

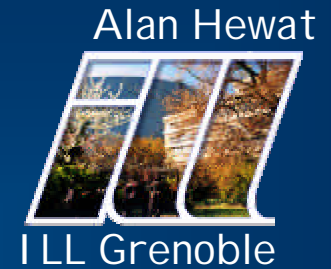
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Alan Hewat



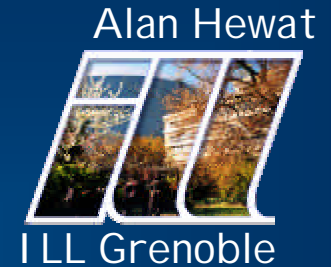
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```
...1011001010001001000100
010100100001001000...0101
011010...0100010010010010
10010001000010....0100101
001011001001010100...1011
0100101011...100100101010
101010101010010101...0010
01010100100...0100001...00
0100101...00101100101010
010101001000100...110010
0011...0010100100100101...
```

● Number Crunching

● Modelling

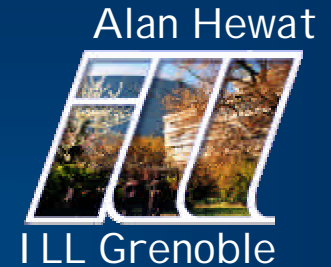
- Neutron Instruments
- Crystal Structures
- Lattice Vibrations
- Wave Functions
- ... etc ... etc

● Example

- Genetic Algorithms
for structure modelling

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- **Number Crunching**

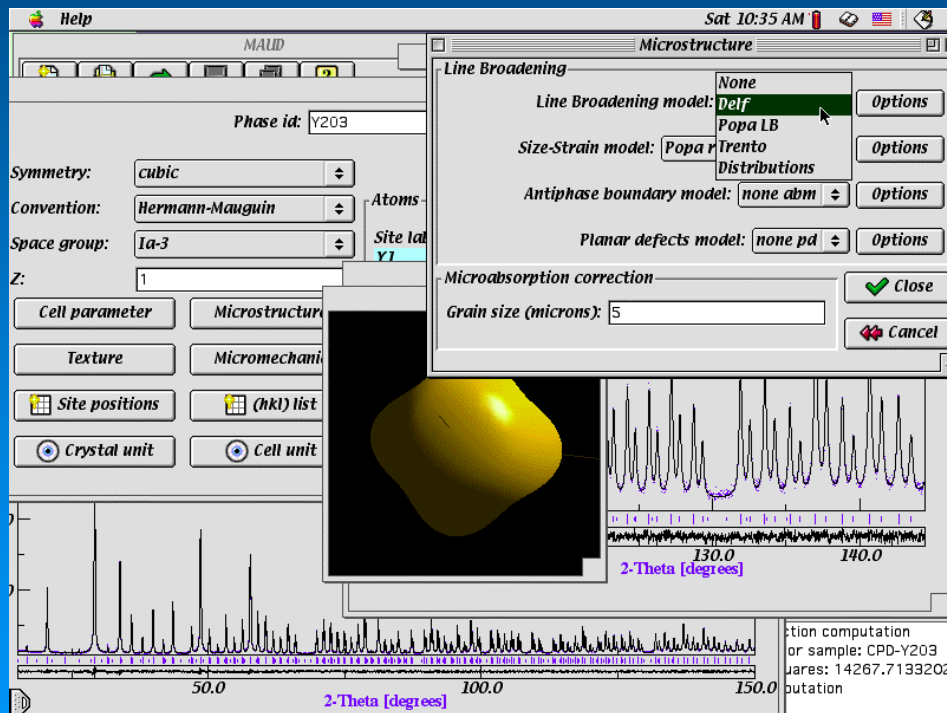
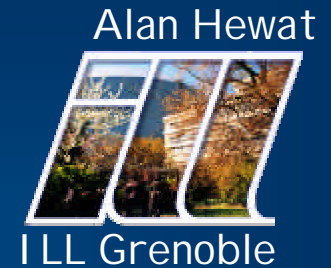
... is still an important application of computers,

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

- BARNES Data analysis via the WWW
- MAD-GUI Instrument control with Java

B.A.R.N.S. Welcome - Microsoft Internet Explorer

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Address <http://barns.ill.fr/>

WEB SERVER FOR I.L.L. APPLICATIONS
If you wish to use this service please enter your name and a nick-name

Last Name
 Nick Name Pwd

Application

ICSD for www

 **Netscape 3.01+ or MSIE 4.0+ is required !!!**

ICSD: Alan HEWAT hewat@ill.fr
 BARNs: Didier RICHARD richard@ill.fr



Alan Hewat



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Data Server

B.A.R.N.S give access to D3-Status - Microsoft Internet Explorer

Address: http://barns.ill.fr/cgi-bin/barns/nph-barns.pl?StartBarns=D3-Status&User=EVERY_bod&Habib=

D3 Status

<p>D3 Status Graphic Version 3.05</p> <p>User: tapan</p> <p>Sample: NaVO</p> <p>Input Stream: None None / None</p> <p>Output file: nav05v 40 lines</p> <p>*rte -1.00 -1.00 -9.00</p> <p>Time: 3000.0 s</p> <p>Rate: Unknown</p> <p>R: Unknown</p> <p>dR: Unknown</p> <p>Server is responding.</p>	<p style="text-align: center;">Primary Spectrometer</p> <p>Monochromator: Heusler Wavelength: 0.8788 Å Filter:</p> <p>Omega: 6.95 deg Theta: 13.91 deg Chi: -0.07 deg</p> <p>HFR: 0 MW Shutters: Closed Closed Mode: Automatic</p> <p>Polar Up: 0.9400+/-0.0010 Polar Down: -.9400+/-0.0010</p> <hr/> <p style="text-align: center;">Secondary Spectrometer</p> <p>Half-Shutter: None Sample Temp: 9999.99 K Field: 0.00 T</p> <p>Omega: -144.31 de Gamma: -24.38 deg Nu: -4.55 deg Phi: 0.00 deg</p> <table style="width: 100%;"> <tr> <td style="width: 50%; text-align: center;">Cryoflipper</td> <td style="width: 50%; text-align: center;">Cryomagnet</td> </tr> <tr> <td>LN2: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 70%, black 70%);"></div> 70%</td> <td>LN2: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 15%, black 15%);"></div> 15%</td> </tr> <tr> <td>LHe: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 70%, black 70%);"></div> 70%</td> <td>LHe: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 45%, black 45%);"></div> 45%</td> </tr> </table> <table style="width: 100%;"> <tr> <td style="width: 50%; text-align: center;">Cold Valve</td> <td style="width: 50%; text-align: center;">VTI</td> </tr> <tr> <td>Set Point: 1.2 Power: 29</td> <td>Reg. Temp: 9999.99 K</td> </tr> <tr> <td>Pressure: 1.2 Mode: Automatic</td> <td>Reg. Heater: 9999.99 *</td> </tr> </table> <p style="text-align: center;"> File Photo Help Halt </p> <p style="text-align: right;"> Mad Status @ 19-Jul-99 09:45:52 Cryo Status @ 1-Jul-1999 20:53:39 </p> <p style="text-align: center;">MAD is active</p>	Cryoflipper	Cryomagnet	LN2: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 70%, black 70%);"></div> 70%	LN2: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 15%, black 15%);"></div> 15%	LHe: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 70%, black 70%);"></div> 70%	LHe: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 45%, black 45%);"></div> 45%	Cold Valve	VTI	Set Point: 1.2 Power: 29	Reg. Temp: 9999.99 K	Pressure: 1.2 Mode: Automatic	Reg. Heater: 9999.99 *
Cryoflipper	Cryomagnet												
LN2: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 70%, black 70%);"></div> 70%	LN2: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 15%, black 15%);"></div> 15%												
LHe: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 70%, black 70%);"></div> 70%	LHe: <div style="width: 100px; height: 10px; background: linear-gradient(to right, blue 45%, black 45%);"></div> 45%												
Cold Valve	VTI												
Set Point: 1.2 Power: 29	Reg. Temp: 9999.99 K												
Pressure: 1.2 Mode: Automatic	Reg. Heater: 9999.99 *												

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Data Server

B.A.R.N.S give access to Ida - Microsoft Internet Explorer

Address http://barns.ill.fr/cgi-bin/barns/nph-barns.pl?StartBarns=Ida&User=EVERY_bod&Habib=



IDA (Internet Data Access)

Select Data by optional search-item

Instrument	Cycle	Year	Month	(ExperimentText)
d2b	3	1999	*	suard

Get a list matching selected items

Transfer the Data to LOCAL or BARNs machine

Cycle	Run (file)	to Run	compressed ?	Download ?
993			<input checked="" type="radio"/> yes <input type="radio"/> no	<input checked="" type="radio"/> yes <input type="radio"/> no

To restore data to your own station :

d2b SEARCH Result for suard

Cycle	Inst	from numer	to numer	from date	to date	string
993	d2b	034471	034475	28-May-99	28-May-99	suard suar
993	d2b	035233	034462	18-Jun-99	25-May-99	suard suar
993	d2b	036108	036112	15-Jul-99	15-Jul-99	suard suar

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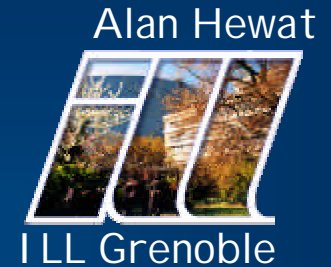
MAUD
Java GUI

The screenshot shows the MAUD Java GUI interface. The main window is titled 'MAUD' and has a menu bar with 'Help'. The status bar at the top right shows 'Sat 10:35 AM'. The 'Phase id' is 'Y203'. The 'Symmetry' is 'cubic', 'Convention' is 'Hermann-Mauguin', and 'Space group' is 'Ia-3'. The 'Z' value is '1'. There are buttons for 'Cell parameter', 'Texture', 'Site positions', 'Crystal unit', 'Microstructure', 'Micromechanics', '(hkl) list', and 'Cell unit'. A 'Microstructure' dialog box is open, showing 'Line Broadening' options: 'Line Broadening model' (Delf), 'Size-Strain model' (Popa r), 'Antiphase boundary model' (none abm), and 'Planar defects model' (none pd). There is also a 'Microabsorption correction' section with 'Grain size (microns): 5'. The dialog has 'Close' and 'Cancel' buttons. The background shows a 3D model of a yellow grain and a diffraction pattern plot with '2-Theta [degrees]' on the x-axis. The plot has markers at 50.0, 100.0, 130.0, and 150.0. A status bar at the bottom right shows 'Computation computation for sample: CPD-Y203' and 'Squares: 14267.7133202'.

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

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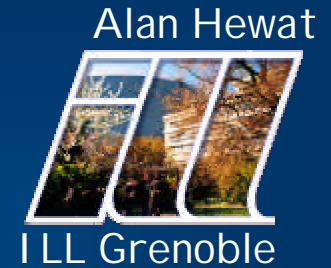
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- Experiments without local contacts ?
 - ... or even without a user manual ... ?
 - Or at least greater independence for users...
 - ...should result in better control of experiments and therefore better experiments...
- Ease of Use (Graphic User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

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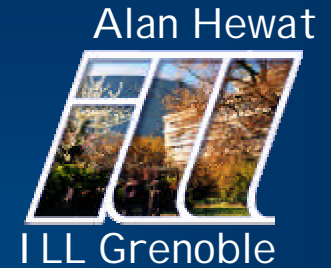
- What will have the greatest impact ?

INFORMATION !!

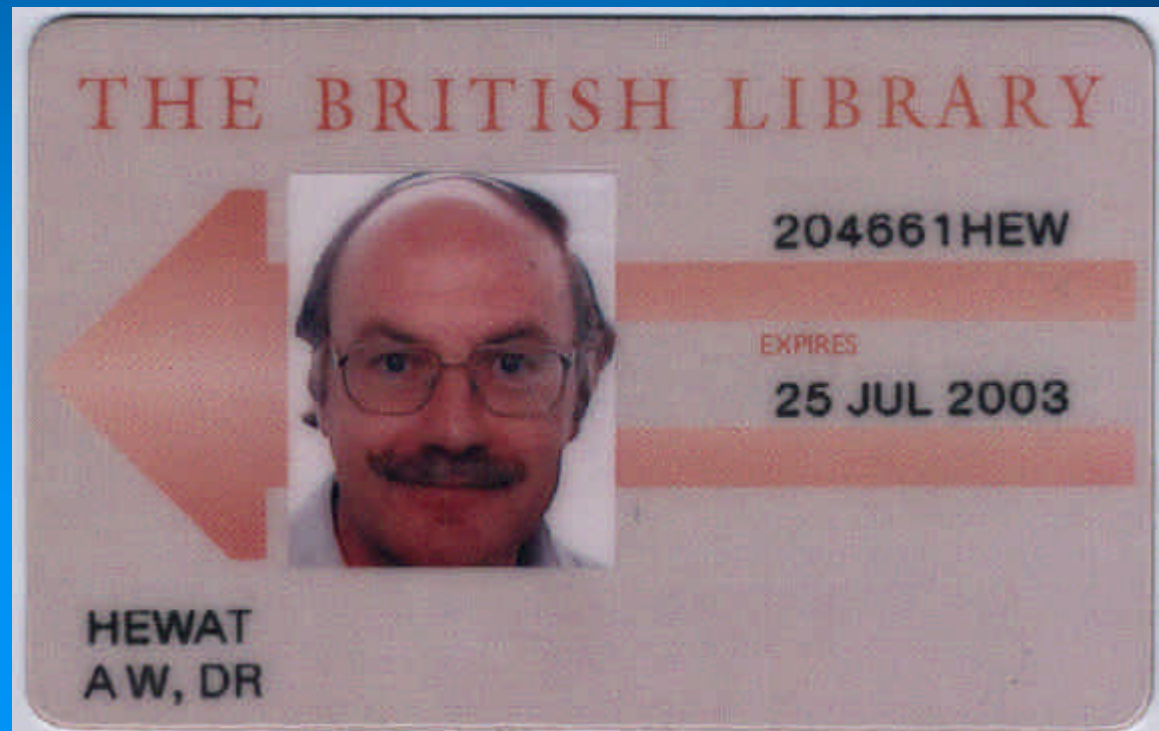
Knowledge is power ?

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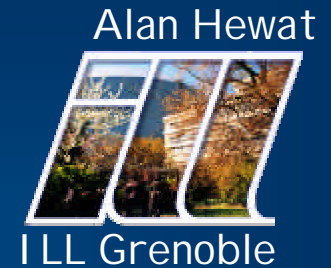


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Advanced Search

Field Qualifiers Search Terms: default operator is AND

ALL	▼	radaelli
AND	▼	ALL
AND	▼	ALL

Year Range

1996/1997	▲
1997/1998	
1998/1999	
Latest	▼

For example: To search for an article on solvent dioxide by A.Smith in the serial "Thin Solid Films"

Select field: Article Title-Serials and type in box 1: **solvent dioxide**

Select field: Author and type in box 2: **smith-a**

Select field: Serial Title and type in box 3: **thin solid films**

Run Search View Search History Clear Search

To save the edited search complete the details below and select Save

Search name:


Search type: Saved Search

Diary Search Daily Weekly Monthly


Day: Day:

e-mail to rio@esrf.fr Select format:


Save



Home



Search Selection



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Address 1=%28%28radaelli%29%29.ITOD%2CINUP.&op1=AND&d=DISC&p=1&r=0&f=S&u=%2FUserdevcgj%2FUserSearch

Search Results

Search Terms: " : 1=RADAELLI.ITOD,I NUP. : 2=1 "
Documents: 1 - 10 of 26

Select	Details
1	<i>Sr Substitution For. Ba in Y (Ba~1~xSr~x)~2Cu~3O~7-d At Varying</i> Licci, F. INTERNATIONAL JOURNAL OF MODERN PHYSICS B, 1999, VOL 13; NUMBER 9/10, page(s): 5
2	<i>Neutron-Diffraction Studies on the Magnetic Ordering Process in the Layered M...</i> Battle, P. D. JOURNAL- PHYSICAL SOCIETY OF JAPAN, 1999, VOL 68; NUMBER 4, page(s): 1462
3	<i>Wigner-crystal and bi-stripe models for the magnetic and crystallographic supers...</i> Radaelli, P. G. PHYSICAL REVIEW -SERIES B-, 1999, VOL 59; NUMBER 22, page(s): 14440-14450
4	<i>Spatial cross-over of polarons across the CMR transition in La~0~.~7~5Ca~0~.~...</i> Lanzara, A. JOURNAL OF SYNCHROTRON RADIATION, 1999, VOL 6; NUMBER 3, page(s): 776-778
5	<i>Nitric oxide and cardiovascular spectral components in the intact, sympathectom...</i> Radaelli, A. HIGH BLOOD PRESSURE AND CARDIOVASCULAR PREVENTION, 1996, VOL 5; NUMBER 3/SU
6	<i>Interference of the alarm reaction on the assessment of postural blood pressure c...</i> Terzoli, L. HIGH BLOOD PRESSURE AND CARDIOVASCULAR PREVENTION, 1999, VOL 5; NUMBER 3/SU
7	<i>Nitric oxide and cardiovascular spectral components in the intact, sympathectom...</i> Radaelli, A. HIGH BLOOD PRESSURE AND CARDIOVASCULAR PREVENTION, 1999, VOL 5; NUMBER 3/SU
8	<i>Influence of @b-adrenergic antagonists on cell proliferation rates in the kidney c...</i> Cardani, R. CHEMICOBIOLOGICAL INTERACTIONS, 1999, VOL 118; NUMBER 3, page(s): 217 - 231

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Advanced Search

Field Qualifiers **Search Terms: default operator is AND**

ALL	radaelli
AND ALL	stripes
AND ALL	

Year Range

All
1993/1994
1994/1995
1995/1996

For example: To search for an article on solvent dioxide by A.Smith in the serial "Thin Solid Films"
 Select field: Article Title-Serials and type in box 1: **solvent dioxide**
 Select field: Author and type in box 2: **smith-a**
 Select field: Serial Title and type in box 3: **thin solid films**

Run Search View Search History Clear Search

To save the edited search complete the details below and select Save

Search name:




Search type: Saved Search

Diary Search Daily Weekly Monthly

Day: Day:

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Search Results

Search Terms: " : 1=RADAELLI AND STRIPES : 2=1 "

Documents: 1 - 3 of 3

Select	Details
1	 <p><i>Stripe Structure and Non-Homogeneity of the CuO₂ Plane by Joint EXAFS and</i> Bianconi, A. JOURNAL DE PHYSIQUE 4, 1997, VOL 7; NUMBER 2; NUMB 4, page(s): C2-735-C2-740 Abstract</p>
2	 <p><i>Anomalous Jahn-Teller Distortions in La_{0.875}Ca_{0.125}MnO₃ System: A</i> Brunelli, M. JOURNAL OF SUPERCONDUCTIVITY, 1997, VOL 10; NUMBER 4, page(s): 315-318</p>
3	 <p><i>Stripe Structure and Non-Homogeneity of the CuO₂ Plane by Joint EXAFS and</i> Bianconi, A. JOURNAL DE PHYSIQUE 4, 1997, VOL 7; NUMBER 2; NUMB 2, page(s): C2-735-C2-740 Abstract</p>

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Full Details

Article Title Stripe Structure and Non-Homogeneity of the CuO~2 Plane by Joint EXAFS and Diffraction

Author(s) Bianconi, A. Saini, N. L. Lanzara, A. Lusignoli, M. Rossetti, T. Radaelli, P. G. Bordet, P. Kwick, A. Oyanagi, H.

Volume Title Proceedings of the 9th International Conference on X-Ray Absorption Fine Structure

Serial Title JOURNAL DE PHYSIQUE 4

Unique Item Number RN034826547 5040.214000

Volume Editor(s) Goulon, J.

Publisher EDITIONS DE PHYSIQUE

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Country of Publication France **Frequency of Publication** Bi-monthly **ISSN** 1155-4339

ISBN None **Dewey Classification Code** 530 **Language** English

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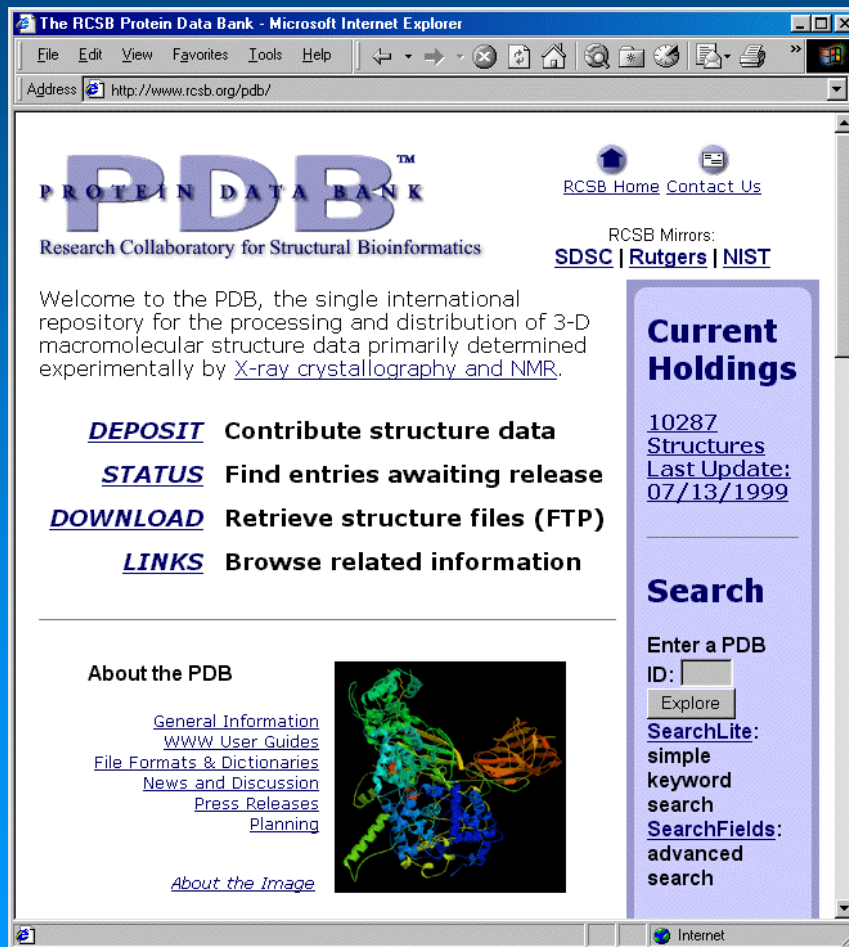
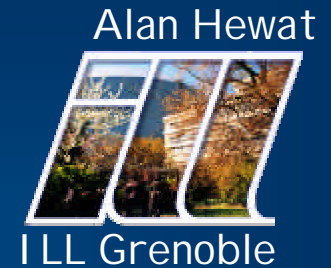


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- WWW Data Bases

- Advantages

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- 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

The RCSB Protein Data Bank - Microsoft Internet Explorer

Address <http://www.rcsb.org/pdb/>

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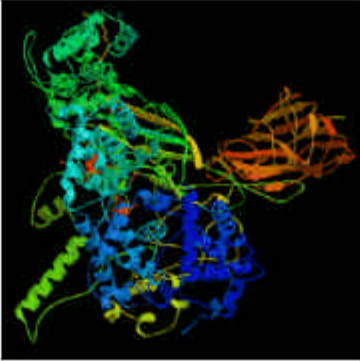
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 Authors of primary citation only!

Contains Chain Type:

	Yes	No	ignore		Yes	No	ignore
Protein:	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	DNA:	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Enzyme:	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	RNA:	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Glycoprotein:	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>	DNA/RNA hybrid:	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
Carbohydrate:	<input type="radio"/>	<input type="radio"/>	<input type="radio"/>				

Compound Information:

PDB HEADER:

Exp. Technique:

Text Search:

Done Internet

PDB Query Result - Microsoft Internet Explorer

Address: <http://www.rcsb.org/pdb/cgi/resultBrowser.cgi>

PDB
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Query Result Browser

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Your query found 6 structures and you have selected 0 structures so far. You can select specific structures by clicking on the checkbox next to their id. If you do not select any structures, certain options will default to all structures. To examine an individual structure select the Explore link!

Pull down to select option:

<input type="checkbox"/>	1LZN	Deposited: 03/23/1999 Exp. Method: Neutron Diffraction Resolution: 1.70 Å	{ EXPLORE }
<i>Classification</i> Hydrolase			
<i>Compound</i> Mol_Id: 1; Molecule: Lysozyme; Chain: A; Ec: 3.2.1.17; Biological_Unit: Monomer; Other_Details: Nitrate Ions Present			
<input type="checkbox"/>	1NTP	Deposited: 09/16/1987 Exp. Method: Neutron Diffraction Resolution: 1.80 Å	{ EXPLORE }
<i>Classification</i> Hydrolase (Serine Proteinase)			
<i>Compound</i> Modified β Trypsin (Monoisopropylphosphoryl Inhibited) (E.C. 3.4.21.4) (Neutron Data)			
<input type="checkbox"/>	2MB5	Deposited: 10/11/1989 Exp. Method: Neutron Diffraction Resolution: 1.80 Å	{ EXPLORE }
<i>Classification</i> Oxygen Storage			
<i>Compound</i> Myoglobin (Carbonmonoxymyoglobin) (Neutron Study)			
<input type="checkbox"/>	3INS	Deposited: 10/14/1988 Exp. Method: Neutron Diffraction; X-ray Diffraction Resolution: 1.50 Å	{ EXPLORE }
<i>Classification</i> Hormone			
<i>Compound</i> 2Zn-Insulin (Joint X-Ray and Neutron Refinement)			
<input type="checkbox"/>	5RSA	Deposited: 04/29/1985 Exp. Method: Neutron Diffraction; X-ray Diffraction Resolution: 2.00 Å	{ EXPLORE }
<i>Classification</i> Hydrolase (Nucleic Acid, RNA)			
<i>Compound</i> Ribonuclease A (E.C. 3.1.27.5) (Joint Neutron and X-Ray)			
<input type="checkbox"/>	6RSA	Deposited: 02/25/1986 Exp. Method: Neutron Diffraction; X-ray Diffraction Resolution: 2.00 Å	{ EXPLORE }
<i>Classification</i> Hydrolase (Nucleic Acid, RNA)			

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Structure Explorer - 1LZN - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <http://www.rcsb.org/pdb/cgi/explore.cgi?pid=14410932458001&page=0&pdbid=1LZN>

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[Geometry](#)
[Other Sources](#)
[Sequence Details](#)

Explore

[SearchLite](#) [SearchFields](#)

Compound: **Mol_Id:** 1; **Molecule:** Lysozyme; **Chain:** A; **Ec:** 3.2.1.17; **Biological_Unit:** Monomer; **Other_Details:** Nitrate Ions Present

Authors: C. I. Bon, M. S. Lehmann, C. Wilkinson

Exp. Method: Neutron Diffraction

Classification: Hydrolase

Source: Gallus Gallus

Primary Citation: Bon, C., Lehmann, M. S., Wilkinson, C.: Quasi-Laue Neutron Diffraction Study of the Water Arrangement in Crystals of Triclinic Lysozyme from Hen Egg-White Lysozyme. *Acta Crystallogr., Sect.D* D55 pp. 978 (1999) [[Medline](#)]

Deposition Date: 03/23/1999 *Release Date:* 04/01/1999

Resolution [Å]: 1.70 *R-Value:* 0.204

Space Group: P 1

Unit Cell: *dim [Å]:* *a* 27.28 *b* 32.04 *c* 34.27
angles [°]: *alpha* 88.80 *beta* 108.80 *gamma* 111.60

Polymer Chains: A *Residues:* 129

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

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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**

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[Other Sources](#)

[Sequence Details](#)

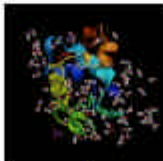
[SearchLite](#) [SearchFields](#)

Interactive 3D Display:

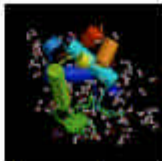
Choose from the following [display options](#):

- [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):


Still Images:




[Ribbons \(250x250\)](#)



[Cylinders \(250x250\)](#)



[Ribbons \(500x500\)](#)



[Cylinders \(500x500\)](#)

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

PDB
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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**

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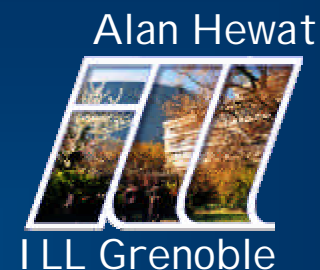
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Display Options

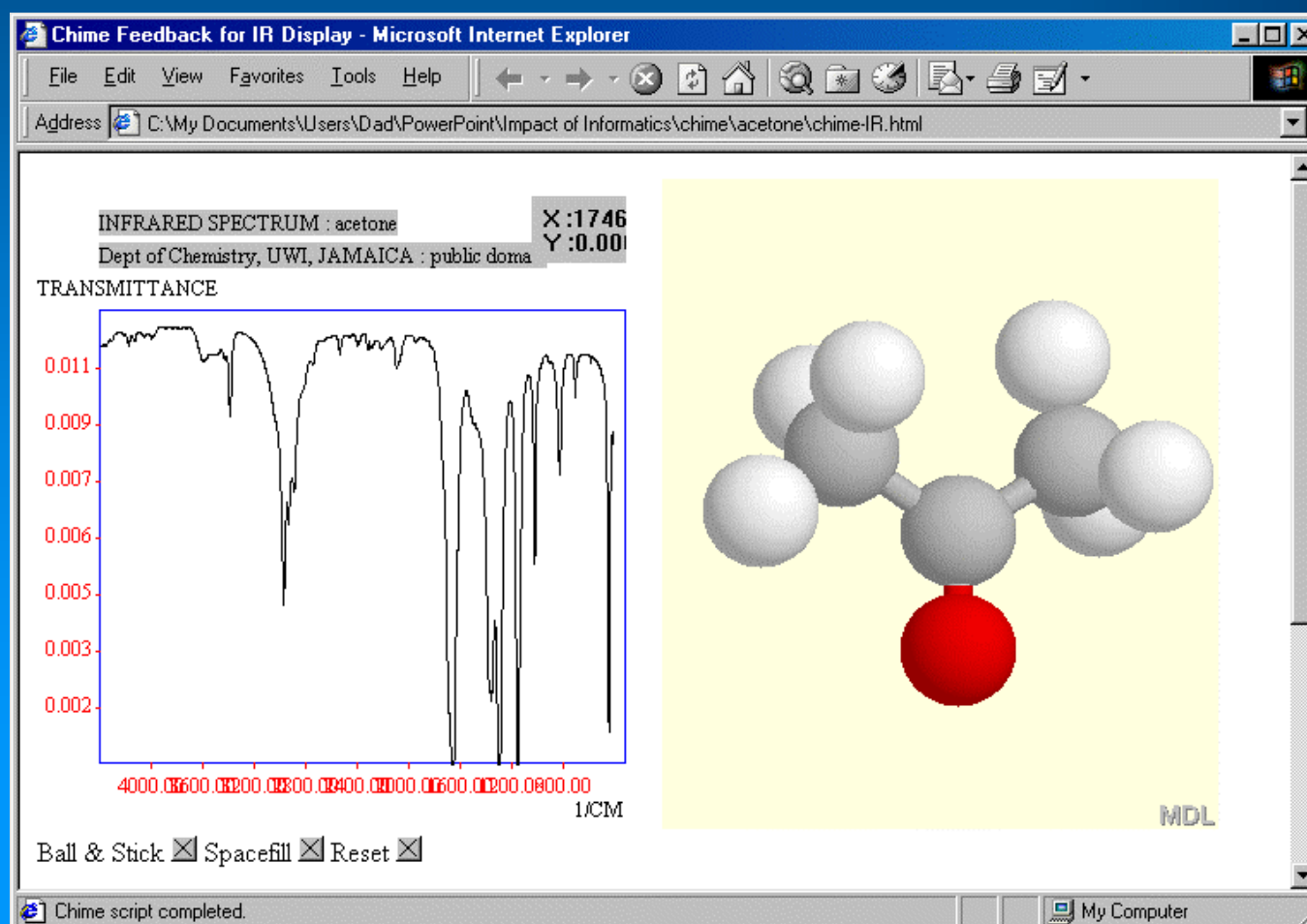
- VRML
- RASMOL
- CHIME
- JAVA

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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)

ICSD for WWW: Query Form - Microsoft Internet Explorer

Address: <http://barns.ill.fr/dif/icsd/icsd.htm>

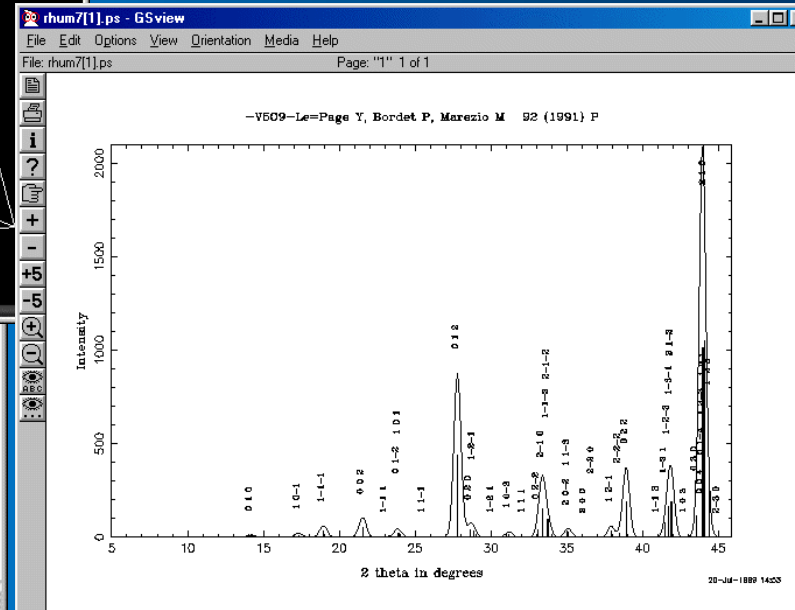
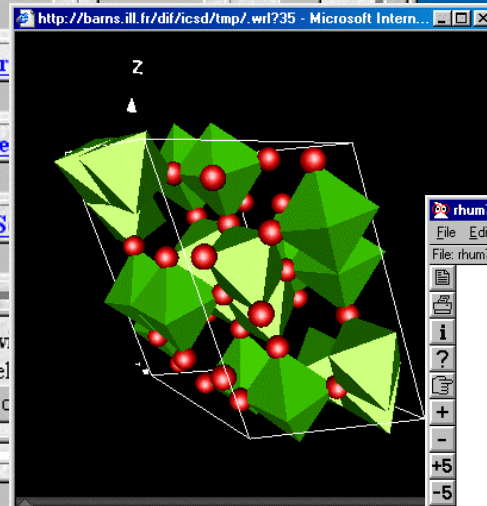
Search filters: Authors, Years, Remarks, S.String, Help, Elements, Ele.Count, Miner, Laue class, System, Space, Z unit/cell, Min.dist., Dist.S.

Full Database, 16 July-1999 w
Expert Query: find (el)
69 selected. List_Entries Endnc

Search results:
1994 Yao - VO2 [P42/ncms]
1993 Oka - VO2 [C12/m1]
1993 Oka - VO2 [C12/m1]
1993 Rogers - VO2 [P42/mnm]
1993 Rogers - VO2 [P121/c1]
1991 Le=Page - V509 [P1-]
1991 Le=Page - V509 [B1-]

Buttons: Details, Bondla, Pattern, Structure, Export, Year, Auth, Form, Group, Mini

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Address <http://barns.ill.fr/dif/icsd/icsd.htm>

Authors <input type="text"/>	Years <input type="text"/>	Remarks <input type="text"/>	S.String <input type="text"/>	Help <input type="button" value="Go"/>
Elements <input type="text" value="v o"/>	Ele. Count <input type="text" value="2"/>	Mineral N. <input type="text"/>	Jrnl Coden <input type="text"/>	ANX Form <input type="text"/>
Laue class <input type="text" value="any"/>	System <input type="text" value="any"/>	Space Gp. <input type="text"/>	Cell vol. <input type="text"/>	Pearson S. <input type="text"/>
Z unit/cell <input type="text"/>	Min. dist. <input type="text"/>	Dist. Select <input type="text"/>	Dist. Range <input type="text"/>	Co-ordin. <input type="text"/>

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Expert Query: find (ele=v and o) and elc=2 ;

69 selected.

<http://barns.ill.fr/dif/icsd/coordn.html> Internet

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Address: <http://barns.ill.fr/dif/icسد/icسد.htm>

Authors <input type="text"/>	Years <input type="text"/>	Remarks <input type="text"/>	S.String <input type="text"/>	Help <input type="button" value="Go"/>
Elements <input type="text" value="V o"/>	Ele.Count <input type="text" value="2"/>	Mineral N. <input type="text"/>	Jrnl Coden <input type="text"/>	ANX Form <input type="text"/>
Laue class <input type="text" value="any"/>	System <input type="text" value="any"/>	Space Gp. <input type="text"/>	Cell vol. <input type="text"/>	Pearson S. <input type="text"/>
Z unit/cell <input type="text"/>	Min.dist. <input type="text"/>	Dist.Select <input type="text"/>	Dist.Range <input type="text"/>	Co-ordin. <input type="text"/>

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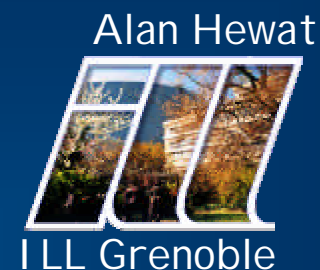
Horiuchi,H. Morimoto,N. Tokonami,M. (1976) J.Solid State Chem. 17 407-424
Crystal structures of Vn O2n-1 (2<n<7)

Horiuchi,H. Morimoto,N. Tokonami,M. (1976) J.Solid State Chem. 17 407-424
Crystal structures of Vn O2n-1 (2<N<7)

Horiuchi,H. Morimoto,N. Tokonami,M. (1976) J.Solid State Chem. 17 407-424
Crystal structures of Vn O2n-1 (2<N<7)

Theobald,F. Cabala,R. Bernard,J. (1976) J.Solid State Chem. 17 431-438
Essai sur la structure de V O2 (B)

<http://barns.ill.fr/dif/icسد/elements.html> Internet



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Authors <input type="text"/>	Years <input type="text"/>	Remarks <input type="text"/>	S.String <input type="text"/>	Help <input type="button" value="Go"/>
Elements <input type="text" value="v o"/>	Ele. Count <input type="text" value="2"/>	Mineral N. <input type="text"/>	Jrnl Coden <input type="text"/>	ANX Form <input type="text"/>
Laue class <input type="text" value="any"/>	System <input type="text" value="any"/>	Space Gp. <input type="text"/>	Cell vol. <input type="text"/>	Pearson S. <input type="text"/>
Z unit/cell <input type="text"/>	Min. dist. <input type="text"/>	Dist. Select <input type="text"/>	Dist. Range <input type="text"/>	Co-ordin. <input type="text"/>

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69 selected.

<http://barns.ill.fr/dif/icsd/coordn.html> Internet

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Authors	Years	Remarks	S.String	Help Go
Elements v o	Ele. Count 2	Mineral N.	Jrnl Coden	ANX Form
Laue class any	System any	Space Gp.	Cell vol.	Pearson S.
Z unit/cell	Min. dist.	Dist. Select	Dist Range	Co-ordin.

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ICSD Choose a format & re-print these Details or Export the file.

Please tell hewat@ill.fr of any errors in these format translations. Take care in particular to check the space group symbol, occupation numbers and anisotropic temperature factors. ICSD sometimes reports Beta(i,j) which are not acceptable in some formats (These **Beta(i,j)** have not been converted to Bij or Uij).

COL ICSD Collection Code 66584 (DATE=R940119/U 0 REL= 35915/
 NAME Vanadium oxide (5/9)
 FORM V5 09
 = 09 V5
 TITL Valence ordering in V5/505/9 below 120K
 AUT Le-Page Y, Bordet P, Marezio M
 REF JSSCB 92 (1991) P. 380-385
 JRNL Journal of Solid State Chemistry
 CELL A=7.0020(20) B=8.3516(20) C=10.9052(23) a=91.91(2) a=108.39(2)
 GA=110.50(2) V=559.4 Z=4
 SYM x,y,z
 SYM -x,-y,-z
 SGR B -1 (0)

PARM	Atom	Nr	Ox	Wy	x	y	z
V	1	+3.6	2F	0.75	0.0	0.75	
V	2	+3.6	4I	0.57992(7)	0.79196(5)	0.92499(4)	
V	3	+3.6	4I	0.43492(7)	0.57526(5)	0.11119(4)	
V	4	+3.6	2F	0.25	0.0	0.75	
V	5	+3.6	4I	0.08668(7)	0.79704(5)	0.92329(4)	
V	6	+3.6	4I	0.93541(7)	0.57951(5)	0.10855(4)	
O	1	-2	4I	0.4864(3)	0.92074(22)	0.29249(17)	
O	2	-2	4I	0.3027(3)	0.67735(21)	0.45282(17)	
O	3	-2	4I	0.3440(3)	0.86266(21)	0.87832(17)	
O	4	-2	4I	0.1759(3)	0.63329(21)	0.04135(16)	
O	5	-2	4I	0.2119(3)	0.97698(21)	0.06285(16)	
O	6	-2	4I	0.0485(3)	0.75928(21)	0.23640(16)	
O	7	-2	4I	0.8721(3)	0.54041(20)	0.40543(16)	

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Address <http://barns.ill.fr/dif/icsd/icsd.htm>

Authors	Years	Remarks	S.String	Help Go
Elements v o	Ele. Count 2	Mineral N.	Jrnl Coden	ANX Form
Laue class any	System any	Space Gp.	Cell vol.	Pearson S.
Z unit/cell	Min. dist.	Dist. Select	Dist Range	Co-ordin.

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69 selected. [List_Entries](#) [Endnote](#) [References](#) [Export_All](#)

1994 Yao - VO2 [P42/ncms] 1993 Oka - VO2 [C12/m1] 1993 Oka - VO2 [C12/m1] 1993 Rogers - VO2 [P42/mnm] 1993 Rogers - VO2 [P121/c1] 1991 Le-Page - V509 [P1-] 1991 Le-Page - V509 [B1-]	Order: Year Auth Form Group Mini
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By default bonds are calculated for a sphere up to 1.25 times the combined ionic radii IR between all ion pairs. You may enter a new sphere radius eg 3.0 or 1.4*IR and a pair of ions eg Cu-O (leave it blank if you want all ion pairs) and re-calculate bond lengths (with angles if required).

Max. bond sphere: between ions: with angles ->

Distances in COL= 66584 (REL= 35915)
 V5 09
 from: V to: 0
 Dmin: 0.01000 Dmax: 1.25000*IR coordination 1 to 999

----- Interatomic distances -----

Origin	Sphere	Distances to neighbours (distance, atom, identifier)							
V 1	2.275	1.923 0 1	1.923 0 1	1.967 0 5	1.967 0 5				
		1.979 0 6	1.979 0 6						
V 2	2.275	1.873 0 3	1.931 0 8	1.938 0 5	1.997 0 6				
		2.051 0 2	2.052 0 7						
V 3	2.275	1.776 0 9	1.879 0 8	1.962 0 7	1.968 0 4				
		2.102 0 2	2.135 0 7						
V 4	2.275	1.939 0 3	1.939 0 3	1.940 0 1	1.940 0 1				
		1.964 0 8	1.964 0 8						
V 5	2.275	1.851 0 5	1.889 0 1	1.916 0 3	2.022 0 2				
		2.031 0 4	2.084 0 9						
V 6	2.275	1.777 0 6	1.948 0 9	1.961 0 4	1.984 0 7				
		2.011 0 2	2.114 0 4						

----- Bonding angles -----

Origin	Angles to neighbours									
V 1	179.98 0 1 0 1	87.76 0 1 0 5	92.24 0 1 0 5							
	91.15 0 1 0 6	88.85 0 1 0 6	92.24 0 1 0 5							
	87.76 0 1 0 5	88.85 0 1 0 6	91.15 0 1 0 6							
	180.00 0 5 0 5	94.06 0 5 0 6	85.94 0 5 0 6							
	85.94 0 5 0 6	94.06 0 5 0 6	179.98 0 6 0 6							
V 2	96.43 0 3 0 8	92.96 0 3 0 5	89.00 0 3 0 6							
	170.17 0 3 0 2	90.28 0 3 0 7	97.37 0 8 0 5							
	173.32 0 8 0 6	88.83 0 8 0 2	85.07 0 8 0 7							

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Address <http://barns.ill.fr/dif/icsd/icsd.htm>

Authors	Years	Remarks	S.String	Help Go
Elements v o	Ele. Count 2	Mineral N.	Jrnl Coden	ANX Form
Laue class any	System any	Space Gp.	Cell vol.	Pearson S.
Z unit/cell	Min. dist.	Dist. Select	Dist Range	Co-ordin.

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<ul style="list-style-type: none"> 1978 Hodeau - V407 [A1-] 1978 Hodeau - V407 [A1-] 1973 Marezio - V407 [A1-] 1973 Marezio - V407 [A1-] 1991 Le=Page - V509 [B1-] 1974 Waltersson - V307 [C12/C1] 1976 Theobald - VO2 [C12/M1] 	<p>Order:</p> <p>Year</p> <p>Auth</p> <p>Form</p> <p>Group</p> <p>Mini</p>
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Note: You can display bond-lengths or structures for **only a single entry at a time**, but you can calculate powder patterns for several simultaneously. (Only 3 can be plotted). Choose any 2 entries with the same space group to **compare structure co-ordinates**.

1978	Hodeau J L, Marezio M
# 1772	V4O7 - Vanadium oxide (4/7) - low-temperature phase ()
Al- (0)	A=5.503(1) B=6.997(2) C=12.256(2) AL=94.86(2) BE=95.17(1) GA=109.39(1) V=440.0
R= 0.04	J.Solid State Chem. 23 (1978) P. 253-263 Remarks: TEM 120

1973	Marezio M, McWhan D B, Dernier P D, Remeika J P
# 7423	V4O7 - VANADIUM OXIDE (4/7) ()
Al- (0)	A=5.509(1) B=7.008(1) C=12.258(2) AL=95.09(1) BE=95.19(1) GA=109.21(1) V=441.5
R= 0.02	J.Solid State Chem. 6 (1973) P. 419-429 Remarks: TEM 298

V1	0.20220	0.14040	0.06216	0.00000	1.00000
V2	0.23620	0.65400	0.06961	0.00000	1.00000
V3	0.68590	0.44060	0.19785	0.00000	1.00000
V4	0.67970	0.94010	0.19961	0.00000	1.00000
O1	0.10720	0.85380	0.01360	0.00000	1.00000
O2	0.59290	0.79270	0.04660	0.00000	1.00000
O3	0.85740	0.49350	0.08610	0.00000	1.00000
O4	0.33120	0.43490	0.13730	0.00000	1.00000
O5	0.52440	0.14530	0.16410	0.00000	1.00000
O6	0.04150	0.06630	0.19440	0.00000	1.00000
O7	0.29560	0.79310	0.22440	0.00000	1.00000

V1	0.21437	0.14740	0.06317	0.00000	1.00000
V2	0.22314	0.65454	0.06686	0.00000	1.00000
V3	0.68224	0.44016	0.19969	0.00000	1.00000
V4	0.68743	0.94206	0.20173	0.00000	1.00000
O1	0.10140	0.85760	0.01500	0.00000	1.00000
O2	0.58520	0.79540	0.05420	0.00000	1.00000
O3	0.85470	0.49370	0.08350	0.00000	1.00000
O4	0.32650	0.43560	0.13740	0.00000	1.00000
O5	0.52570	0.14370	0.16430	0.00000	1.00000
O6	0.03090	0.06390	0.19770	0.00000	1.00000
O7	0.29530	0.79210	0.22450	0.00000	1.00000

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Address <http://barns.ill.fr/dif/icsd/icsd.htm>

Authors	Years	Remarks	S.String	Help Go
Elements v o	Ele. Count 2	Mineral N.	Jrnl Coden	ANX Form
Laue class any	System any	Space Gp.	Cell vol.	Pearson S.
Z unit/cell	Min. dist.	Dist. Select	Dist Range	Co-ordin.

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69 selected. [List_Entries](#) [Endnote](#) [References](#) [Export_All](#)

1994 Yao - VO2 [P42/ncms] 1993 Oka - VO2 [C12/m1] 1993 Oka - VO2 [C12/m1] 1993 Rogers - VO2 [P42/mnm] 1993 Rogers - VO2 [P121/c1] 1991 Le=Page - V509 [P1-] 1991 Le=Page - V509 [B1-]	Order: Year Auth Form Group Mini
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[inorg. crystal](#)
[structures](#)

Alan Hewat



ILL Grenoble

ICSD-for-WWW
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ICSD for WWW: Result - Microsoft Internet Explorer

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

Edit the data then click on **Plot** to see the pattern. You may need help setting up to [view postscript files](#). Most problems with the [data format](#) are due to an incorrect [Space Group](#), but **try switching off the gzip option** if it is selected below.

```
TITLE -V509-Le=Page Y, Bordet P, Marezio M 92 (1991) P
CELL 7.0020 8.3516 10.9052 91.91 108.39 110.50
SPCGRP B -1
ATOM V 1 0.75000 0.00000 0.75000 1.00000 0.00000
ATOM V 2 0.57992 0.79196 0.92499 1.00000 0.00000
ATOM V 3 0.43492 0.57526 0.11119 1.00000 0.00000
ATOM V 4 0.25000 0.00000 0.75000 1.00000 0.00000
ATOM V 5 0.08668 0.79704 0.92329 1.00000 0.00000
```

Technique: Neutron Diffractometer

Wavelength: Custom 1.909 Å

Width U V W

2theta range 5.0 to 45.0

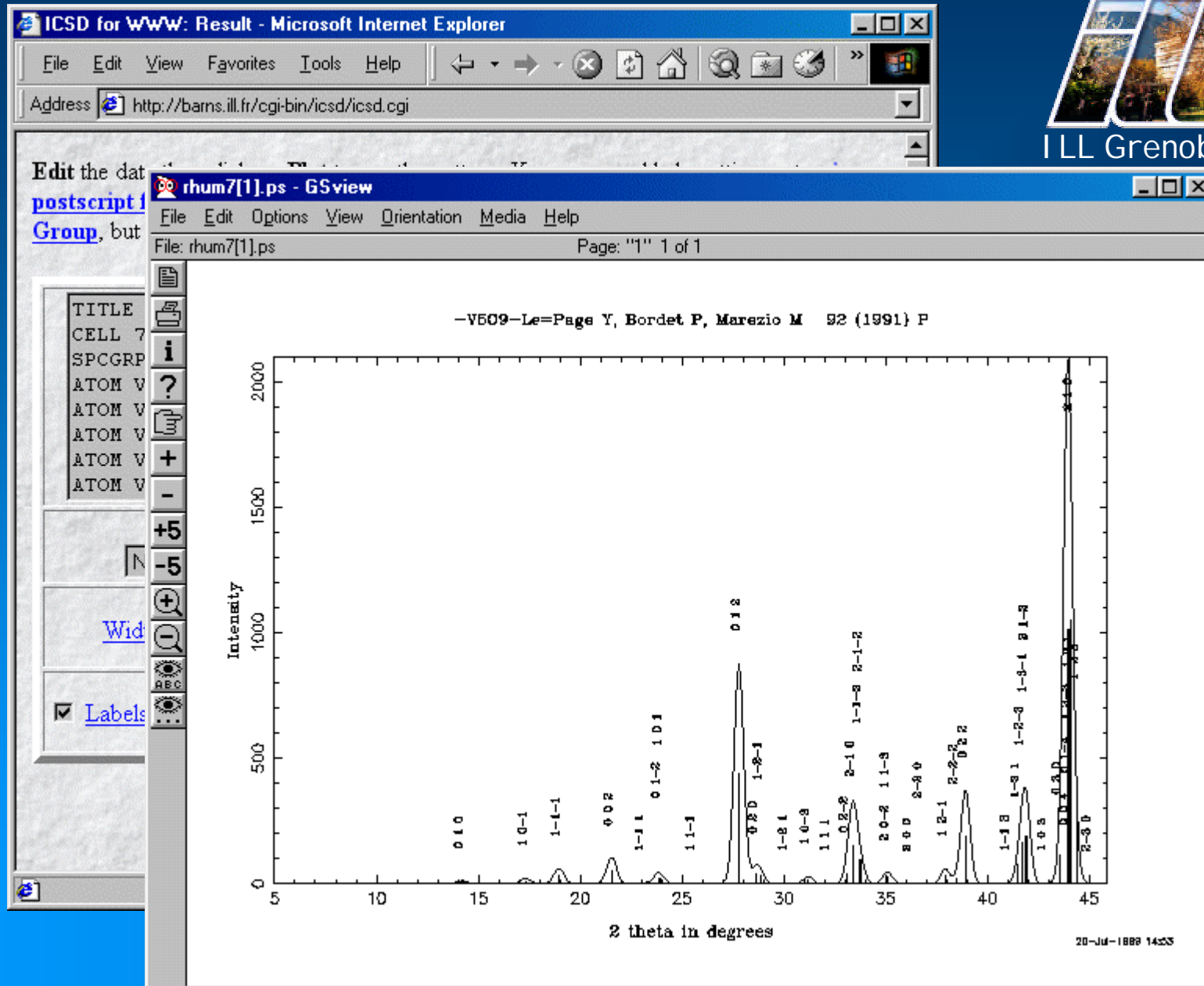
2Theta Zero Step

Labels Dispers Color Gzip **Plots/Page** 1

Defaults
Plot

Re-plot or Copy the postscript profile Print-out the listing.
Postscript plotting using **Lazy** by Benjamin Nunes (MIT).

Internet



ICSD for WWW: Query Form - Microsoft Internet Explorer

Address <http://barns.ill.fr/dif/icsd/icsd.htm>

Authors	Years	Remarks	S.String	Help Go
Elements v o	Ele. Count 2	Mineral N.	Jrnl Coden	ANX Form
Laue class any	System any	Space Gp.	Cell vol.	Pearson S.
Z unit/cell	Min. dist.	Dist. Select	Dist Range	Co-ordin.

Full Database, 16 July-1999 with 50479 Entries. [Help](#) & [News](#)

Expert Query: find (ele=v and o) and elc=2 ;

69 selected. [List_Entries](#) [Endnote](#) [References](#) [Export_All](#)

1994 Yao - VO2 [P42/ncms] 1993 Oka - VO2 [C12/m1] 1993 Oka - VO2 [C12/m1] 1993 Rogers - VO2 [P42/mnm] 1993 Rogers - VO2 [P121/c1] 1991 Le=Page - V509 [P1-] 1991 Le=Page - V509 [B1-]	Order: Year Auth Form Group Mini
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[Details](#) [Bondla](#) [Pattern](#) [Structure](#) [Export](#)

Search the Database [Internet](#)

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ICSD for WWW: Result - Microsoft Internet Explorer

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
```

<input checked="" type="checkbox"/> Axes	<input checked="" type="checkbox"/> Cell	<input type="checkbox"/> Transp	<input checked="" type="checkbox"/> Black B/G
<input type="checkbox"/> Smooth	<input type="checkbox"/> Names	<input type="checkbox"/> Wirefrm	<input checked="" type="checkbox"/> Gzip
Atom type: Small Spheres	Bond type: Polys+Sticks		
Multiple Cells:	x: 1	y: 1	z: 1
Bonds ??? eg: Cu-O Cu1-O,F Cu2-O 1,1,0	<input type="text"/>	Min Bond: 0.9	Max Bond: 2.8
		<input type="button" value="Defaults"/>	<input type="button" value="Display"/>

or VRML structure CCSL output

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

Internet

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ICSD for WWW: Result - Microsoft Internet Explorer

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: 1

Bonds ??? eg: Min Bond: 0.9 Max Bond: 2.8

Cu-O Defaults Disp

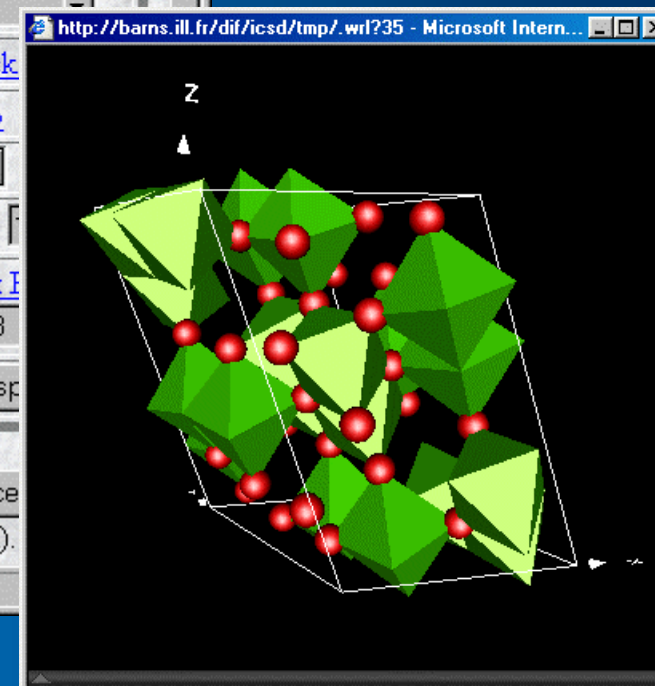
Cu1-O,F

Cu2-O 1,1,0

Re-display or Save VRML structure Print CCSL output Valence

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

Internet





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ICSD for WWW: Result - Microsoft Internet Explorer

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

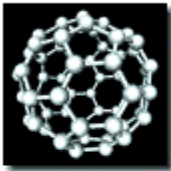
Edit the data, select the model, bonding etc. & click on **Display**. You may need help viewing [VRML files](#). Most [problems](#) are due to an incorrect [Space Group](#).

```

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 0.11118 0.00000 1.00000
A V4 0.25000
A V5 0.08668
  
```

[Axes](#) [C](#)
 [Smooth](#) [N](#)
Atom type: Small Spher
Multiple Cells:
Bonds ??? eg:
Cu-O
Cu1-O,F
Cu2-O 1,1,0

ICSD for WWW: xtal-3d Valence-Sums - Microsoft Internet Explorer

 **Brown-Shannon Valence-Sums from xtal-3d**

Note that you will only obtain valence-sums for the atom-pairs specified in the [Bonds](#) box, using the default [parameters R,B](#), and then only after you **Display** the structure.

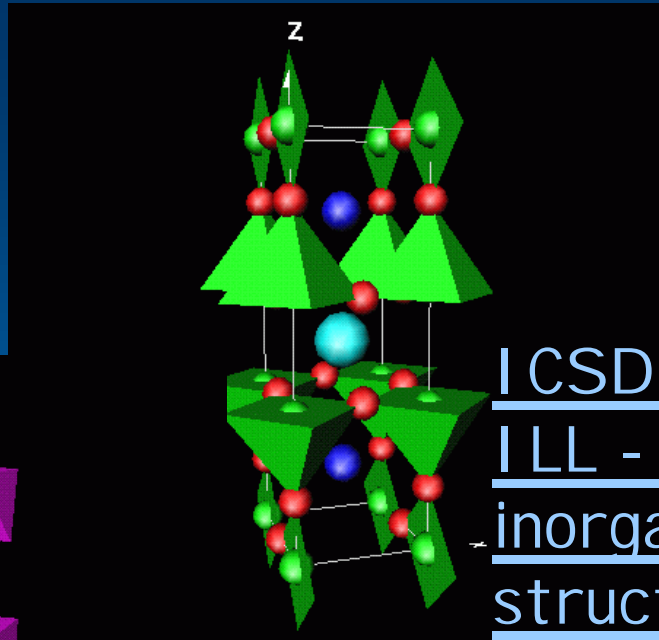
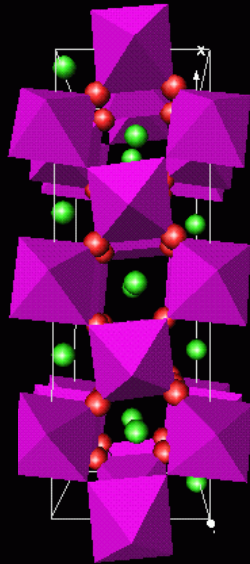
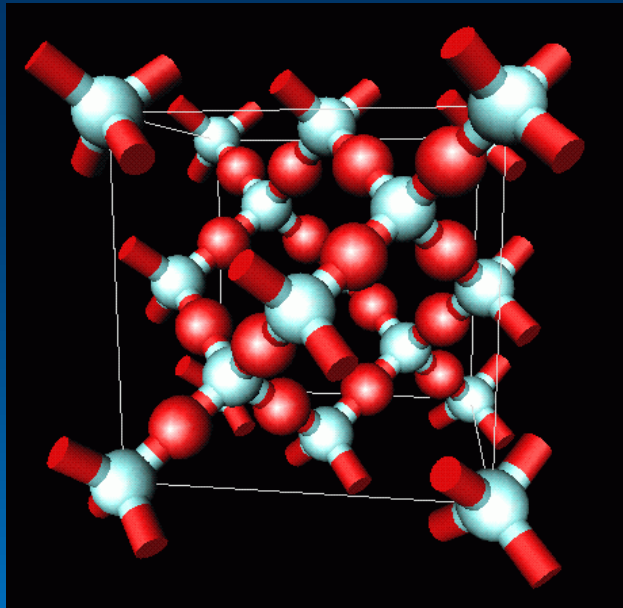
```


Bond-valence sum for V1 is 3.74 assuming Ro=1.784 B=0.370 for V 4+ to O -2
Bond-valence sum for V2 is 3.16 assuming Ro=1.743 B=0.370 for V 3+ to O -2
Bond-valence sum for V3 is 3.80 assuming Ro=1.784 B=0.370 for V 4+ to O -2
Bond-valence sum for V4 is 3.66 assuming Ro=1.784 B=0.370 for V 4+ to O -2
  
```

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

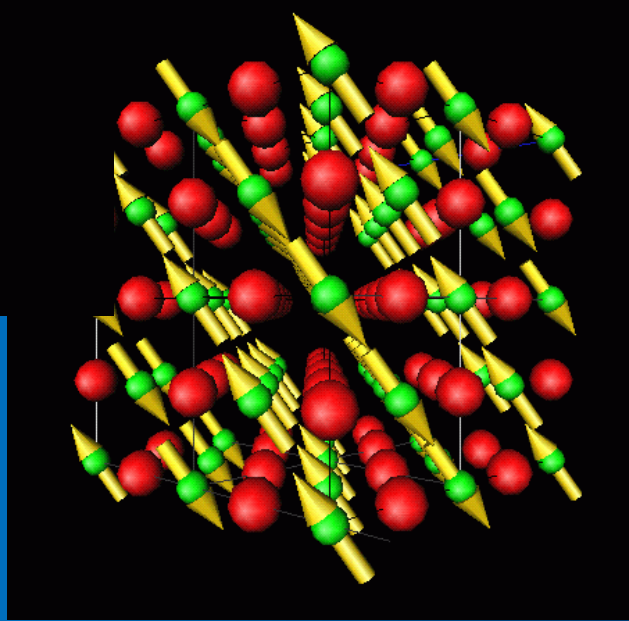
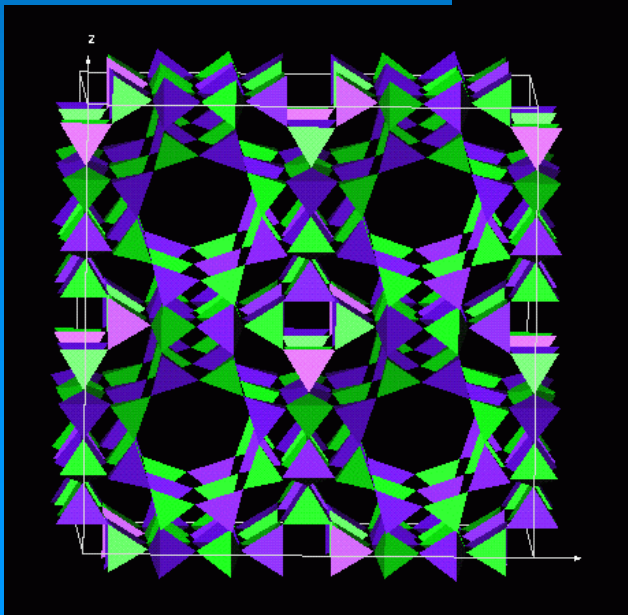
VRML drawing with xtal-3d by Marcus Hewat (UJF/ASU/Lyon-I).

Internet



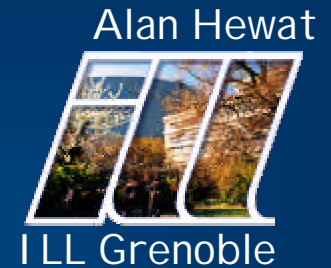
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The Impact of Informatics

Alan Hewat, Diffraction Group, 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.

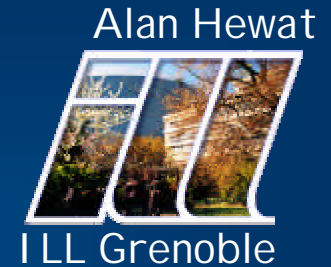
*www.ill.fr/dif/3D-crystals/index.html



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[inorganic crystal structures](#)

The Impact of Informatics

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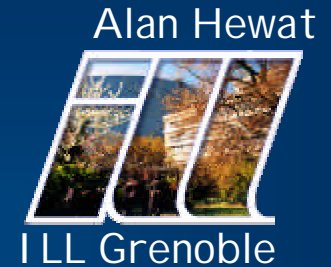


Laboratories running ICSD-for-WWW

- ILL/ESRF
- CDS UK (UK academic community)
- CCP14 Daresbury UK
- CICS Spain (Spanish Scientific Research Council)
- ORNL (Oak Ridge National Laboratory, USA)
- NI ST 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

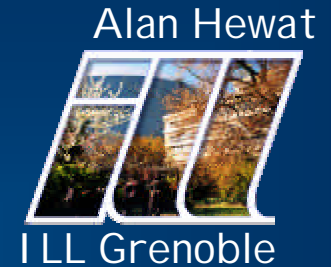
● Who pays ?

- 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