

Powder Diffraction

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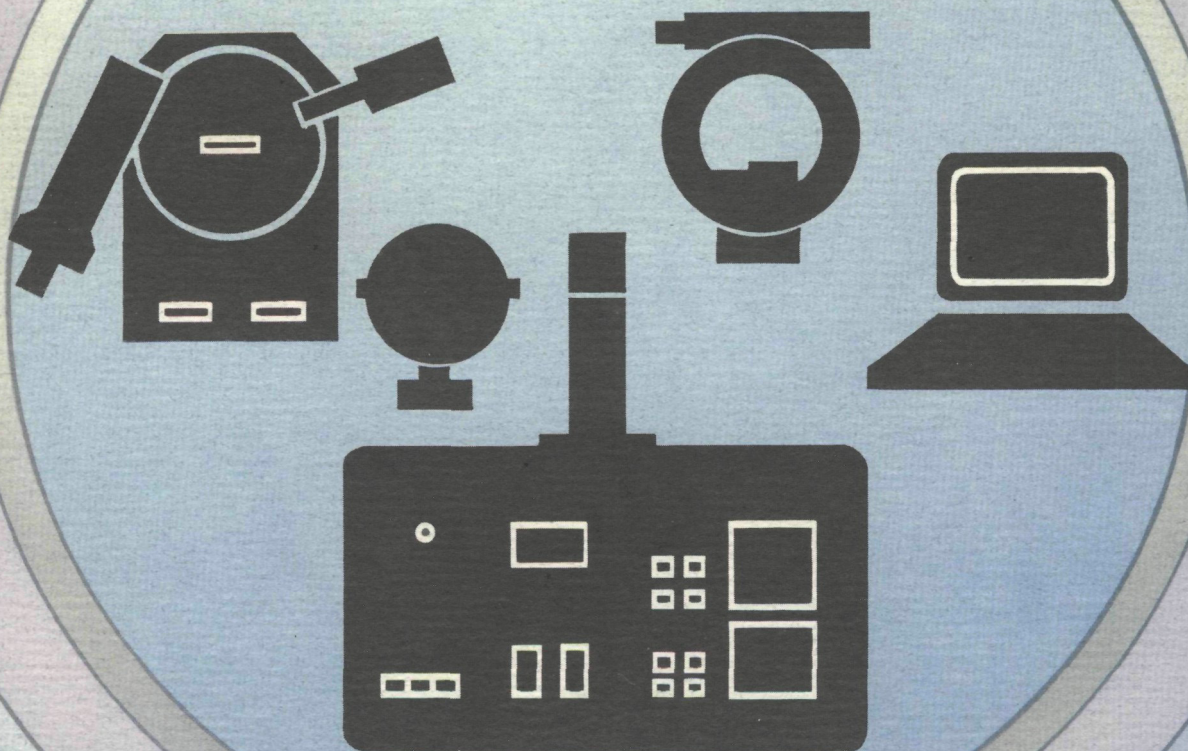
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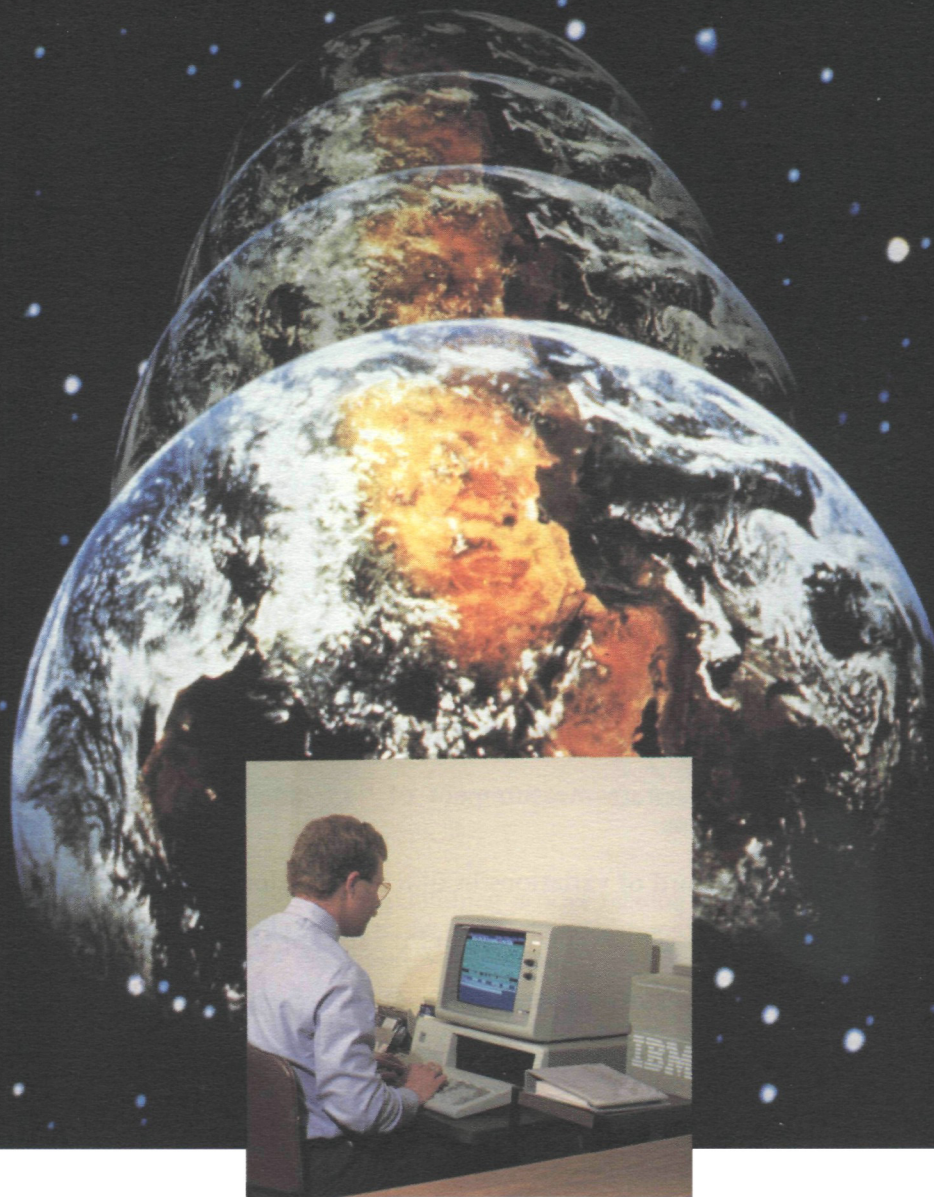
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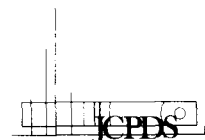
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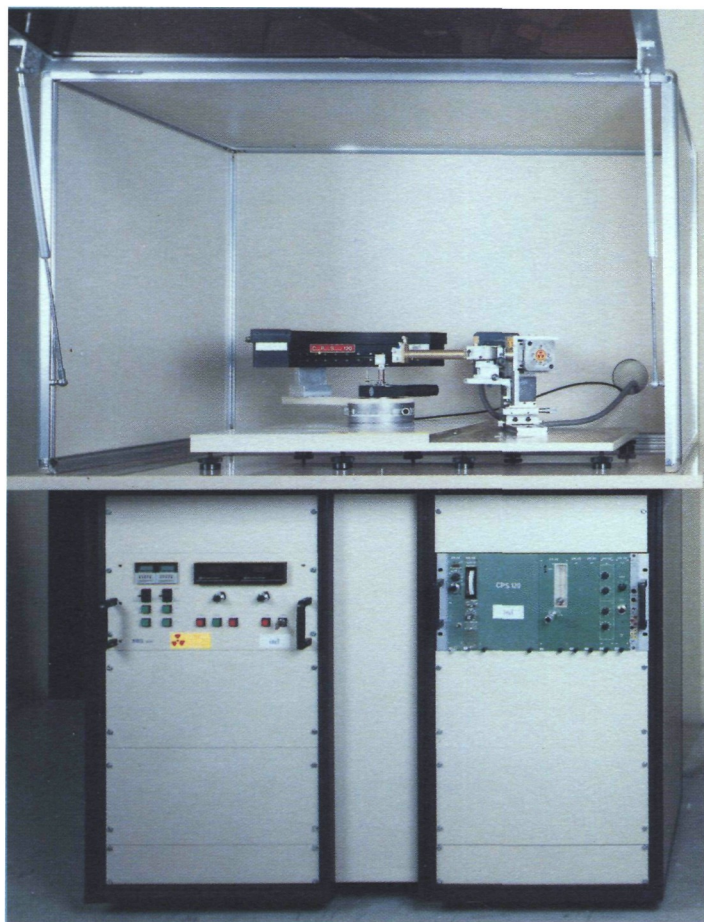
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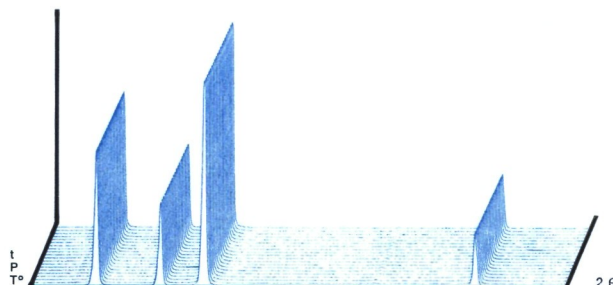
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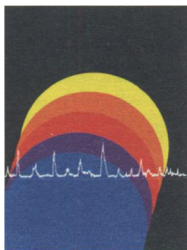
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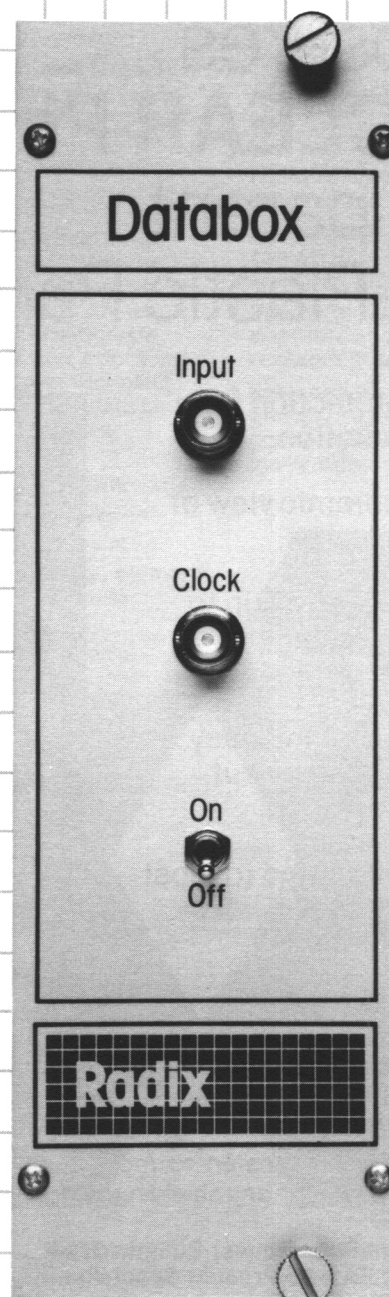
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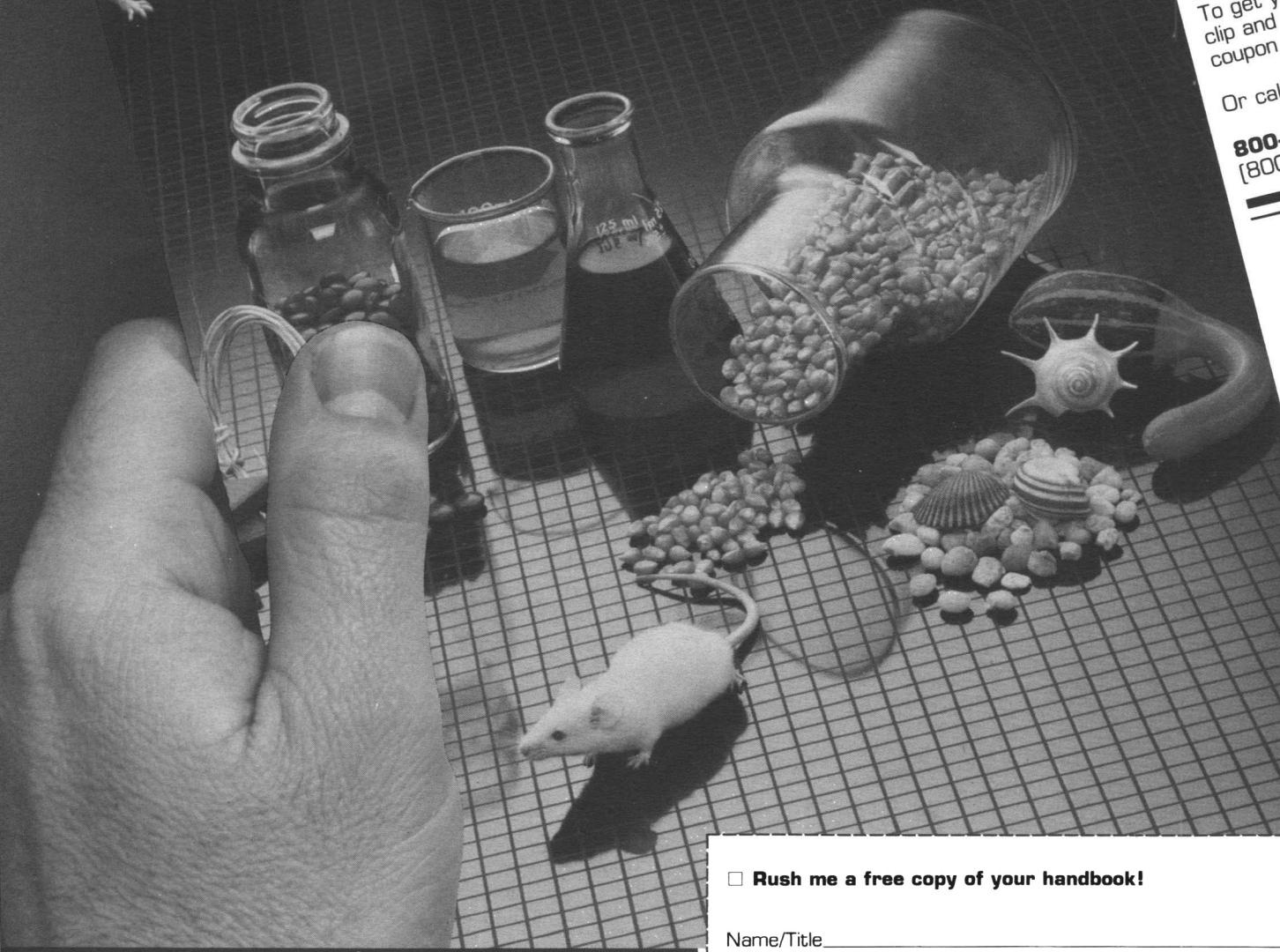
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Further information on the NBS Crystal Data Distribution Package is available from:

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The database is of interest to scientists of many disciplines.

- **Analytical Chemistry:** Identify chemical compounds using one tiny crystal, non-destructive
- **Materials Science:** Find materials having desired physical and structural properties and design new materials
- **Crystallography:** Save time and money... prevent redeterminations of crystal structures by checking to see if done previously
- **Mineralogy:** Study symmetry and pseudosymmetry of minerals with any given composition range
- **Ceramics and Metallurgy:** Identify phases even

with incomplete diffraction data

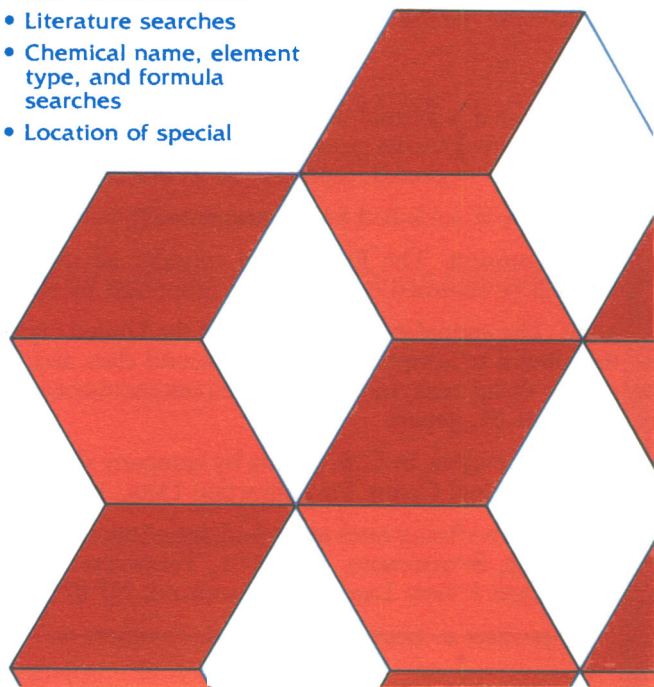
- **Inorganic and Organic Chemistry:** Characterize reaction products and intermediates uniquely and quickly

The NBS Crystal Data Distribution Package is also of special interest to powder diffractionists, electron diffractionists, solid-state and structural chemists, and technical information specialists. Other typical uses include:

- Compound identification and characterization
- Literature searches
- Chemical name, element type, and formula searches
- Location of special

chemical classes or types of materials

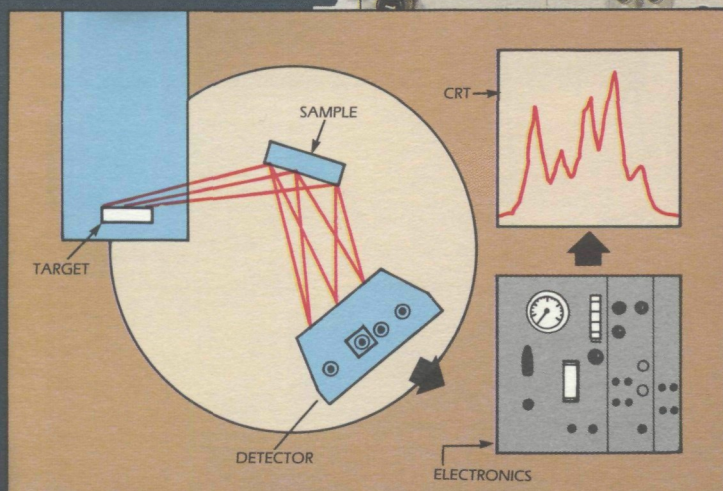
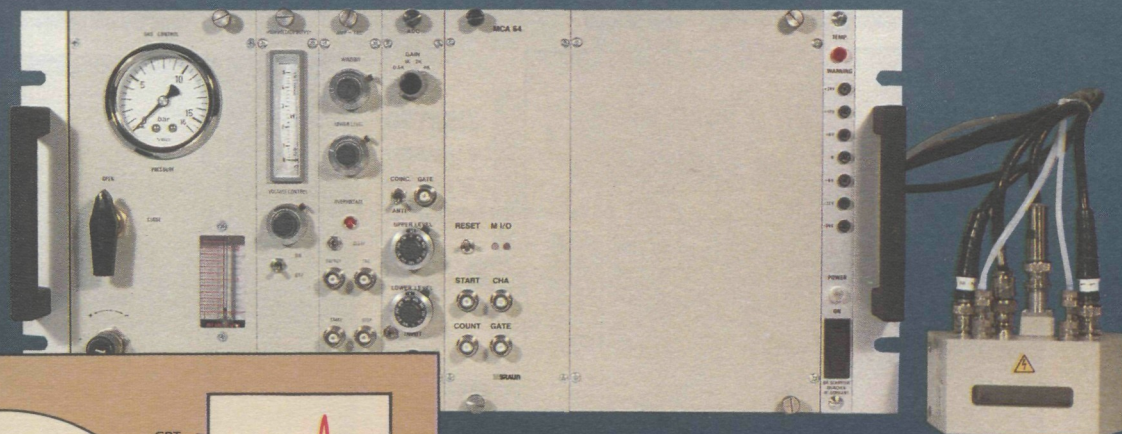
- Identification of compounds having specified properties
- Source of data for scientific and statistical research studies
- Searches on space groups, density ranges, crystal systems, and many other parameters



PD8

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- Guinier diffractometer
- Scattering experiments
- Time resolved diffraction.

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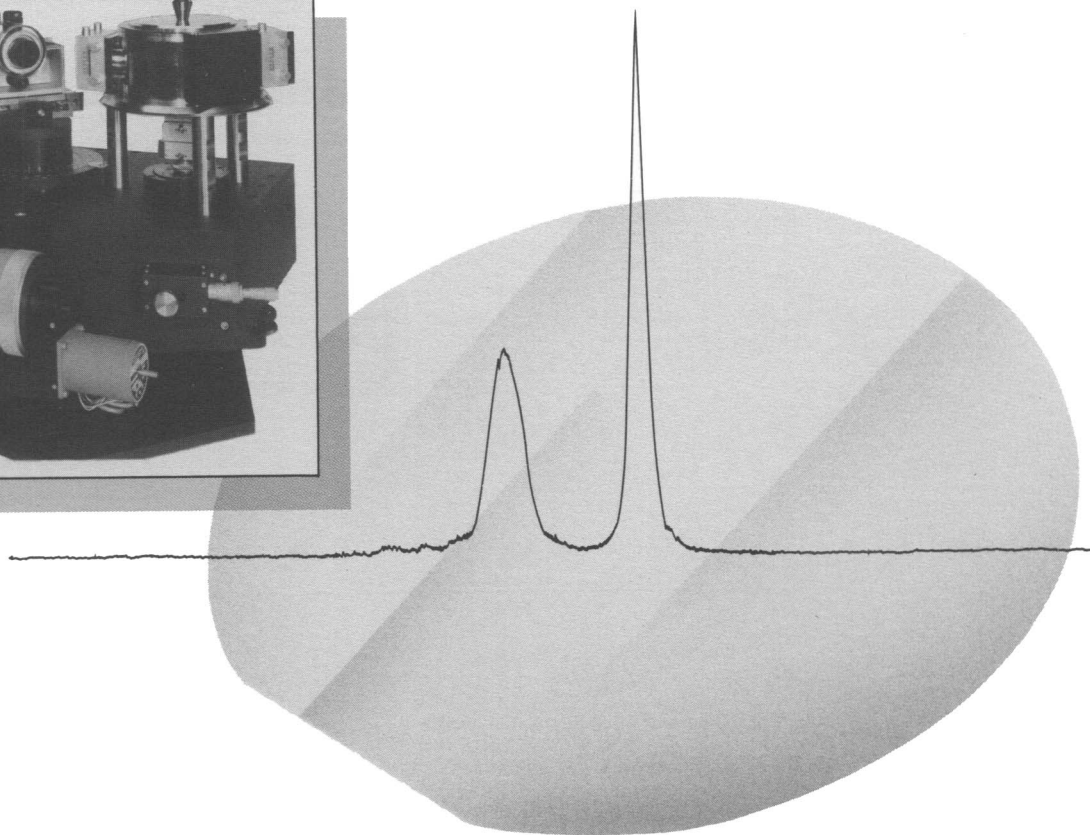
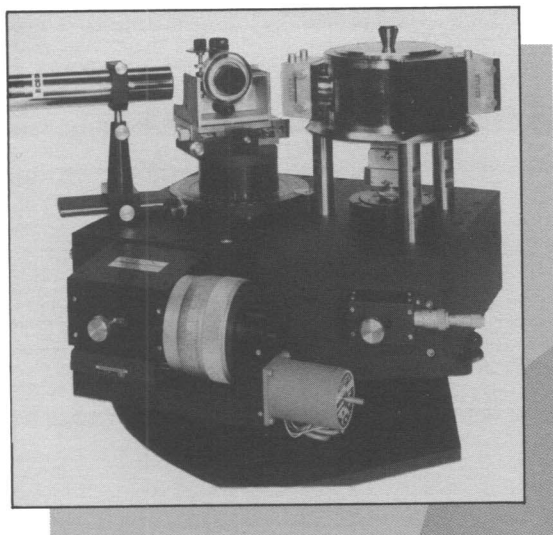
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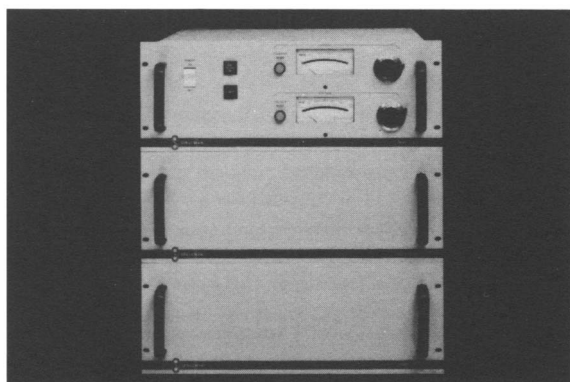
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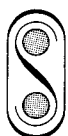
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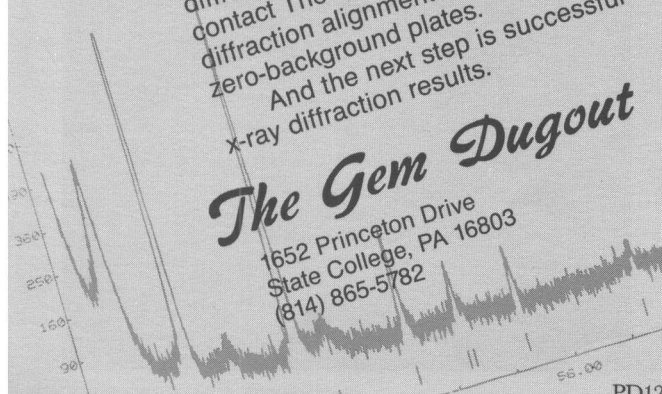
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PD11

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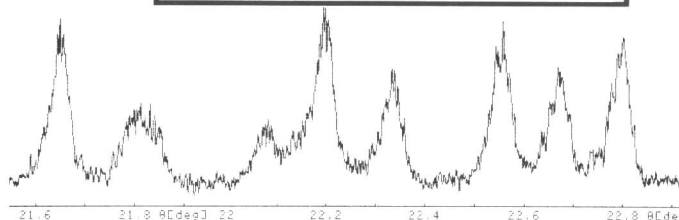
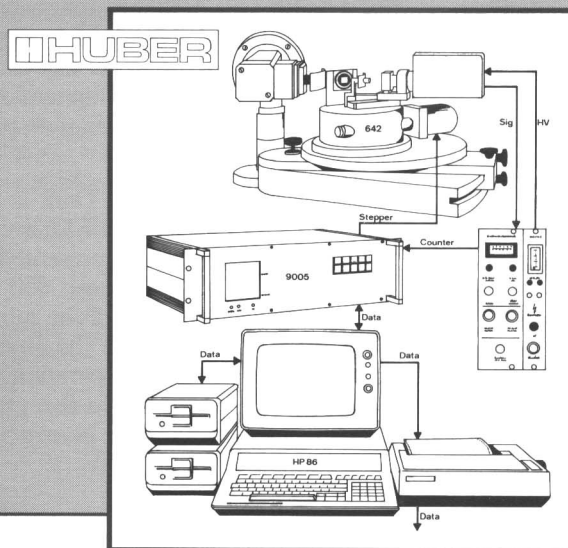
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PD13

Mineral Powder Diffraction File Data Book & Search Manual

850 *new* patterns

3400 patterns total

2700 species

Data Book

- Enlarged and revised for Sets 1–35
- Ordered alphabetically on mineral name

Search Manual contains sections on

- Chemical Name
- Hanawalt Numerical
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- Mineral Name

Since its inception almost 50 years ago, the Powder Diffraction File has always been well served in the area of mineral species. In 1974 the first special mineral based publication was produced, this being in the form of a book of minerals containing about 2,600 selected patterns in numerical sequence. A supplement to this edition was produced in 1981. In 1980 an alphabetically ordered data book was produced followed by a group data book in 1983. Each of these products has proven very popular both with the community of mineralogists as well as others involved in general qualitative phase identification.

The International Centre for Diffraction Data is now pleased to announce a new Mineral Powder Diffraction File containing about 2,700 species represented by 3,400 patterns. This selection includes about 850 new patterns added since 1980. This revision of the mineral file has been produced by the Editors of the International Centre for Diffraction Data in cooperation with the Minerals Subcommittee, and has been further guided by nomenclature recommendations of the International Mineralogical Association.

The Mineral Powder Diffraction File Data Book is ordered alphabetically on mineral name, thus grouping together patterns of the same mineral including hydrates, polytypes, order-disorder and chemical varieties, and obviating the need for an index. All data have been reedited with special reference to nomenclature, chemical formula, indexing and other crystallographic data. Physical data is also recorded including opaque optical data where available.

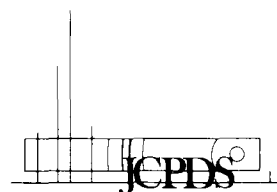
The Search Manual supplied with the new Data Book is based on the latest Hanawalt search/matching techniques including special provisions for finding patterns recorded using the Debye-Scherrer technique and data from highly oriented materials.

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PD14

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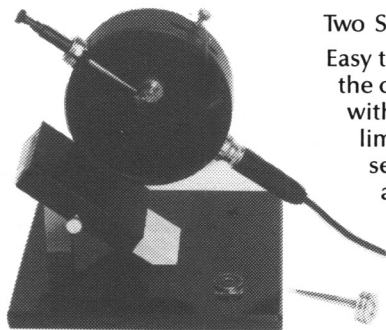
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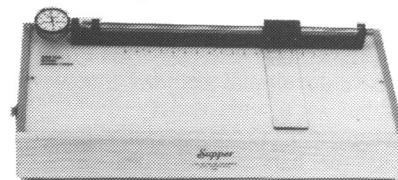
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PD16

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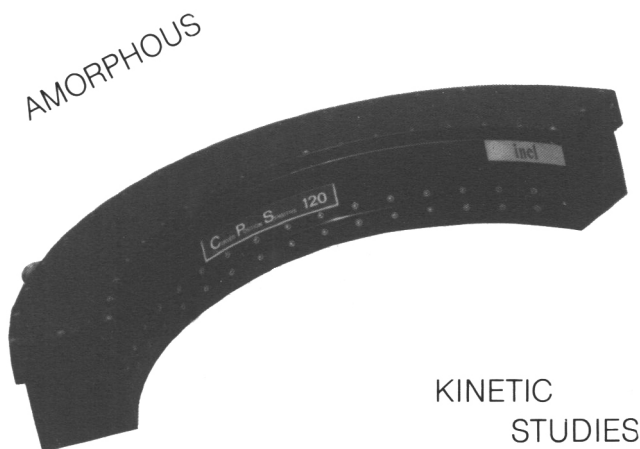
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PD19

XIV

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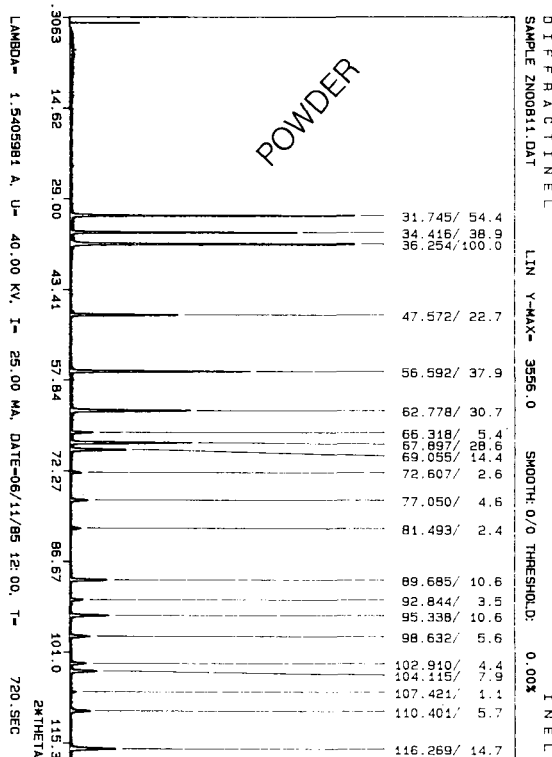
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PD21

Editorial

Presentation of Reference Data in *Powder Diffraction*

One of the purposes for creating *Powder Diffraction* was to provide a medium for the publication of new diffraction data. The first three issues have included data produced by the Research Associateship of the International Centre for Diffraction Data and other laboratories. The papers illustrate several formats which can be followed in the presentation of powder data.

Many compounds examined in the modern laboratory produce patterns superior to those presently in the Powder Diffraction File. Often, there is little time in the rush of the project to devote much effort to preparing a formalized description of compound, the data, and the documentation. Consequently, much useful data is lost to the scientific community. I would like to suggest a procedure to rescue these data and provide recognition to the experimentalist who collects the data.

The data published by the Research Associateship exemplifies the useful documentation organized in a concise manner along with the complete listing of the diffraction pattern. These tables can serve as a model to diffractionists who wish to prepare data sets for submission. Of course, the diffraction data is the most important component of the information, but it is more valuable with as much documentation as is possible. Conditions and diffraction parameters for the data collection and the description of the compound, both its chemistry and synthesis, need to be supplied by the submitter. Crystallographic data should also be supplied as far as it is known. If the pattern can be indexed and refined to determine the best-fit cell parameters, the information is desirable. However, all patterns submitted will be processed through the EXAIDS review program, and this check will confirm the indexing as well as much of the other information supplied and produce a refined cell along with the figures-of-merit. For any diffractionist who will take the time to supply this basic data to the editorial staff, we will process the data through EXAIDS and prepare the data tables and supporting information for a short article in *Powder Diffraction* if the data prove to be an improvement on the existing pattern.

The International Centre for Diffraction Data does have a standard form which is used by many diffractionists for submission of data. Copies of this form will be supplied on request. The Notes for Authors published in the first

issue also contains guidelines for documenting powder data. These guidelines were prepared by a committee of the American Crystallographic Association and accepted by the International Union of Crystallography. They were published in detail in National Bureau of Standards Special Publication 567 (1980). These guidelines resulted when a committee examined the quality of powder data available at the time and made recommendations to improve the status of these data. One of the major recommendations was the preservation of the original diffraction data, i.e. the 2θ values, and the analysis of errors based on these values. This decision was based on the linearity of errors on the 2θ scale and on the non-linearity of errors on the d-spacing scale. The effect is to require that the 2θ values be reported along with the rest of the data, so that EXAIDS can properly evaluate the accuracy of the data.

Diffractionists should not be discouraged from submitting data just because it does not meet all the requirements listed in the guidelines or match the quality of the data produced by the Research Associateship. This quality of data demands a considerable amount of time in the data collection. Any data set which is an improvement of existing data is useful. Some compounds may never yield this quality of data. For experimentalists who have a stock of compounds for which data should be collected, but who have no support for the time, may wish to consider the Grant-in-Aid program of the International Centre. It is designed to provide funding to support the data collection in just such situations.

This request for submission of experimental data is not meant to discourage the preparation of more detailed papers describing crystal-chemical studies and data analysis. It is not the desire of *Powder Diffraction* to establish a required format for all data presentation. However, such a format may encourage a lot of diffractionists to publish data which they would not otherwise take the time to prepare. If this effort does prove successful, we will start a section devoted to data sets and assign this section to a special editor for data. Go to your files, pull out those data sets and send in the necessary information.

Deane K. Smith
Editor-in-Chief