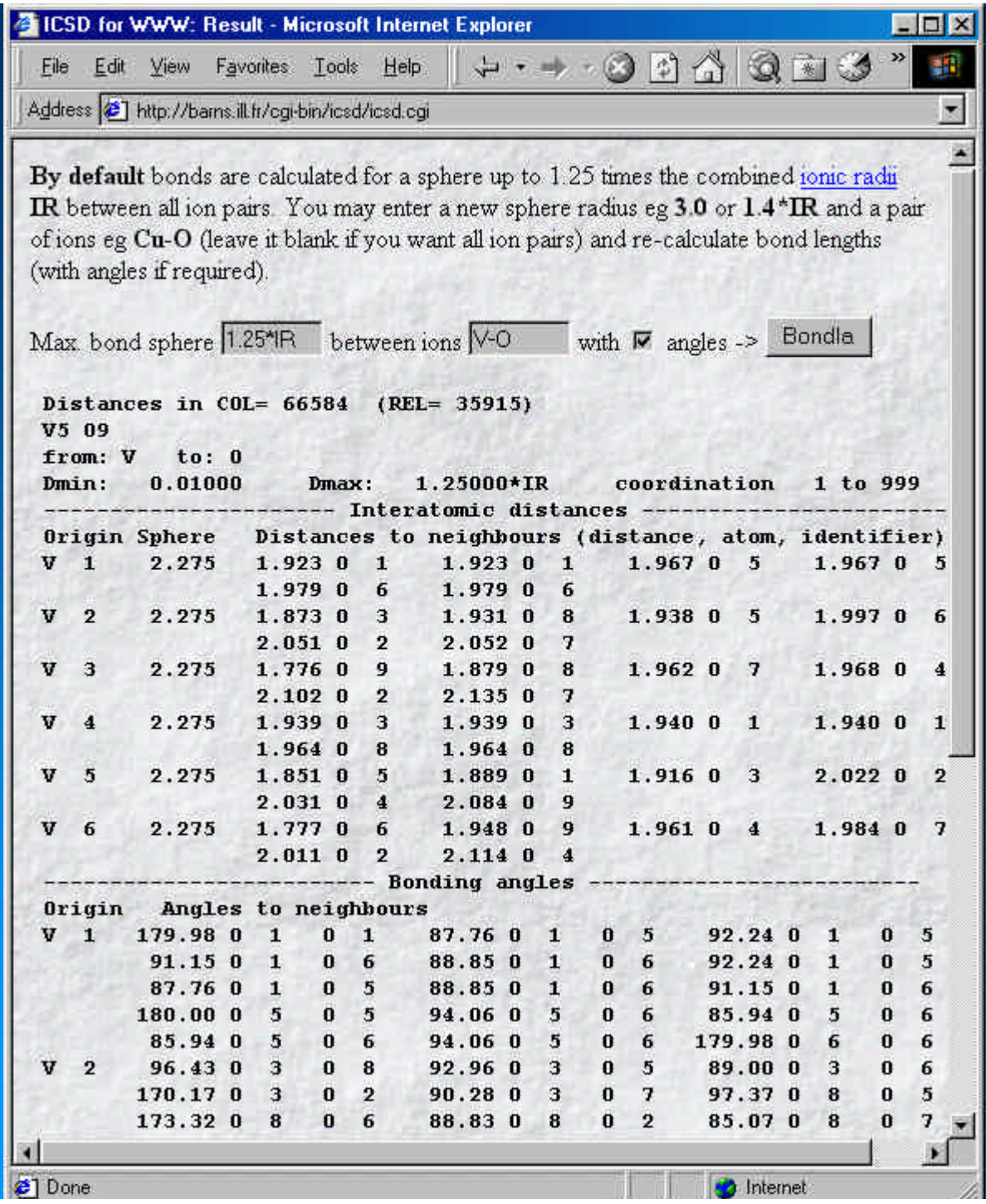
Calculate Bond Lengths and Angles



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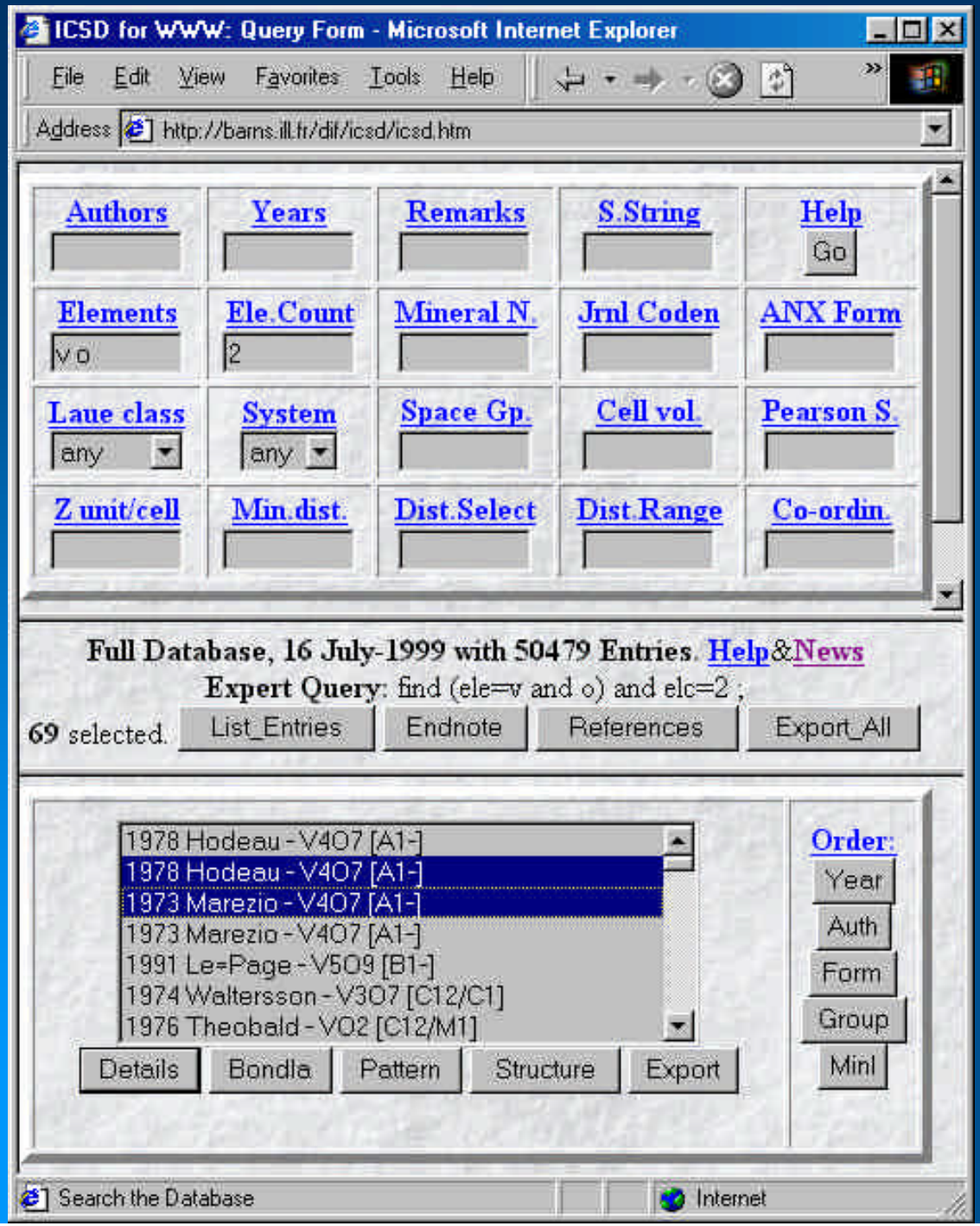
Calculate Bond Lengths and Angles



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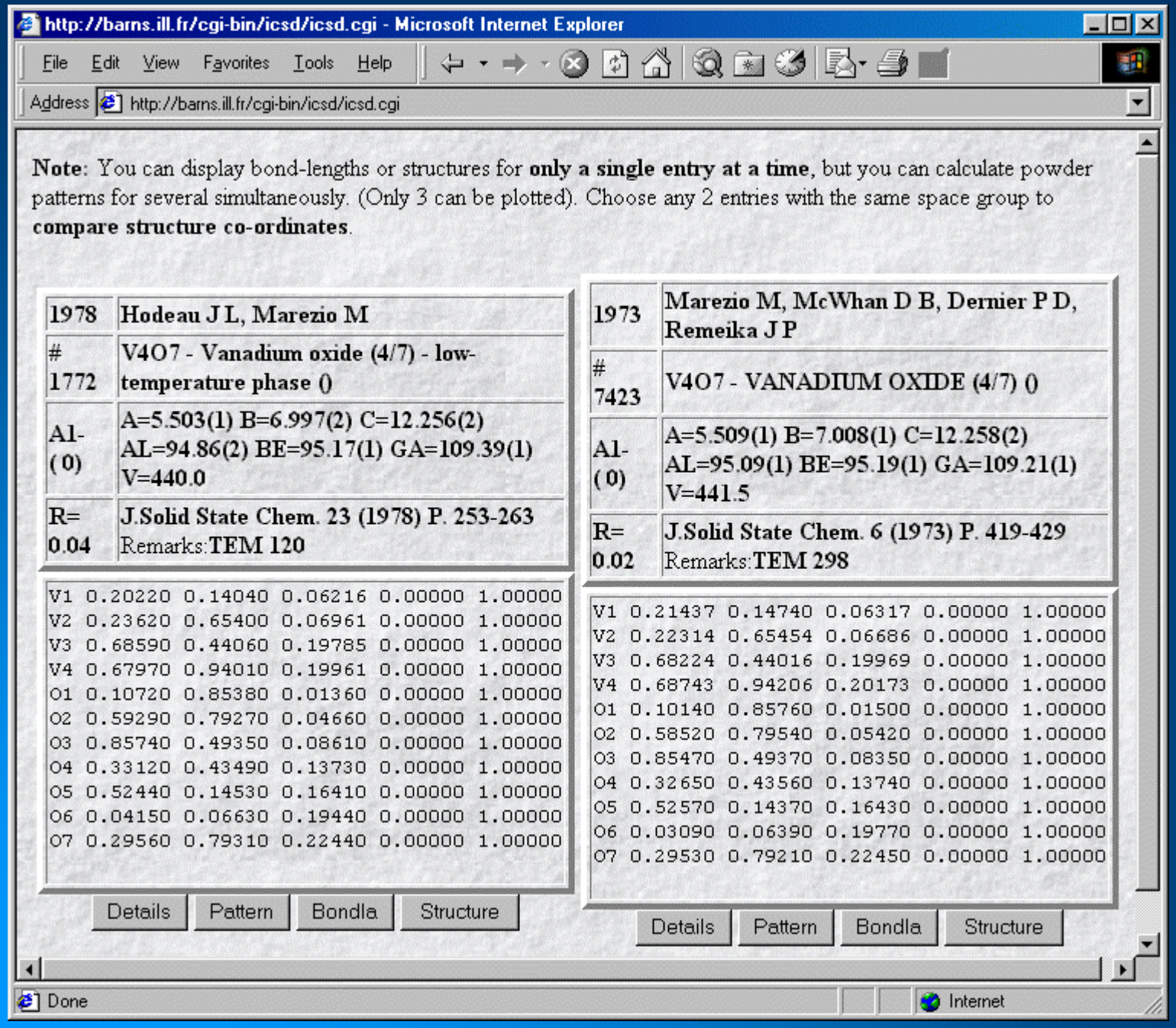
Compare similar structures



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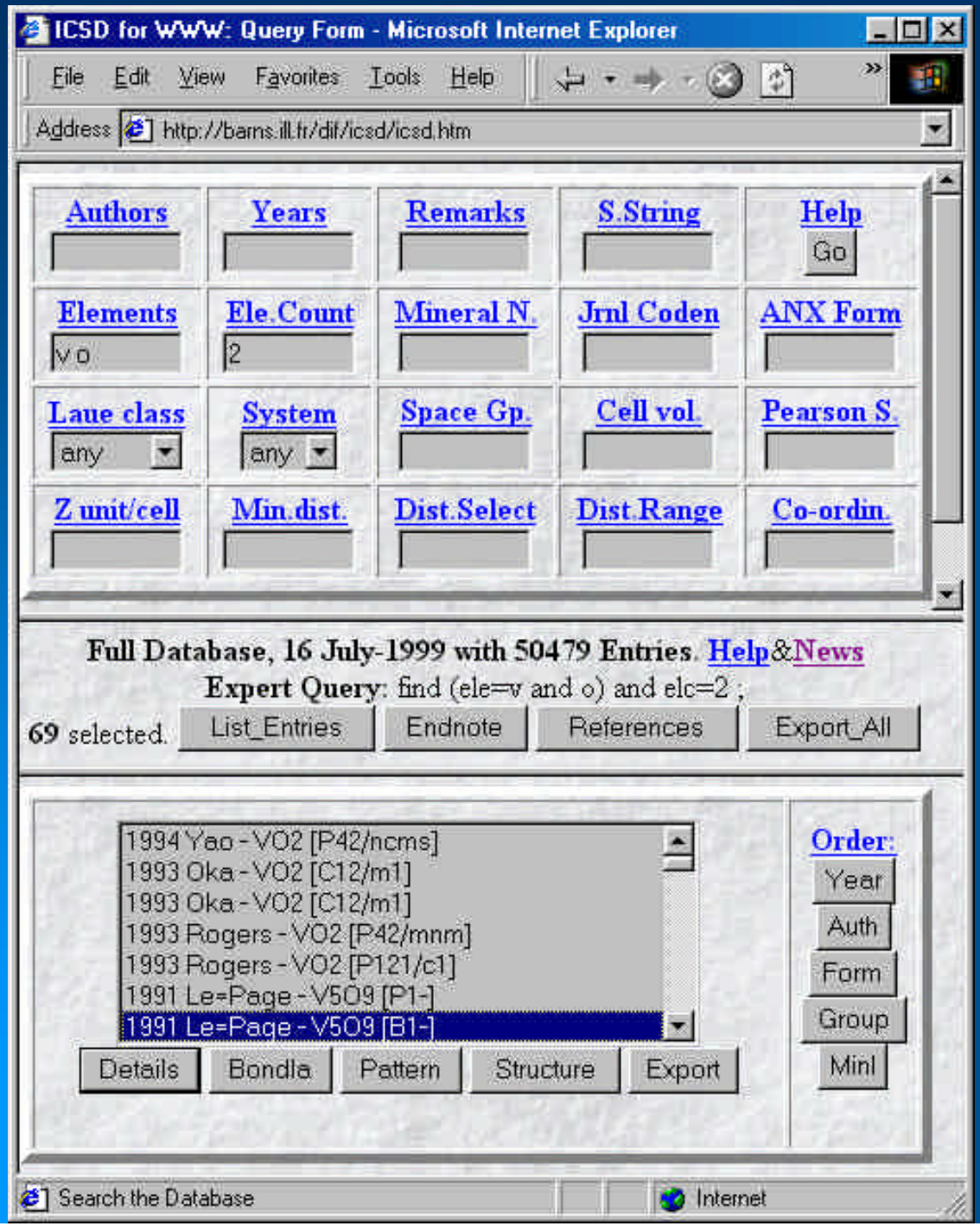
Compare similar structures



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Calculate the indexed powder pattern

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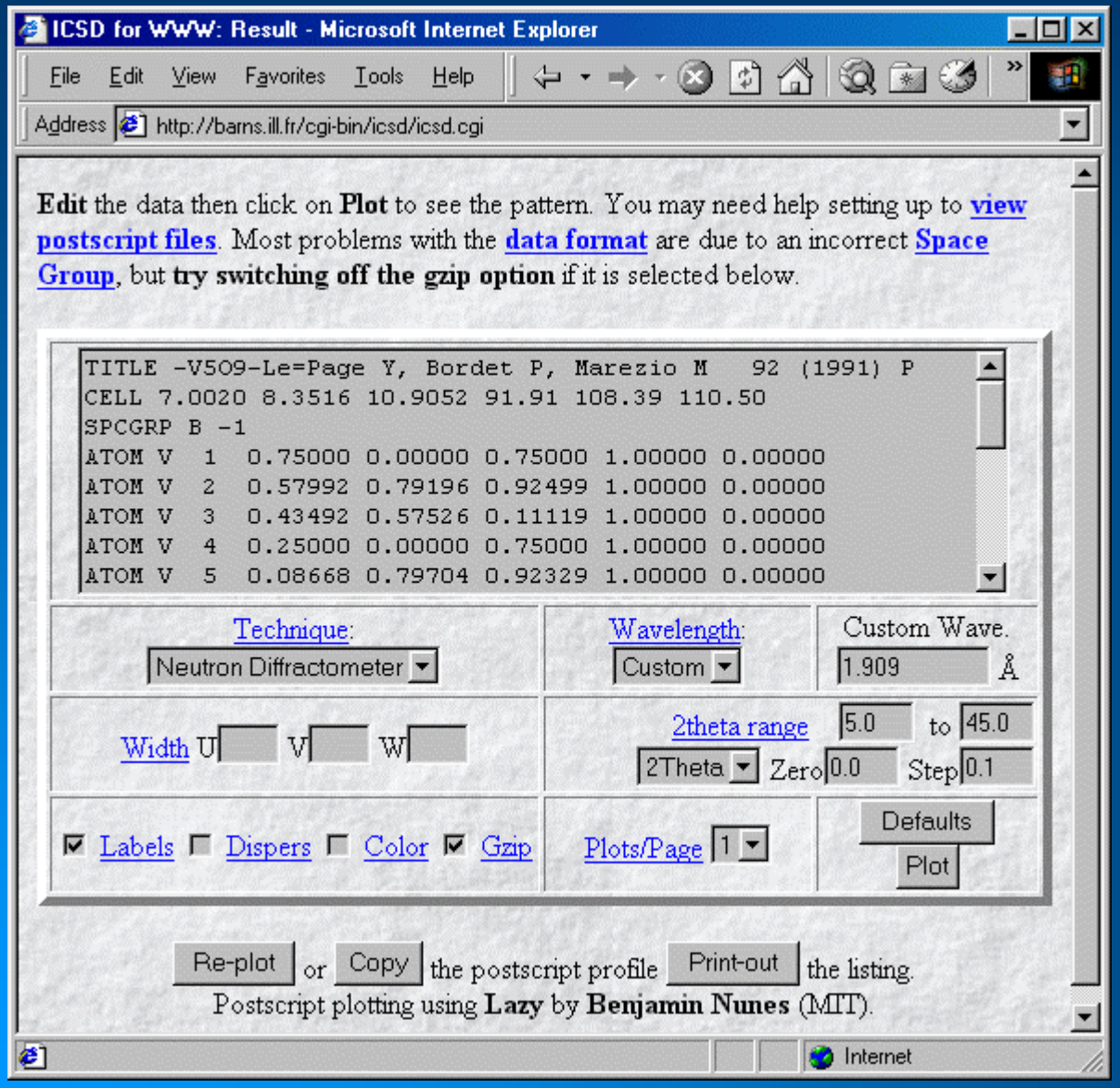

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Calculate the indexed powder pattern

Select neutrons, Xrays wavelength, peak width etc

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ICSD for WWW: Result - Microsoft Internet Explorer

File Edit View Favorites Tools Help

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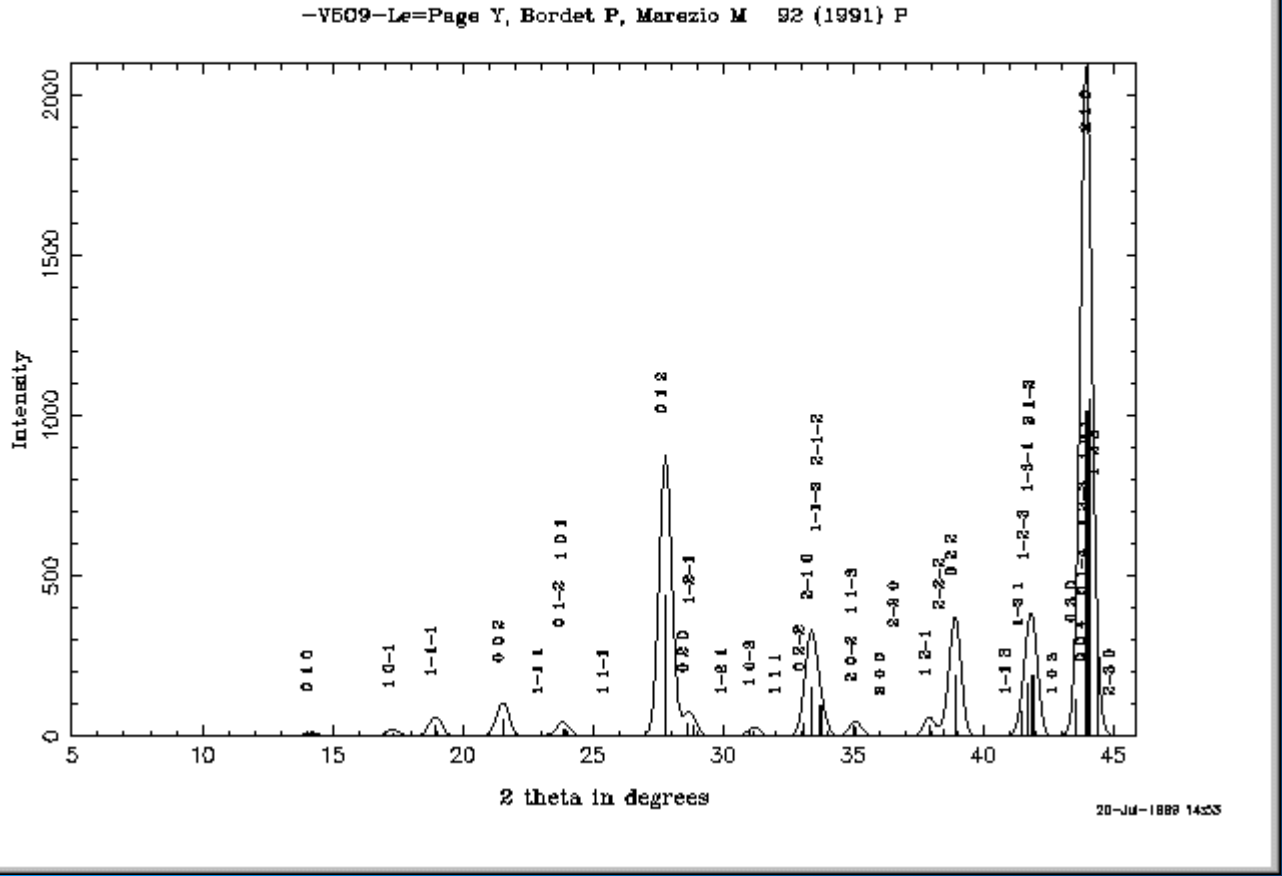

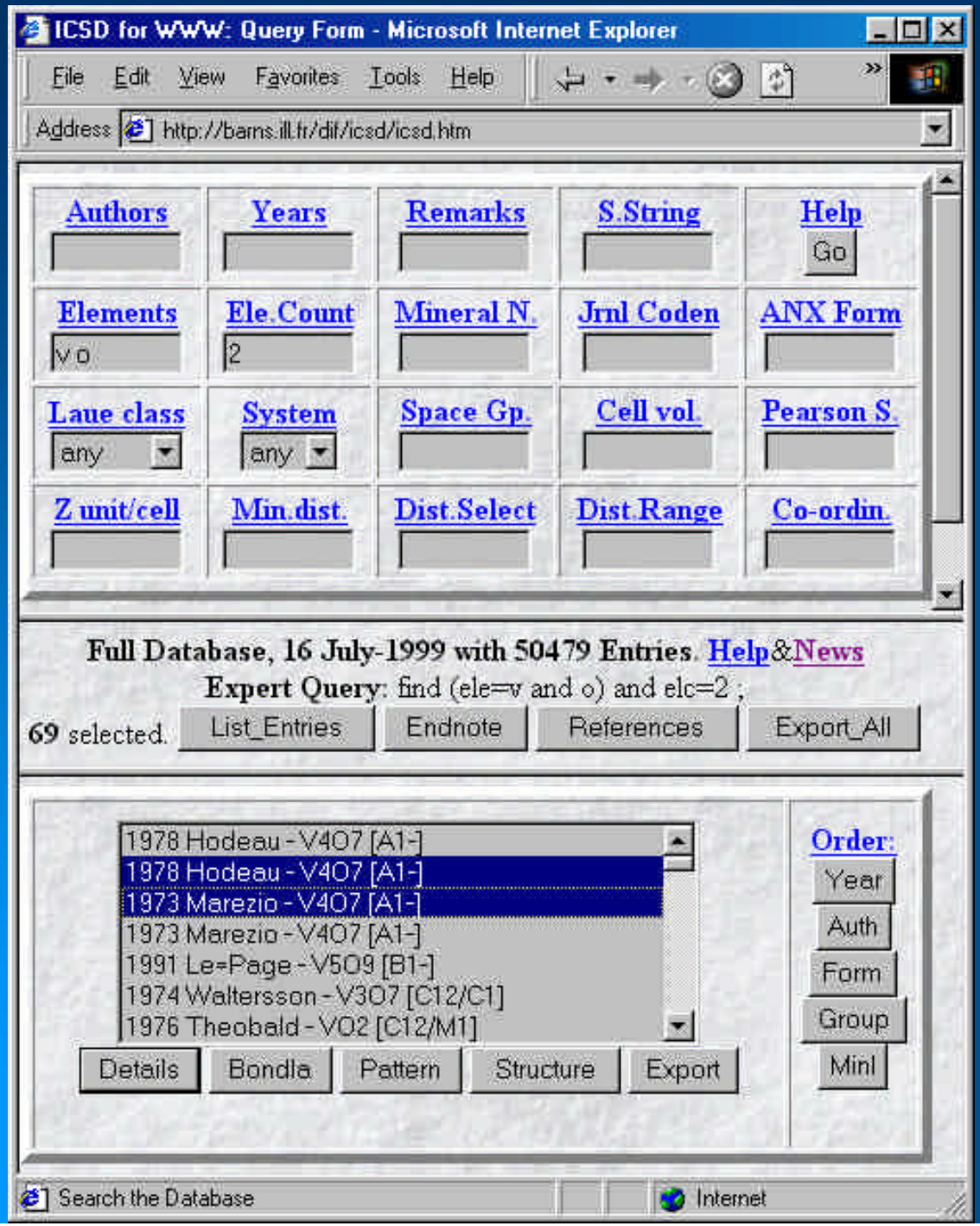

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Compare powder patterns for similar structures

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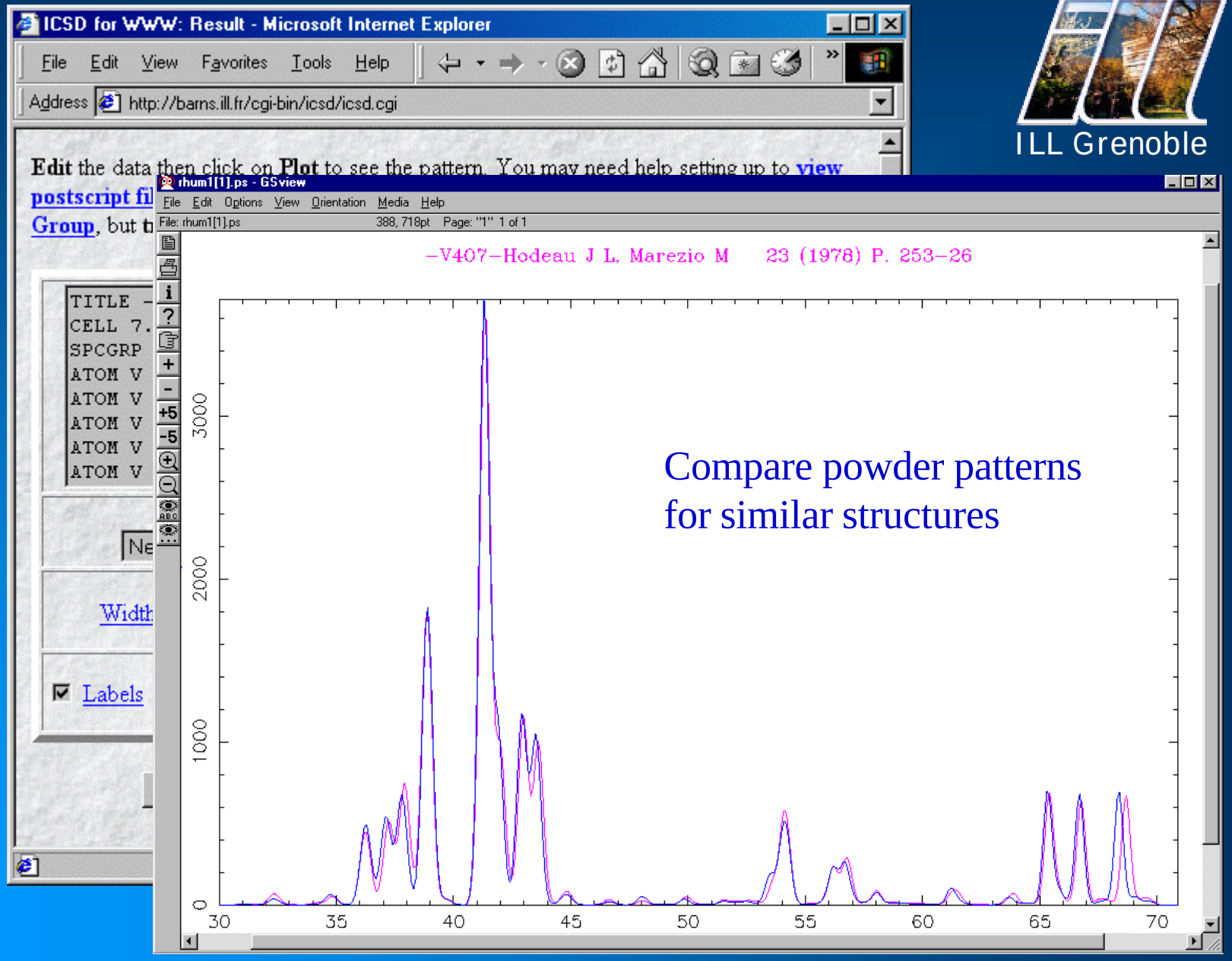

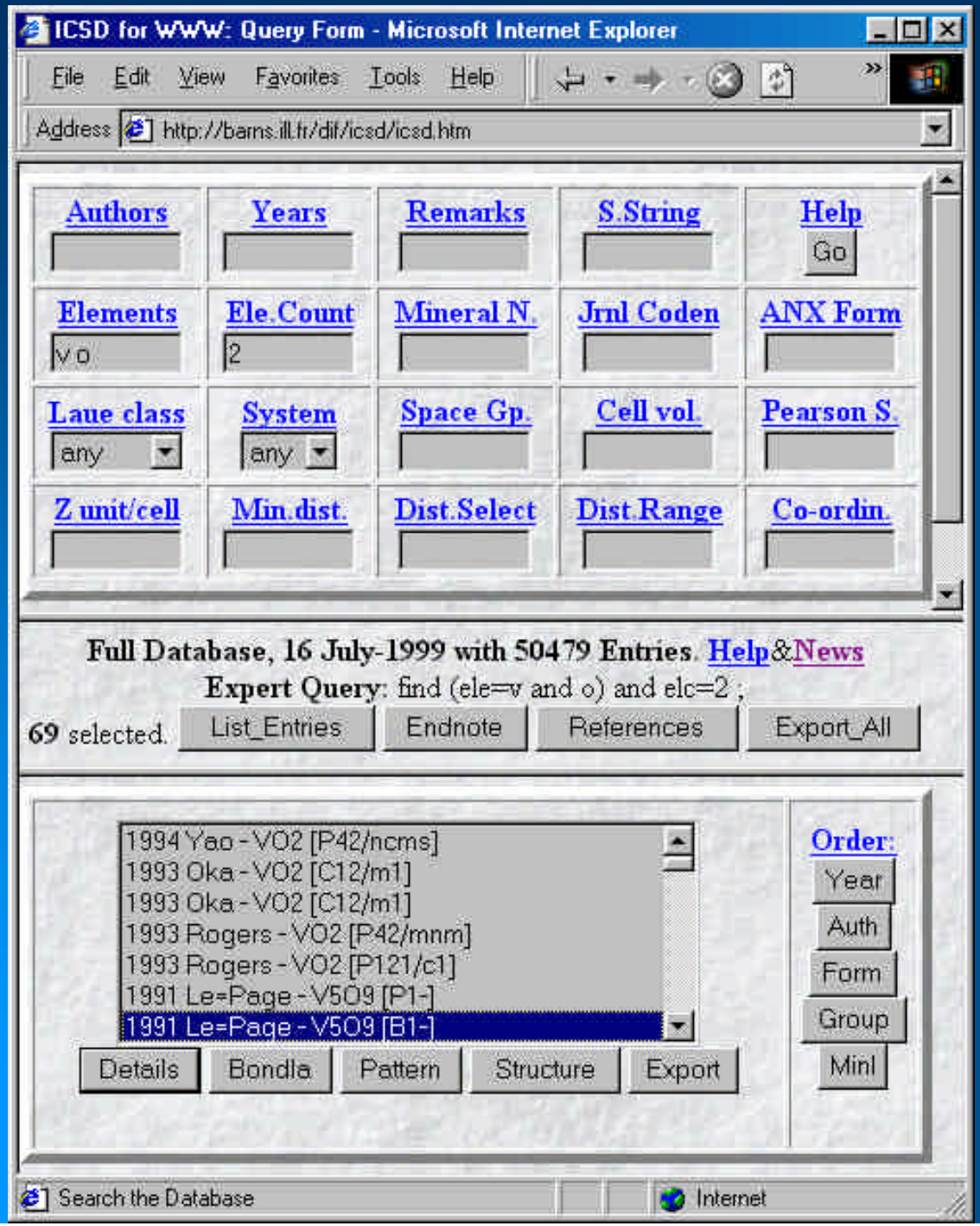

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Display a 3D structure

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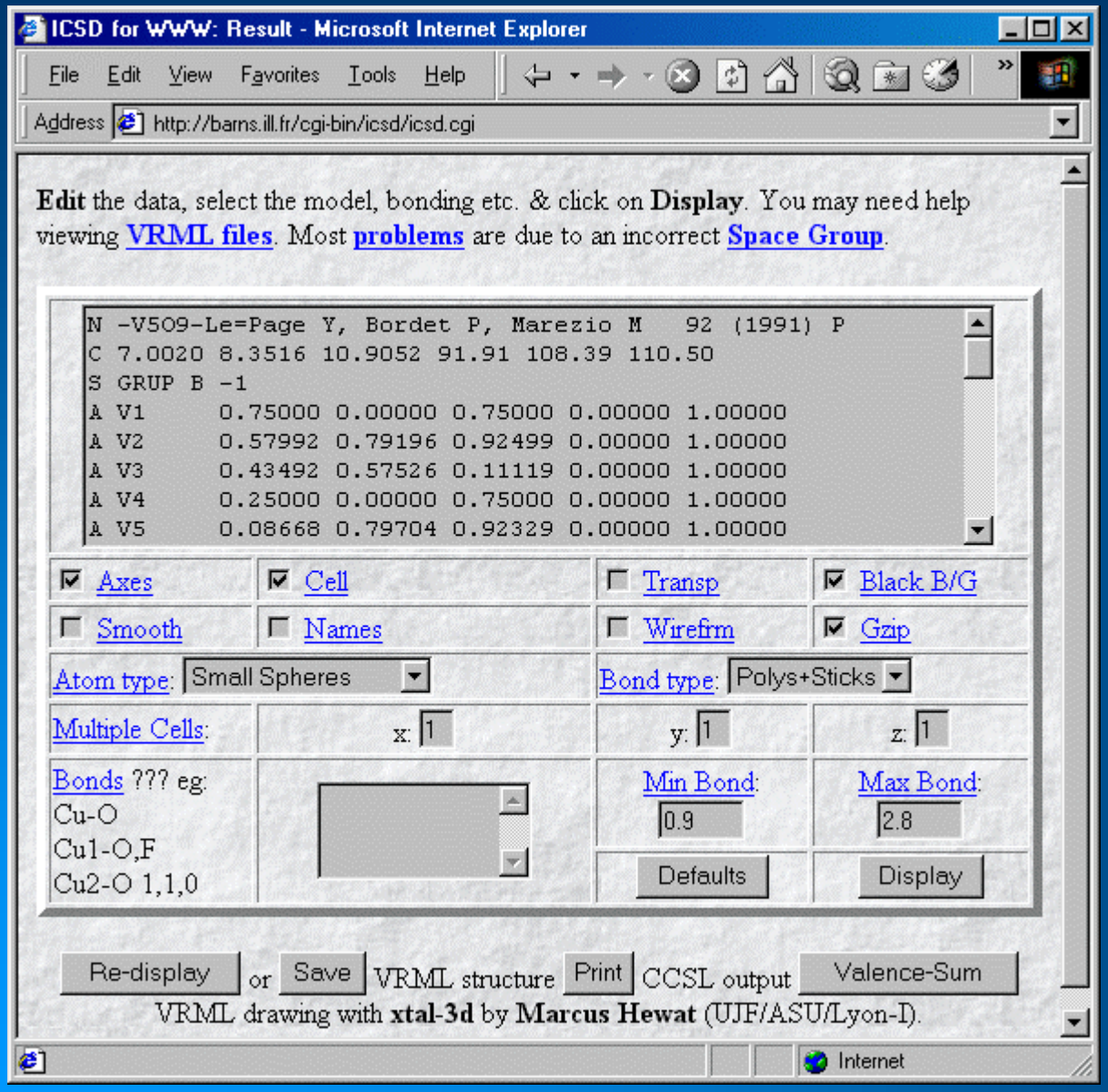

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Display a 3D structure

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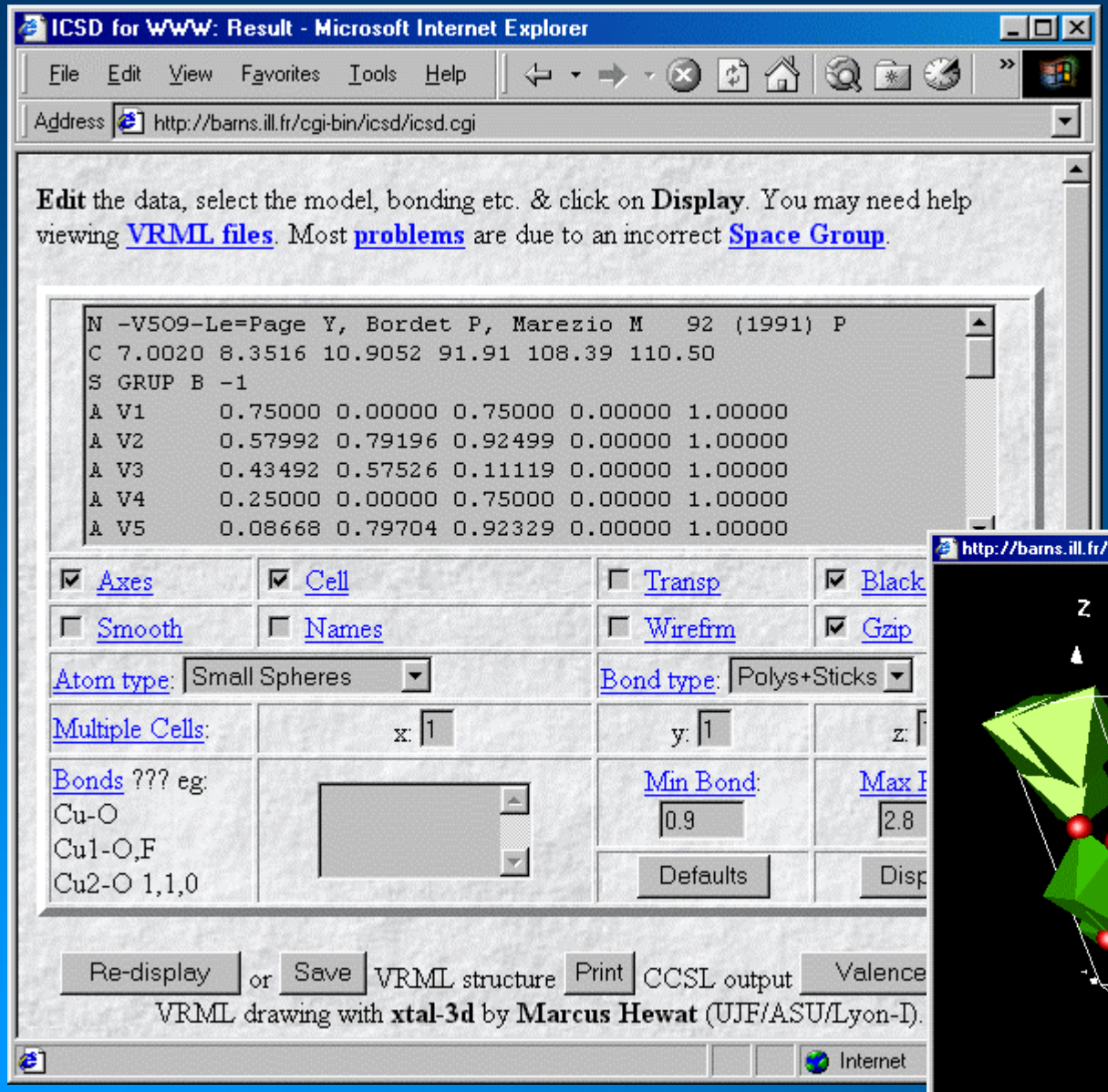

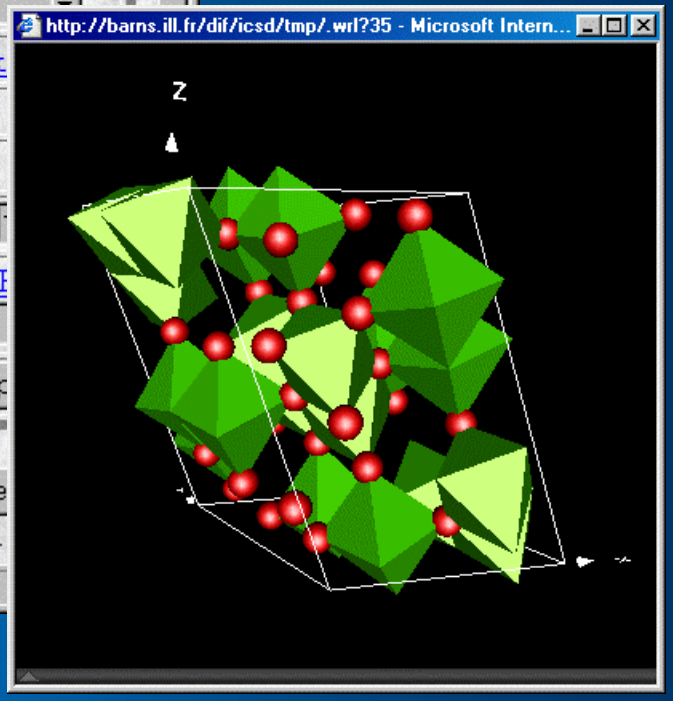

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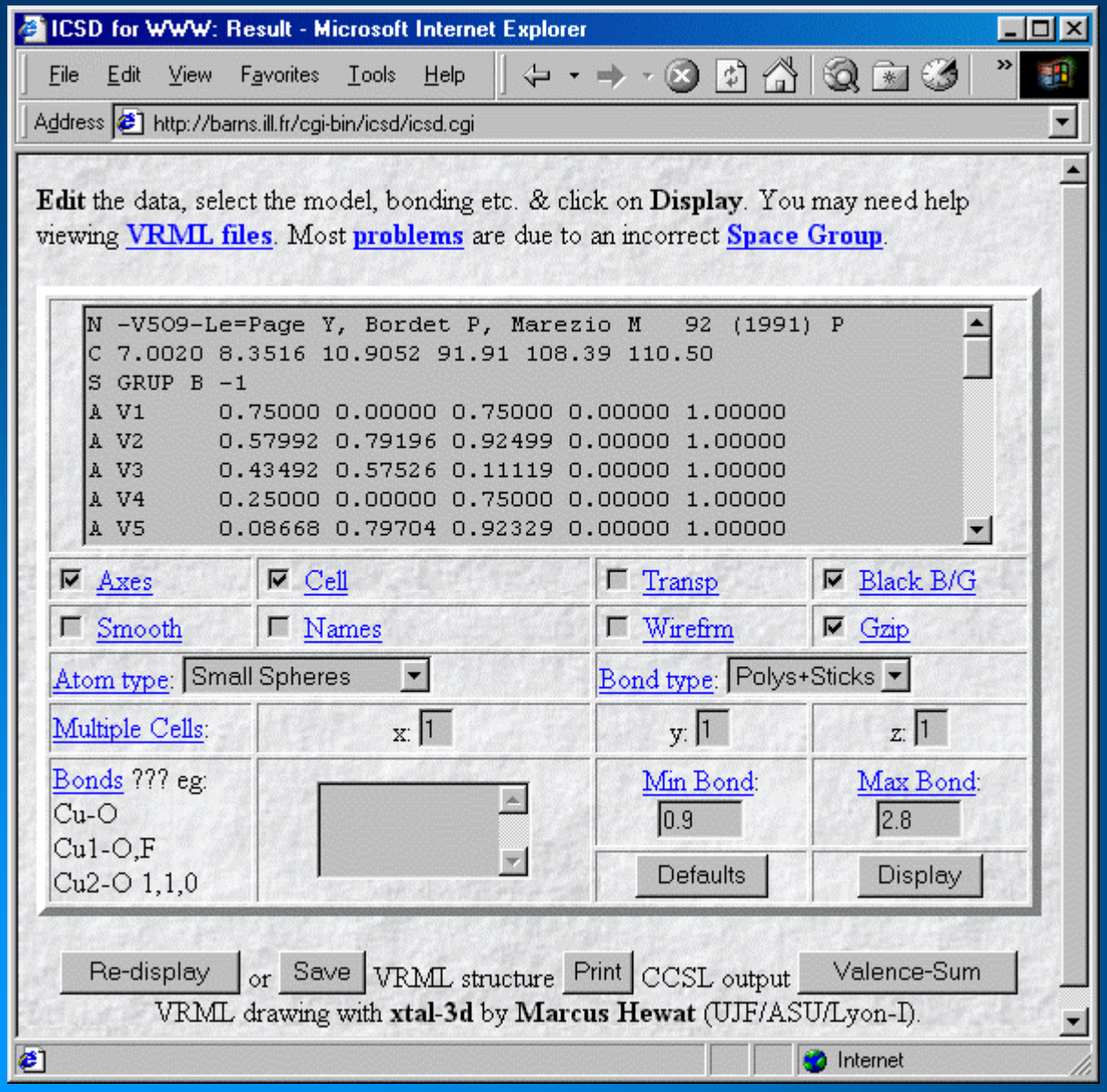

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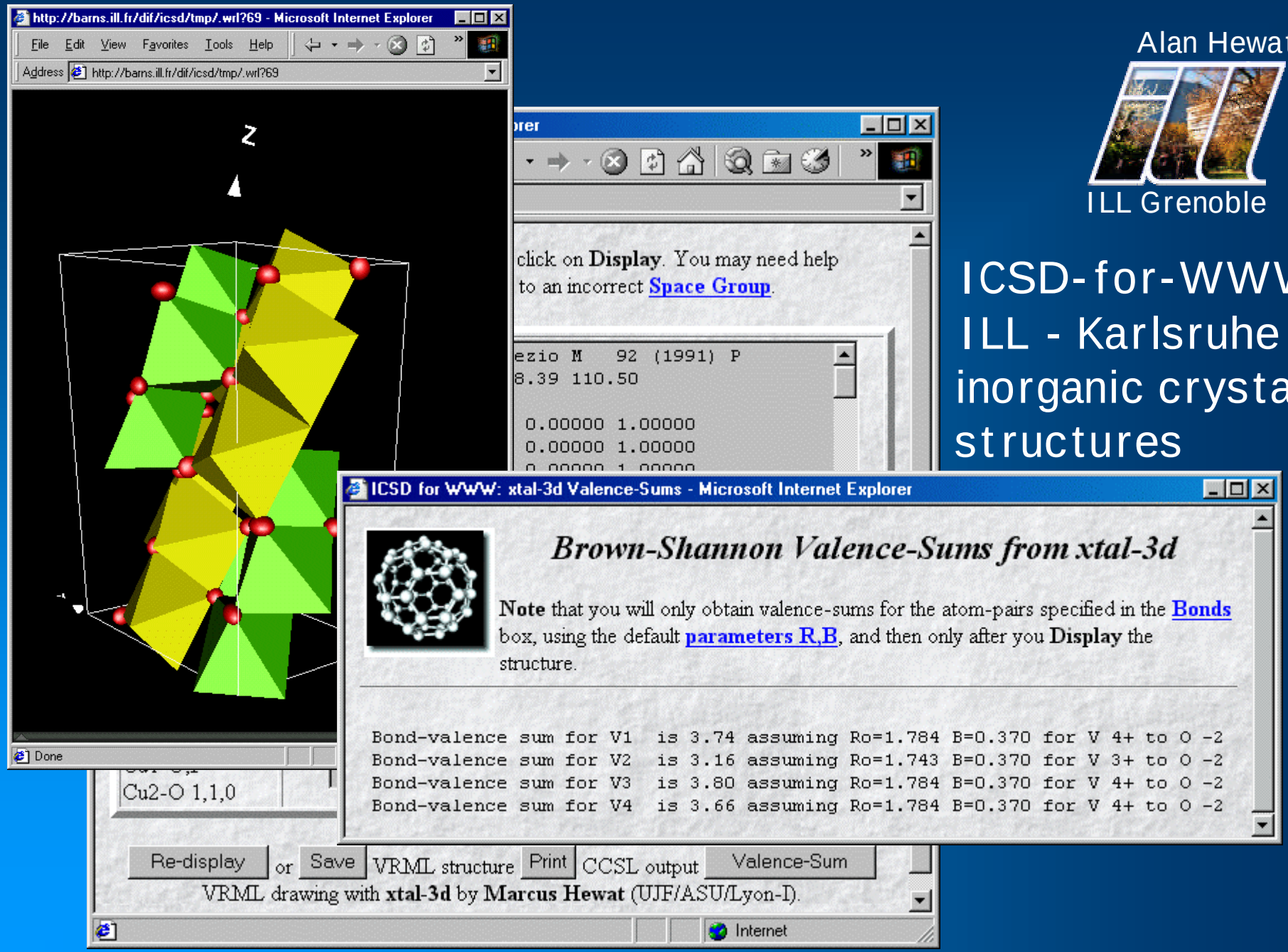
Calculate Brown-Shannon valence sums and color V^{3+} & V^{4+}



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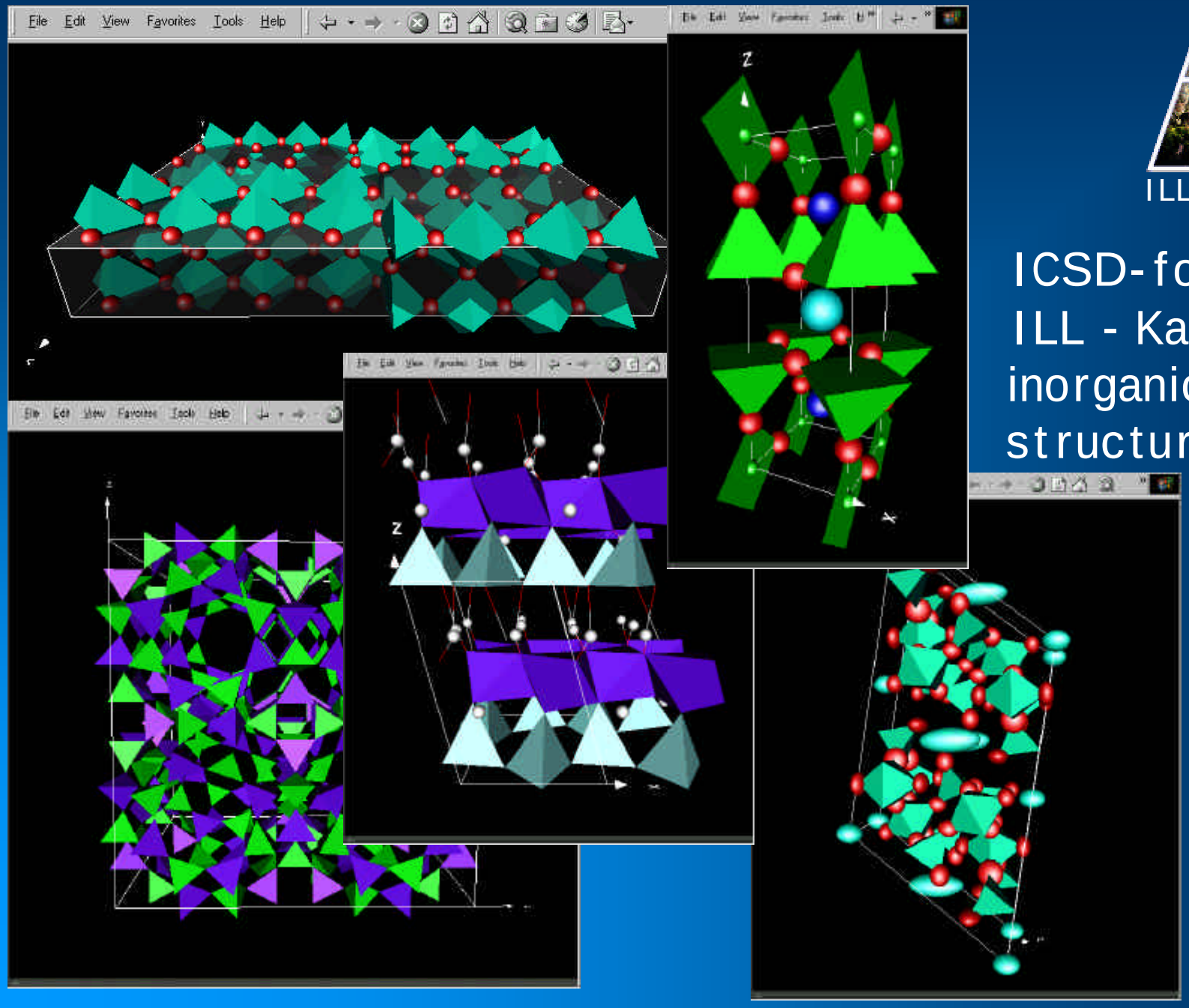

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What's New with ICSD-for-WWW

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Science 12 March 1999

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

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Laboratories running ICSD-for-WWW

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

What's New with ICSD-for-WWW

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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...

What's New with ICSD-for-WWW

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- Who Pays ?
  - National Grants eg
    -EPSRC Daresbury
    -New US Protein Data Base on WWW
  - Individual Labs.
    -Cost comparable to journal subscription
    -Ask your library to subscribe to ICSD-for-WWW
  - Individual users eg
    -cf ICSD-DOS license - locked to individual user/machine
  - Pay-Per-Use system
    -"Jeton" or "Token" system cf British Library

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- How do we collect and check data ?
  - Users enter new data via WWW form
    - New US Protein Data Base on WWW
  - Journal Editors enter data via WWW
    - In return for advertising the journal ?
  - Volunteers check new data
    - Already there are such volunteers
  - New automatic programs check data

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