

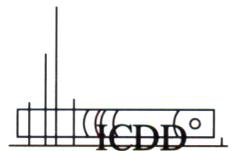


# Powder Diffraction

An international  
journal of materials  
characterization

Volume 12 Number 4 December 1997

33-1161		SiO <sub>2</sub>		Silicon Oxide		Quartz, syn		
Rad. CuKα <sub>1</sub>	λ 1.540598	Filter Mono.	d-sp Diff.	Int	hkℓ	dÅ	Int	hkℓ
Cut off	Int.	Diffractionmeter	W <sub>max</sub> 3.6					
Ref. <i>Natl. Bur. Stand. (U.S.) Monogr. 25, 18 61 (1981)</i>								
Sys. Hexagonal		S.G. P3,21 (154)						
a 4.9133(2)	b	c 5.4053(4)	A	Z 3	mp	C 1.1001		
α	β							
Ref. <i>Ibid.</i>								
D <sub>1</sub> 2.65	D <sub>2</sub> 2.66							
Color Colorless	noβ 1.544	SS/FOM F <sub>50</sub> =77(013,31)	Sign + 2V					
Pattern taken at 25 C. Sample from the Glass Section at NBS,	Ref. Swanson, Fuyat, <i>Natl. Bur. Stand. (U.S.)</i>	ey 1.553	McCarthy, C., North Dakota State					
Gaithersburg, Maryland, USA. Ground single-crystals of optical qual-			ity. Pattern reviewed by Holzer, USA, <i>ICDD Grant-in-Aid</i> (1990).					
University, Fargo, North Dakota, USA, <i>ICDD Grant-in-Aid</i> (1990).			Agrees well with experimental and calculated patterns. O <sub>2</sub> Si type.					
Quartz group. Also called: silica. Also called: low quartz. Silicon used			as internal standard. PSC: hP9. To replace 5-490 and validated for cal-					
culated pattern. Plus 6 additional reflections to 0.9089.								



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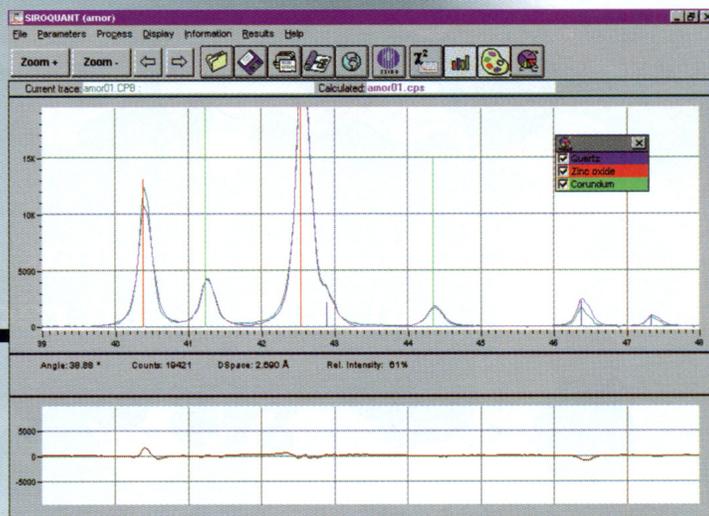
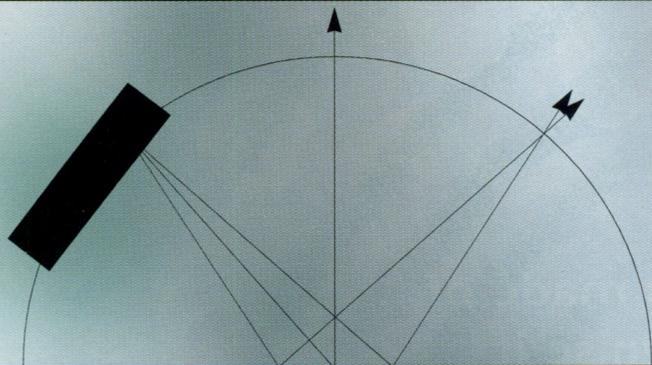
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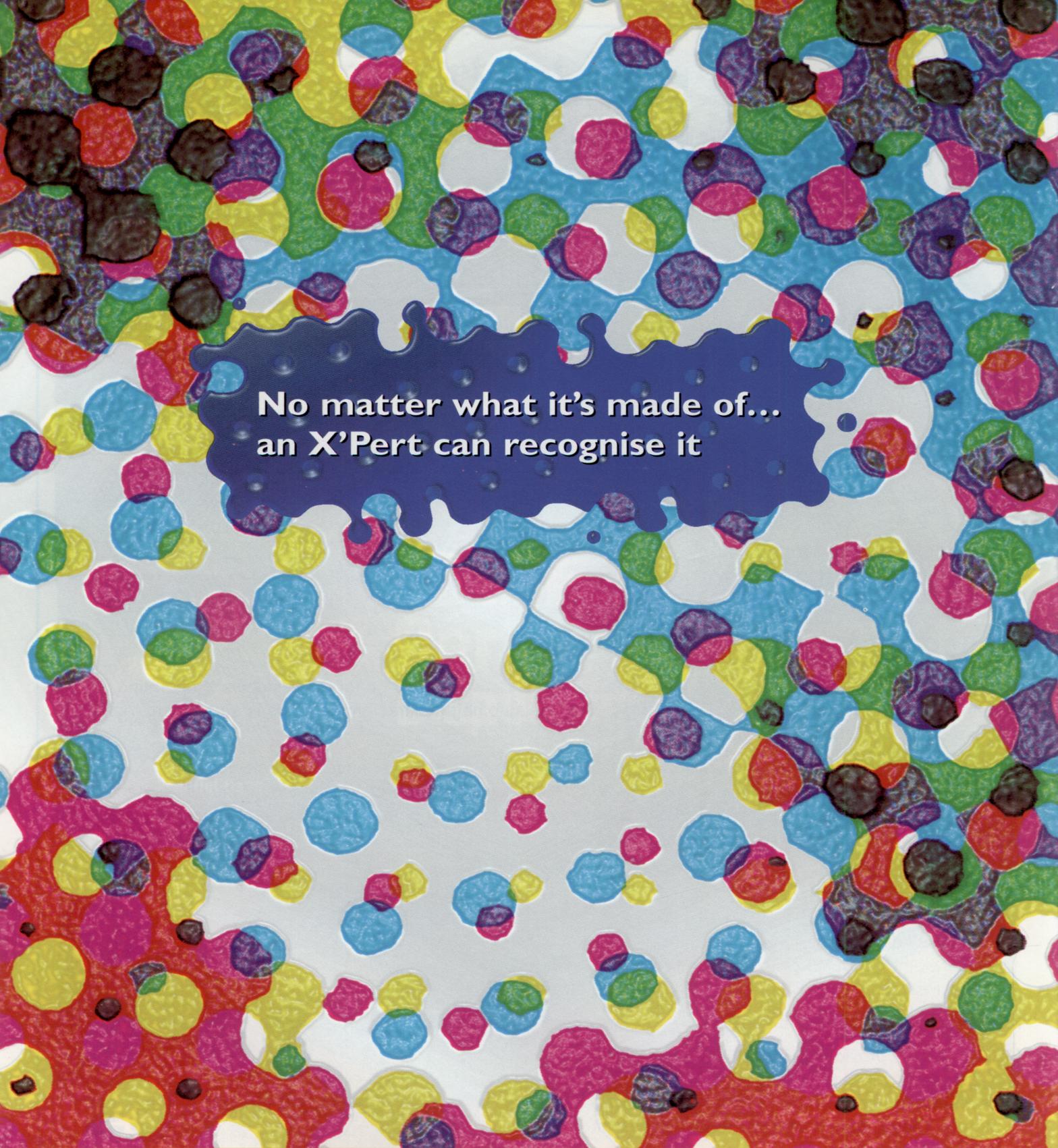
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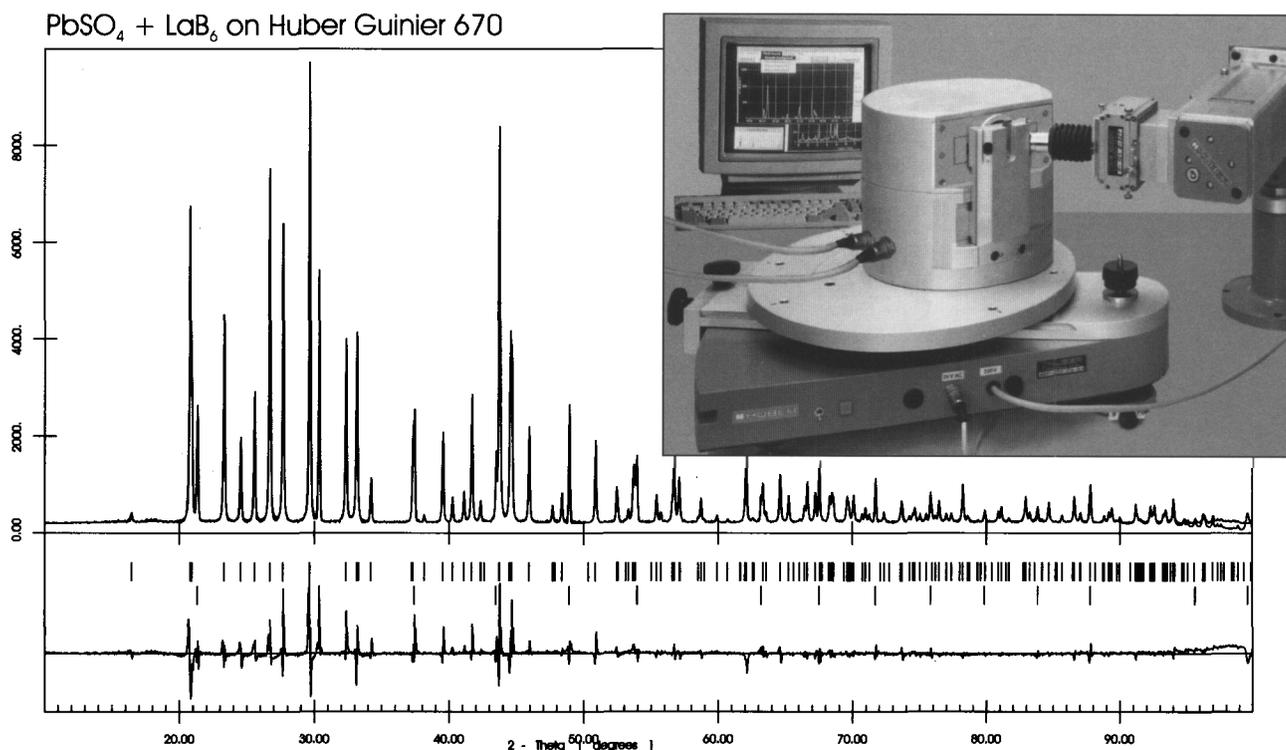
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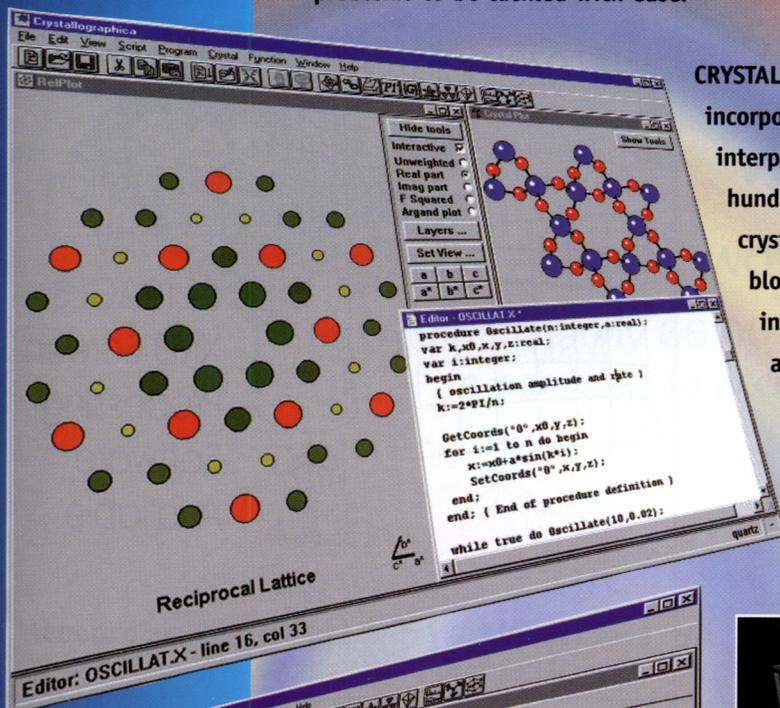
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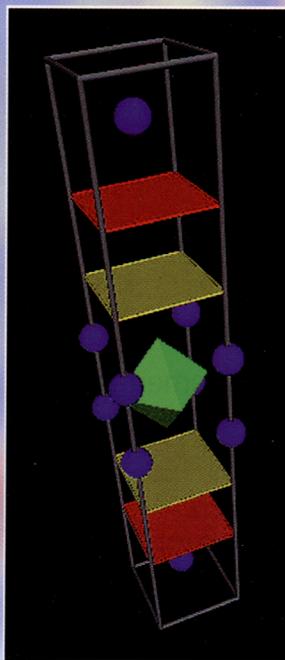
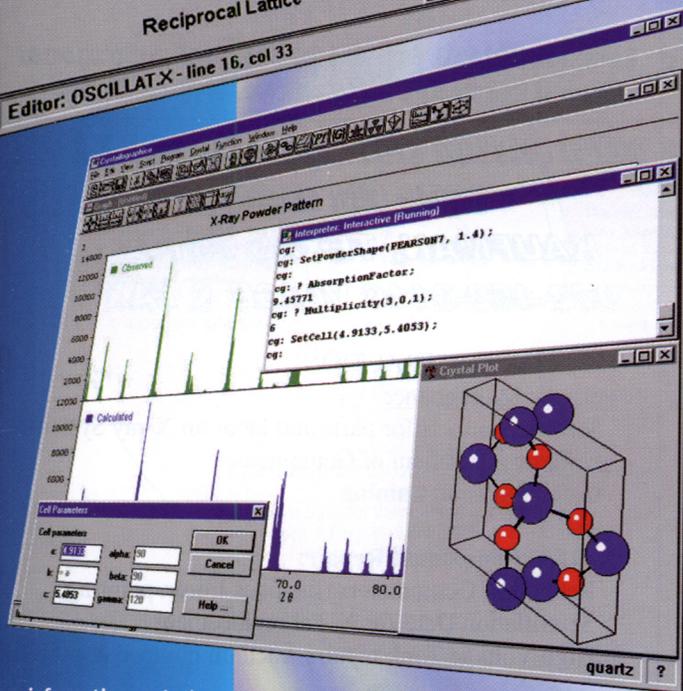


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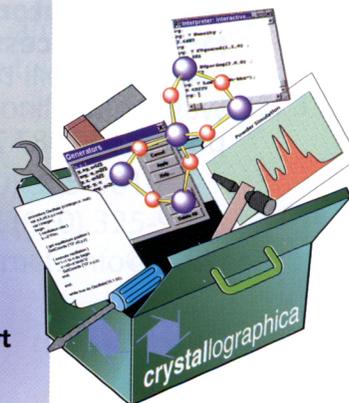
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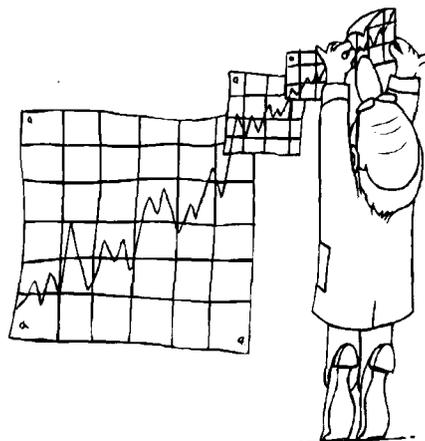
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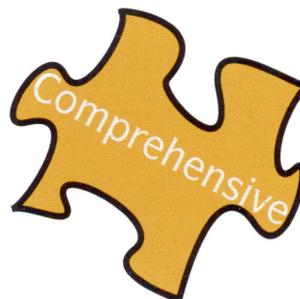
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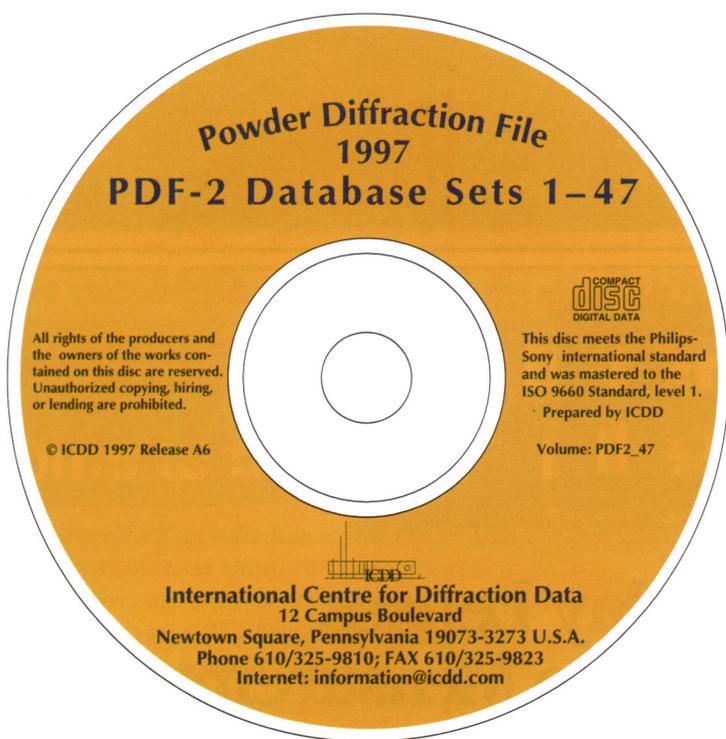


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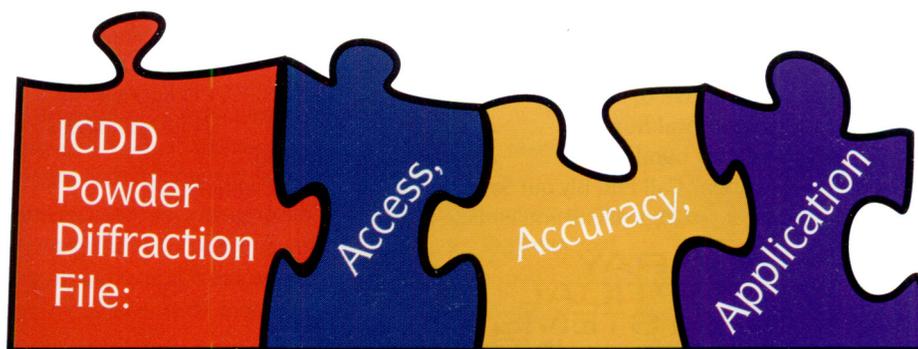
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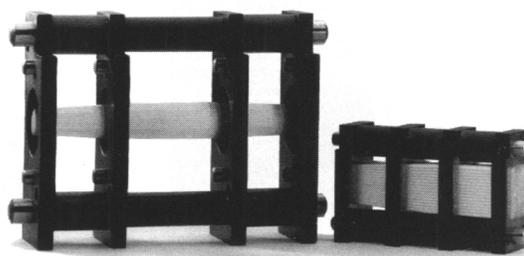
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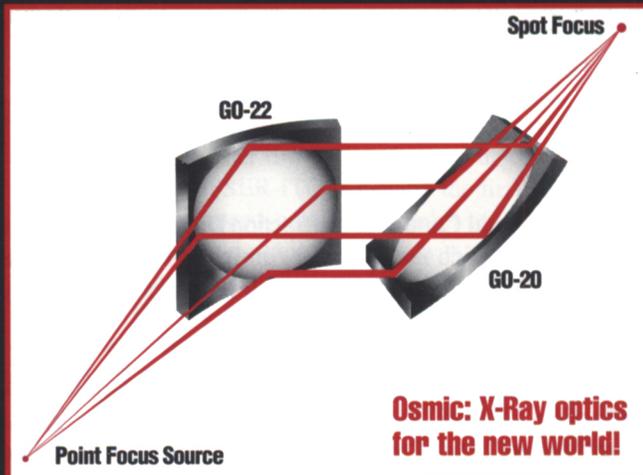
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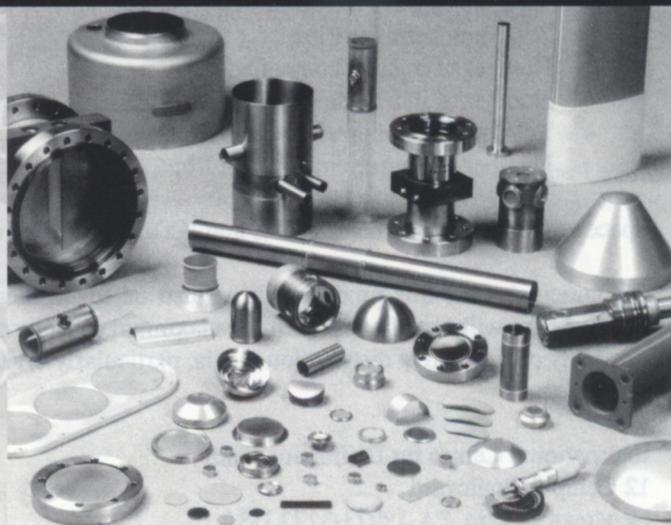
- Depend on us as the only fully integrated source for beryllium sheet and foil products. All critical operations are performed in-house for seamless excellence.
- We're your partner in joining and coating metals. When your project involves joining a metal to a metal, you can count on us.
- Come to us for all your UHV beryllium product needs: x-ray windows, chambers, beam pipes and more.
- Rely on our expert engineering. We like challenges. Taking your design concept into reality would be our pleasure.

**Count on us for your tough jobs.** Keep in mind that we're the only fully integrated source for beryllium products for the analytical, medical, and scientific industries. Challenge us with your "cutting edge" requirements. We look forward to hearing from you.

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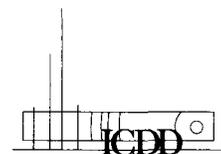
# International Centre for Diffraction Data

Newtown Square Corporate Campus

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Newtown Square, Pennsylvania, 19073-3273, U.S.A.

Phone 610/325-9810 ♦ FAX 610/325-9823 ♦ Internet INFORMATION@ICDD.COM



## ANNOUNCEMENT

The International Centre for Diffraction Data and Fachinformationszentrum, Karlsruhe, Germany, (FIZ), have signed an agreement which marks the beginning of an important relationship between the two organizations. As a result of this relationship with FIZ, ICDD will release a significantly enhanced powder diffraction database in September of 1998.

The first enhancement, and the one potentially with the longest term impact, is the cross-correlation of the Powder Diffraction File (PDF) and the Inorganic Crystal Structure Database (ICSD). Today, automated search/match algorithms are limited to listing the best matched phases in order of "goodness of fit." The automated ability to access the atomic coordinates and then generate the calculated patterns for potential phases identified in an unknown mixture opens a new era in phase ID. Least squares refinement of the calculated patterns will permit the next generation of algorithms to test and resolve postulates concerning preferred orientation and solid solution shifting in establishing the match. With this new ability, algorithms will be able to, fully automatically and unambiguously, identify the actual phases in an unknown, when the appropriate information is in both of the databases (DBs). In addition, all of the other information potentially contained in the powder patterns can be readily extracted as part of the phase ID - i.e. semi-quantitative analysis from the calculated  $I/I_c$  values, concentration of components in identified solid solutions, all degrees of preferred orientation in a specimen, the crystallite size and strain of each of the phases exhibiting line broadening, etc. The integration of the crystal structure information with the PDF will bring on a new era of phase analysis for licensed users of both databases.

For the present, the 1998 release of the PDF will be enhanced by the addition of approximately 40,000 calculated patterns obtained from ICSD. This enhancement does NOT require that users have an ICSD license - the calculated patterns are a permanent addition to the PDF and there will be NO INCREASE IN THE PRICE OF THE PDF. The enhanced database will follow the same format as the previous PDF-2 database. We expect the combination database to contain:

Total number of entries	~ 115,000
Number of organic compounds	~ 20,000
Number of inorganic compounds	~ 95,000
Total number of entries with $I/I_c$	~ 50,000
Number of unique entries with $I/I_c$	~ 37,000

Space requirements for the data files and ICDD index files will require approximately 580 MB of space.

We anticipate that this product will be distributed, in the short term, using conventional CD-ROM technology. However, we will rapidly approach the maximum capacity of the CD-ROM. Consequently, we will be exploring the feasibility of alternative distribution media, particularly DVD technology. We will keep you informed of our progress in this area.

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Please visit our web site @ [www.icdd.com](http://www.icdd.com)