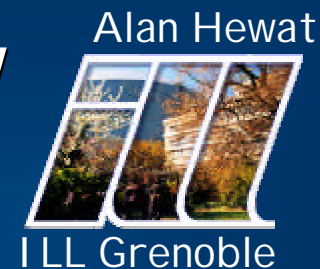


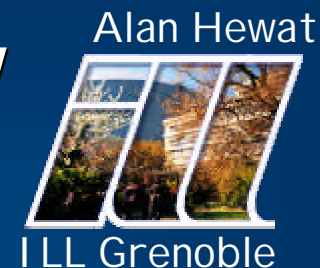
What's New with ICSD-for-WWW

WWW Inorganic Crystal Structure Database - ILL/FIZ



What's New with ICSD-for-WWW

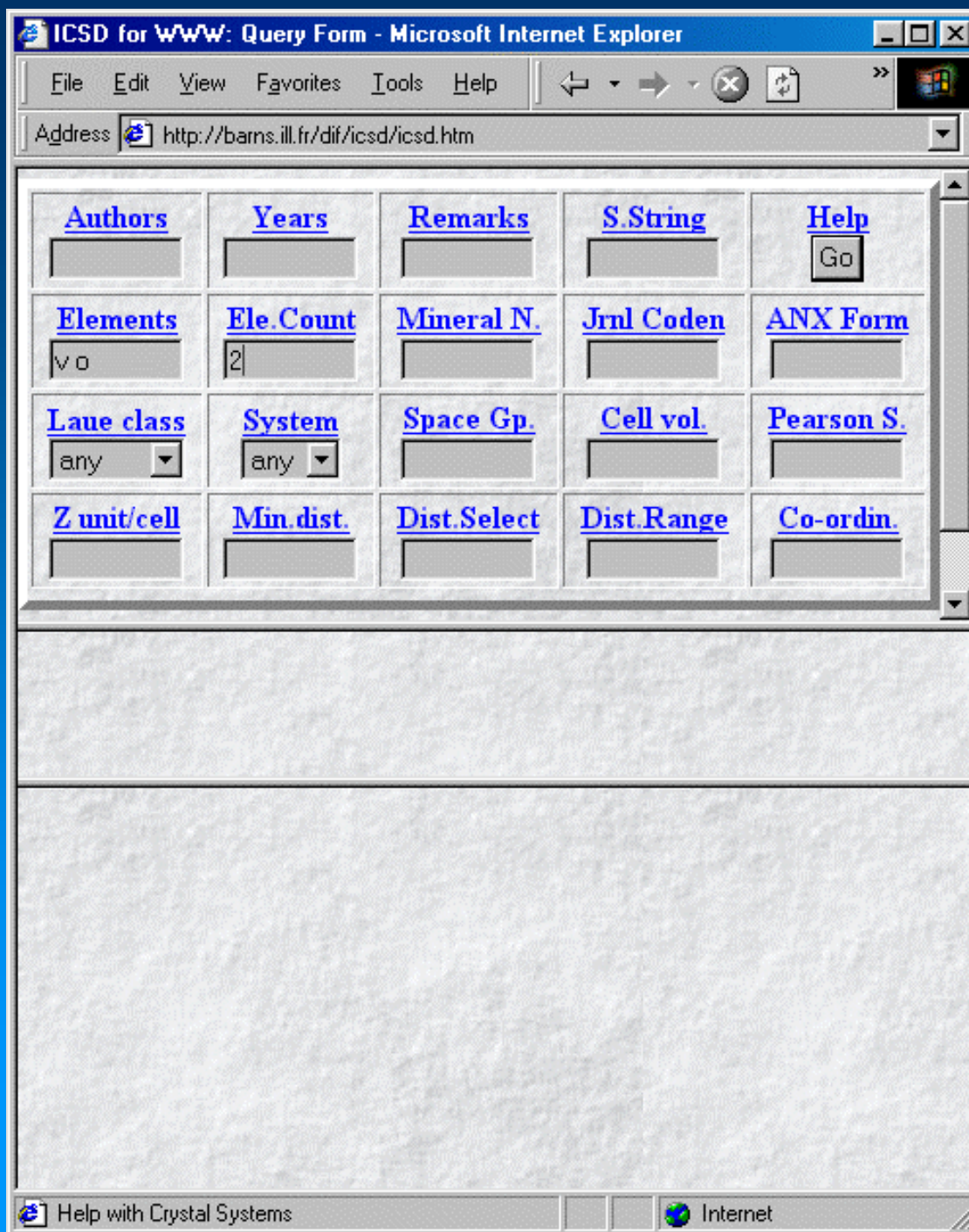
WWW Inorganic Crystal Structure Database - ILL/FIZ



- 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 ?





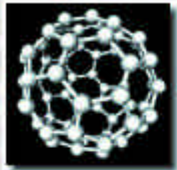


ICSD-for-WWW
 ILL - Karlsruhe
 inorganic crystal
 structures

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 Al_2O_3 , you should as well specify an element count of **2**, or perhaps elements **Al2 O3** (note the separating 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).

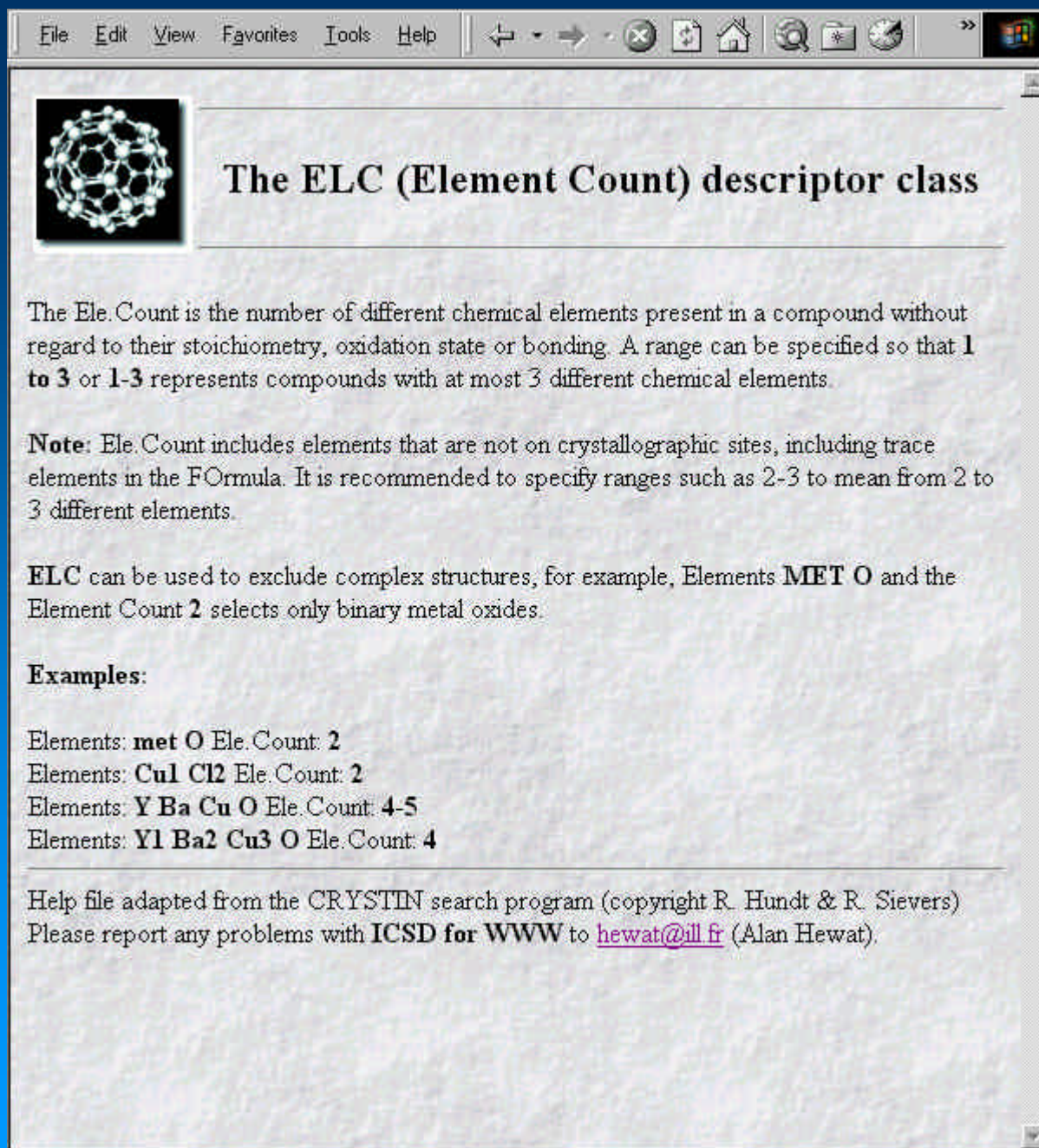
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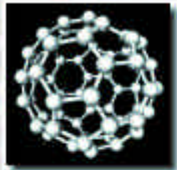
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Help with any field
 (Click on its title)

● 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

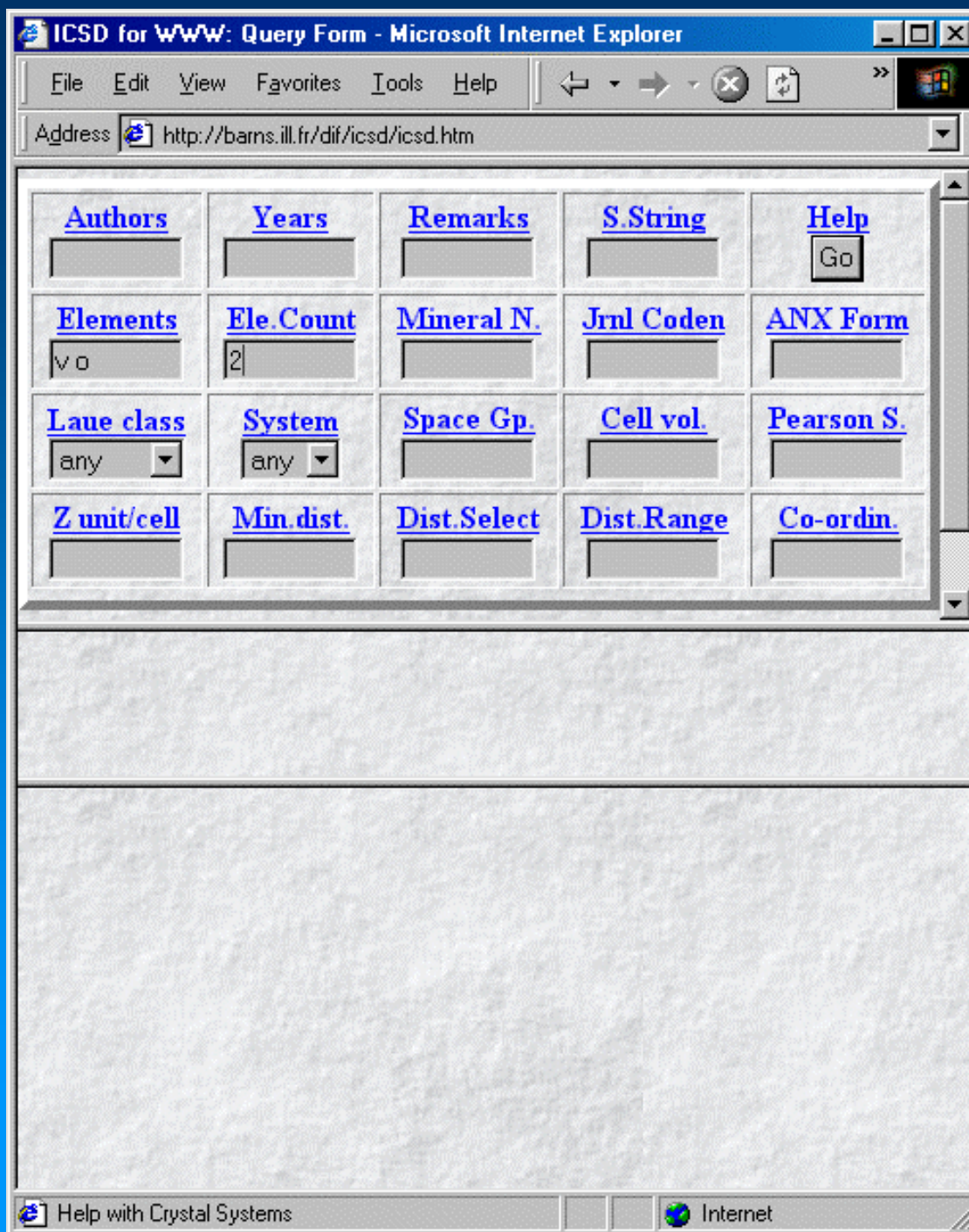


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Help with any field
(Click on its title)

- Help with Elements
- Help with N° Elements



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Search for vanadates

Elements = V O
 Number elements = 2

ICSD for WWW: Query Form - Microsoft Internet Explorer

File Edit View Favorites Tools Help

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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ICSD for WWW: Query Form - Microsoft Internet Explorer

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"/>

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

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

69 selected.

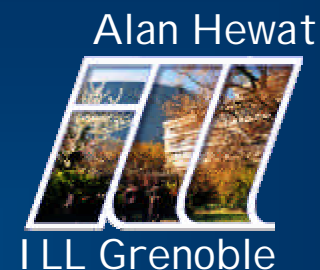
Horiuchi,H. Morimoto,N. Tokonami,M. (1976) J.Solid State Chem. 17 407-424
Crystal structures of Vn O2n-1 (2<n<7)

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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List References

ICSD for WWW: Query Form - Microsoft Internet Explorer

File Edit View Favorites Tools Help

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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69 selected.

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

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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]	Order: Year Auth Form Group Minl
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-]	

[Details](#) [Bondla](#) [Pattern](#) [Structure](#) [Export](#)

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ICSD-for-WWW ILL - Karlsruhe inorganic crystal structures

List Entries

Entries can be sorted

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

ICSD for WWW: Result - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <http://bams.ill.fr/cgi-bin/icسد/icسد.cgi>

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 V₅/50₉ 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)	

Done Internet

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List Details of Entry

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ICSD for WWW: Result - Microsoft Internet Explorer

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

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

ICSD
Lazy P.
Xtal-3d
PowderCell
GSAS
FullProf
Shel-X
CIF

...t@ill.fr of any errors in these format translations. Take care in particular
...ace group symbol, occupation numbers and anisotropic temperature
...ometimes reports Beta(i,j) which are not acceptable in some formats
... have not been converted to Bij or Uij).

COL ICSD Collection Code 1536 (DATE=R800101/U 0 REL= 1199/
NAME Vanadium oxide (6/13)
FORM V6 013
= 013 V6
TITL Structural re-investigation of the low-temperature phase of
V₅/6 O₅/1₅/3
AUT Kawada I, Ishii M, Saeki M, Kimizuka N, Nakano-Onoda M, Kato K
REF ACBCA 34 (1978) P. 1037-1039
JRNL Acta Crystallographica B (24,1968-38,1982)
CELL A=11.96(1) B=3.713(3) C=10.07(2) $\alpha=90.0$ $\beta=100.9(2)$ $\gamma=90.0$
V=439.1 Z=2
SGR P 1 21/A 1 (14)

PARM	Atom	Nr	Ox	Wy	x	y	z
V	1	+4.33	4E	0.35201(7)	0.03851(23)	-0.00144(8)	
V	2	+4.33	4E	0.41203(4)	0.00155(26)	0.36403(6)	
V	3	+4.33	4E	0.71537(4)	-0.00113(26)	0.36664(6)	
O	1	-2	4E	0.1775(2)	0.0076(10)	0.0003(3)	
O	2	-2	4E	0.8818(2)	-0.0018(11)	0.3885(2)	
O	3	-2	4E	0.2510(2)	0.0012(11)	0.4092(2)	
O	4	-2	2B	0.5	0.0	0.0	

ICSD-for-WWW ILL - Karlsruhe inorganic crystal structures

List or Export Details
in many formats

- ICSD
- Lazy Pulverl x
- CCSL
- PowderCell
- GSAS
- FullProf
- Shel-X
- CIF

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.

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

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

1994 Yao - VO2 [P42/ncms]	Order: Year Auth Form Group Mini
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-]	

[Details](#) [Bondla](#) [Pattern](#) [Structure](#) [Export](#)

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ICSD-for-WWW
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Calculate Bond Lengths
 and Angles

ICSD for WWW: Result - Microsoft Internet Explorer

Address: <http://bams.ill.fr/cgi-bin/icسد/icسد.cgi>

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							

Done Internet

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Calculate Bond Lengths
 and Angles

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](#)

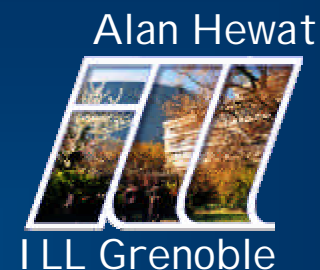
Expert Query: find (ele=v and o) and elc=2 ;

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

1978 Hodeau - V407 [A1-]	Order: Year Auth Form Group Mini
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]	

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Compare similar
 structures



Compare similar structures

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

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	1973	Marezio M, McWhan D B, Dernier P D, Remeika J P
#	V4O7 - Vanadium oxide (4/7) - low-temperature phase ()	#	V4O7 - VANADIUM OXIDE (4/7) ()
Al-	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	Al-	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=	J.Solid State Chem. 23 (1978) P. 253-263 0.04 Remarks:TEM 120	R=	J.Solid State Chem. 6 (1973) P. 419-429 0.02 Remarks:TEM 298

V1	0.20220	0.14040	0.06216	0.00000	1.00000	V1	0.21437	0.14740	0.06317	0.00000	1.00000
V2	0.23620	0.65400	0.06961	0.00000	1.00000	V2	0.22314	0.65454	0.06686	0.00000	1.00000
V3	0.68590	0.44060	0.19785	0.00000	1.00000	V3	0.68224	0.44016	0.19969	0.00000	1.00000
V4	0.67970	0.94010	0.19961	0.00000	1.00000	V4	0.68743	0.94206	0.20173	0.00000	1.00000
O1	0.10720	0.85380	0.01360	0.00000	1.00000	O1	0.10140	0.85760	0.01500	0.00000	1.00000
O2	0.59290	0.79270	0.04660	0.00000	1.00000	O2	0.58520	0.79540	0.05420	0.00000	1.00000
O3	0.85740	0.49350	0.08610	0.00000	1.00000	O3	0.85470	0.49370	0.08350	0.00000	1.00000
O4	0.33120	0.43490	0.13730	0.00000	1.00000	O4	0.32650	0.43560	0.13740	0.00000	1.00000
O5	0.52440	0.14530	0.16410	0.00000	1.00000	O5	0.52570	0.14370	0.16430	0.00000	1.00000
O6	0.04150	0.06630	0.19440	0.00000	1.00000	O6	0.03090	0.06390	0.19770	0.00000	1.00000
O7	0.29560	0.79310	0.22440	0.00000	1.00000	O7	0.29530	0.79210	0.22450	0.00000	1.00000

Details Pattern Bondla Structure

Details Pattern Bondla Structure

Done Internet

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

Authors	Years	Remarks	S.String	Help Go
Elements Vo	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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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](#)

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Calculate the indexed
 powder pattern

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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

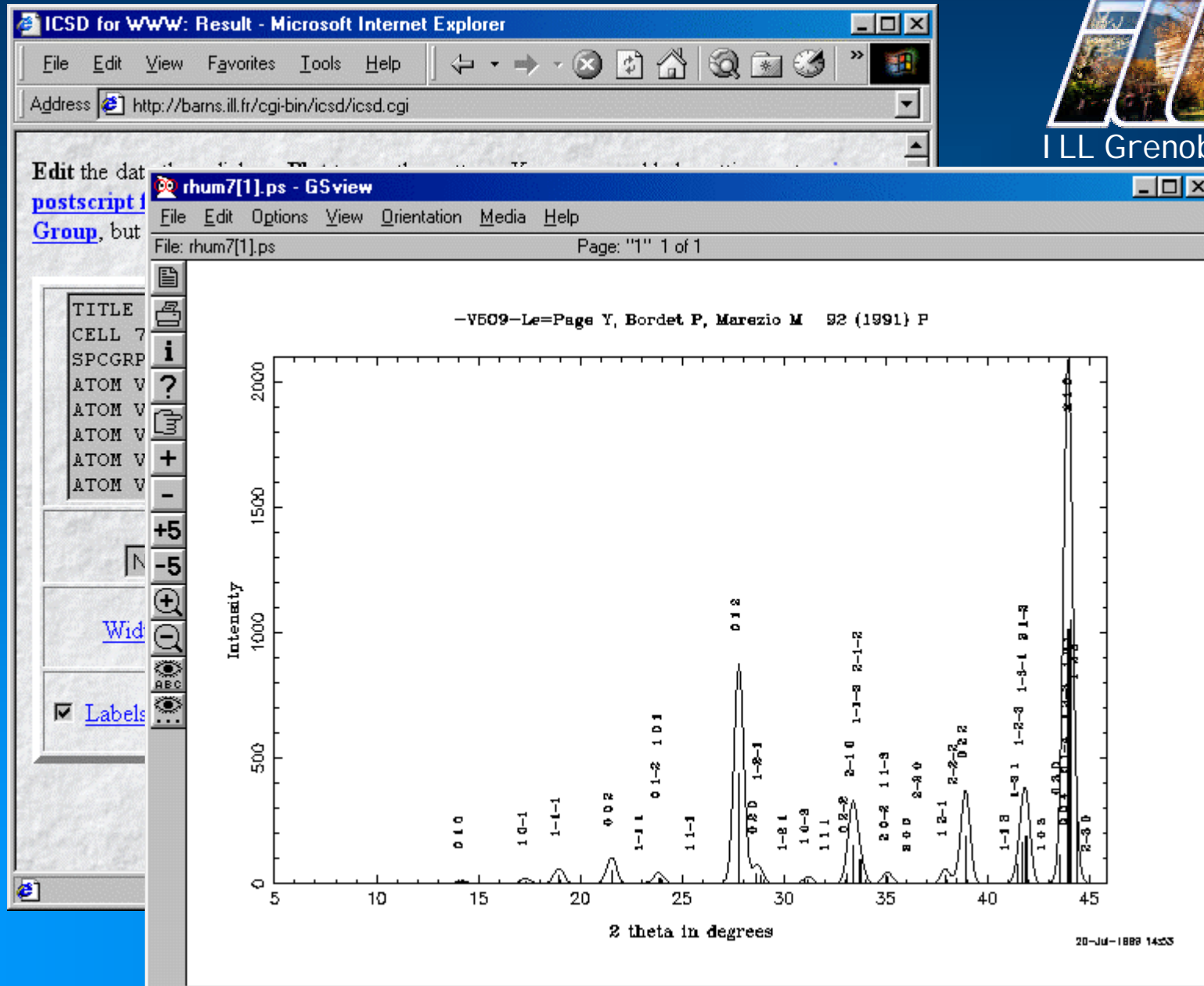
Re-plot or Copy the postscript profile Print-out the listing.
Postscript plotting using **Lazy** by Benjamin Nunes (MIT).

Internet

ICSD-for-WWW
ILL - Karlsruhe
inorganic crystal
structures

Calculate the indexed
powder pattern

Select neutrons, Xrays
wavelength, peak width
etc



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](#)

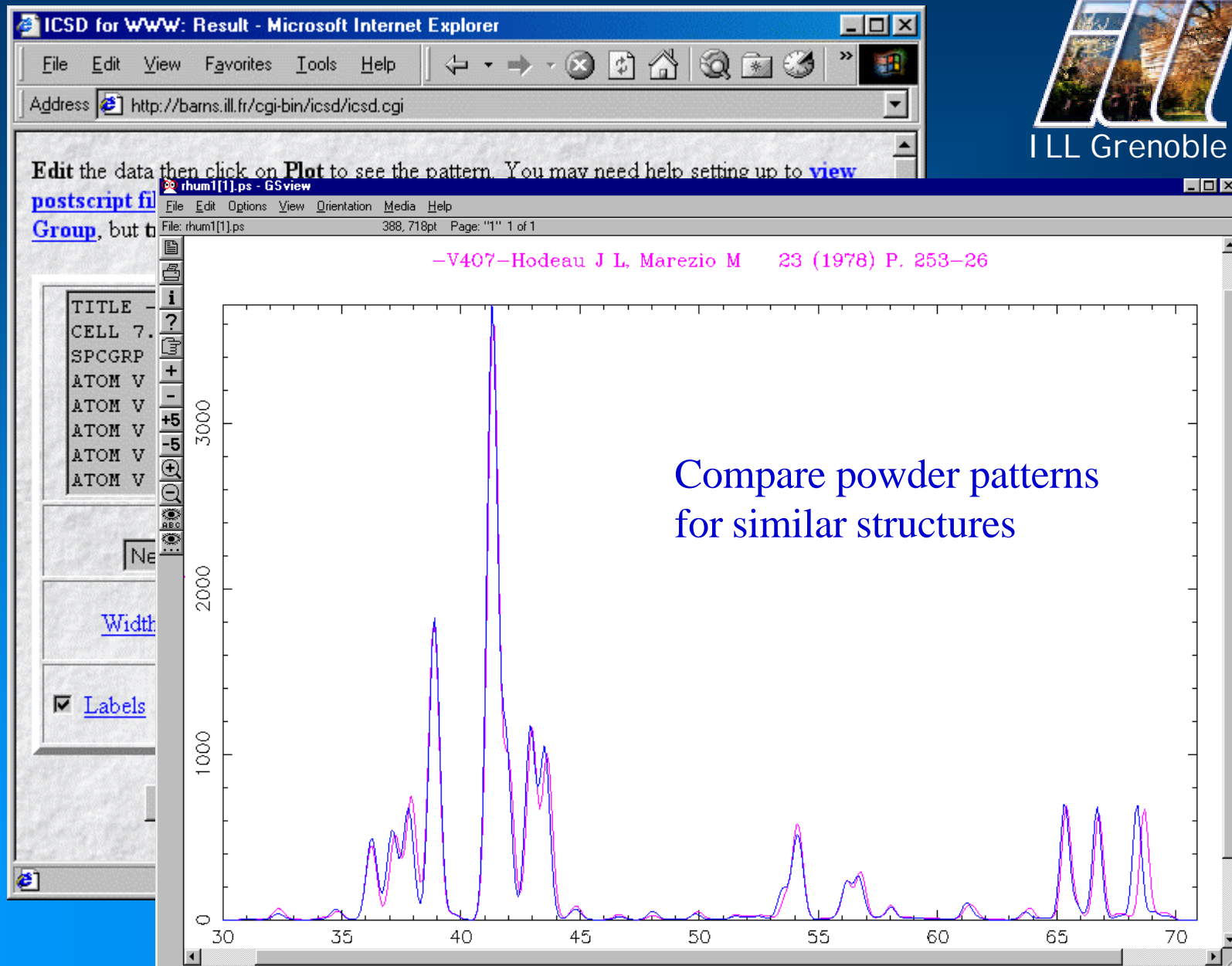
<ul style="list-style-type: none"> 1978 Hodeau - V407 [A1-] 1978 Hodeau - V407 [A1-] 1973 Marezio - V407 [A1-] 1973 Marezio - V407 [A1-] 1991 Le=Page - V509 [B1-] 1974 Waltersson - V307 [C12/C1] 1976 Theobald - VO2 [C12/M1] 	<p>Order:</p> <p>Year</p> <p>Auth</p> <p>Form</p> <p>Group</p> <p>Mini</p>
--	---

[Details](#) [Bondla](#) [Pattern](#) [Structure](#) [Export](#)

Search the Database Internet

ICSD-for-WWW
 ILL - Karlsruhe
 inorganic crystal
 structures

Compare powder
 patterns for similar
 structures



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
--	--

[Details](#) [Bondla](#) [Pattern](#) [Structure](#) [Export](#)

Search the Database [Internet](#)

ICSD-for-WWW
 ILL - Karlsruhe
 inorganic crystal
 structures

Display a 3D structure



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 B/G](#)
 [Smooth](#)
 [Names](#)
 [Wirefrm](#)
 [Gzip](#)
[Atom type:](#) Small Spheres
 [Bond type:](#) Polys+Sticks
[Multiple Cells:](#) x: 1 y: 1 z: 1
[Bonds ??? eg:](#) Cu-O
 [Min Bond:](#) 0.9
 [Max Bond:](#) 2.8
 Cu1-O,F
 Cu2-O 1,1,0
 Defaults Display

Re-display or Save VRML structure Print CCSL output Valence-Sum
 VRML drawing with **xtal-3d** by **Marcus Hewat** (UJF/ASU/Lyon-I).

ICSD-for-WWW ILL - Karlsruhe inorganic crystal structures

Display a 3D structure

Alan Hewat



ILL Grenoble

ICSD-for-WWW ILL - Karlsruhe inorganic crystal structures

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

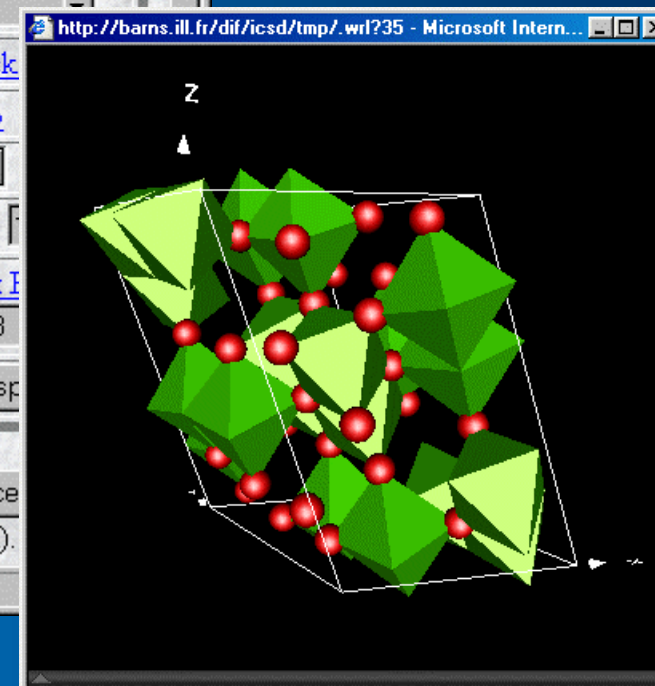
Cu-O Defaults Disp

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).



Alan Hewat



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 B/G](#)
 [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
Cu1-O,F
Cu2-O 1,1,0

Defaults Display

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

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

Internet

ICSD-for-WWW
ILL - Karlsruhe
inorganic crystal
structures

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

Alan Hewat



ILL Grenoble

ICSD-for-WWW ILL - Karlsruhe inorganic crystal structures

http://barns.ill.fr/dif/icsd/tmp/.wrl?69 - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address http://barns.ill.fr/dif/icsd/tmp/.wrl?69

Done

Cu2-O 1,1,0

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

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

Internet

er

click on **Display**. You may need help to an incorrect [Space Group](#).

```
ezio M 92 (1991) P
8.39 110.50
0.00000 1.00000
0.00000 1.00000
0.00000 1.00000
```

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.

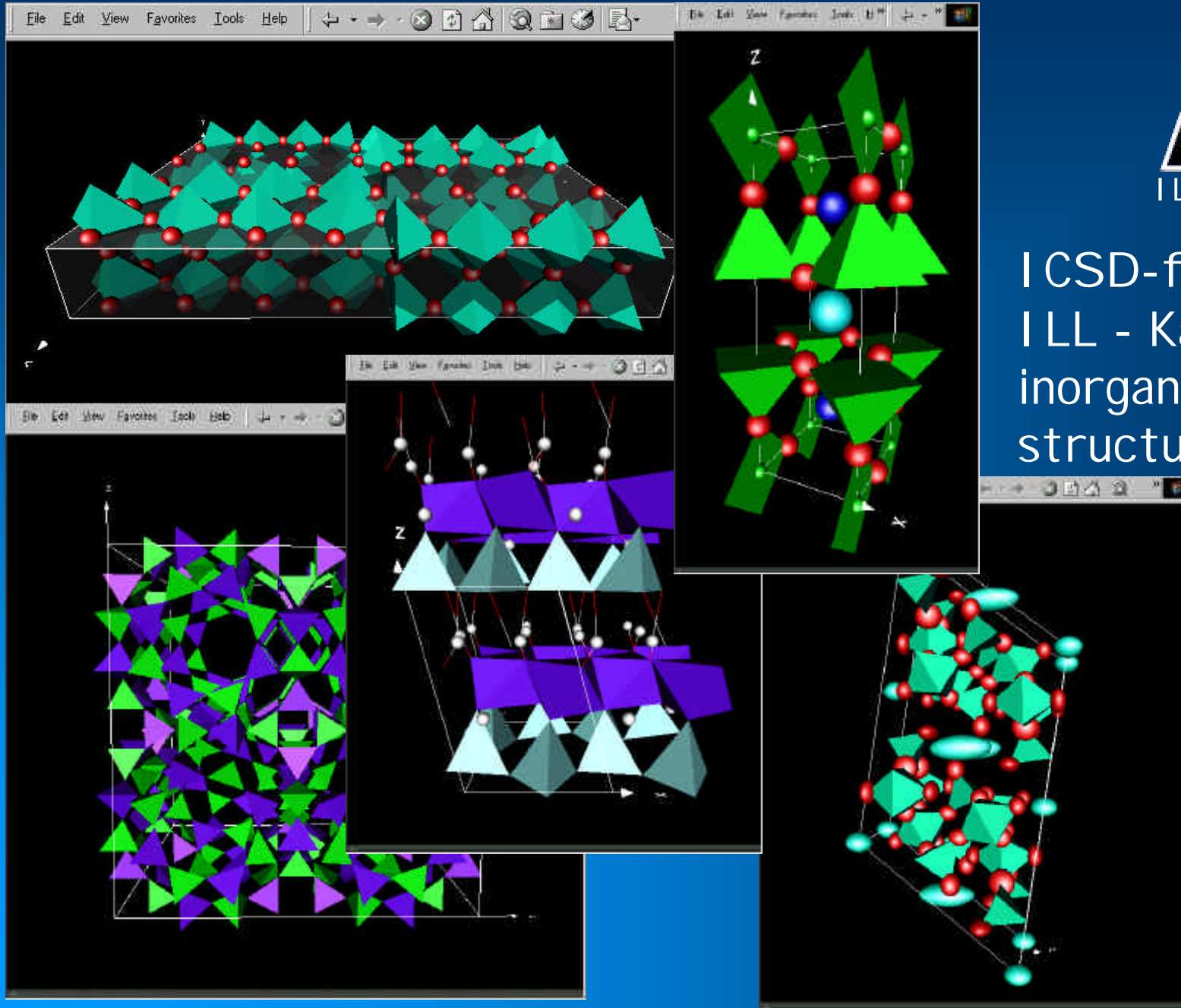
```
Bond-valence sum for V1 is 3.74 assuming Ro=1.784 B=0.370 for V 4+ to O -2
Bond-valence sum for V2 is 3.16 assuming Ro=1.743 B=0.370 for V 3+ to O -2
Bond-valence sum for V3 is 3.80 assuming Ro=1.784 B=0.370 for V 4+ to O -2
Bond-valence sum for V4 is 3.66 assuming Ro=1.784 B=0.370 for V 4+ to O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


Alan Hewat



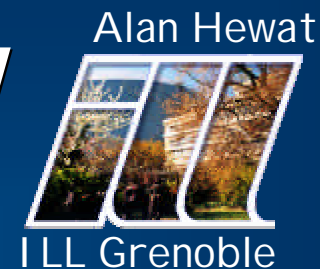
ILL Grenoble

ICSD-for-WWW
ILL - Karlsruhe
inorganic crystal
structures



What's New with ICSD-for-WWW


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

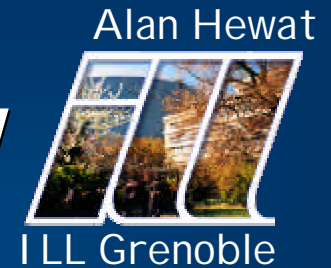
ICSD-for-WWW
ILL - Karlsruhe
inorganic crystal
structures



Laboratories running ICSD-for-WWW

- 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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\$....\$....\$...\$...\$.

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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

- 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



What's New with ICSD-for-WWW

- 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

Alan Hewat



ILL Grenoble