ANNOUNCEMENT

The International Centre for Diffraction Data (ICDD) and Fachinformationszentrum, Karlsruhe, Germany (FIZ), have signed an agreement which marks the beginning of an important relationship between the 2 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 Struture 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, fully automatically and unambiguously, to identify the actual phases in an unknown, when the appropriate information is in both of the databases. In addition, all of the other information potentially contained in the powder patterns can be readily extracted as part of the phase ID—that is, semi-quantitative analysis from the calculated I/Ic 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/Ic	~ 50,000
Number of unique entries with I/Ic	~ 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 direct-view device (DVD) technology. We will keep you informed of our progress in this area.

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Please visit our website @ www.icdd.com

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