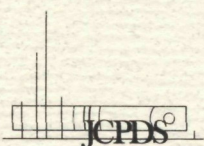


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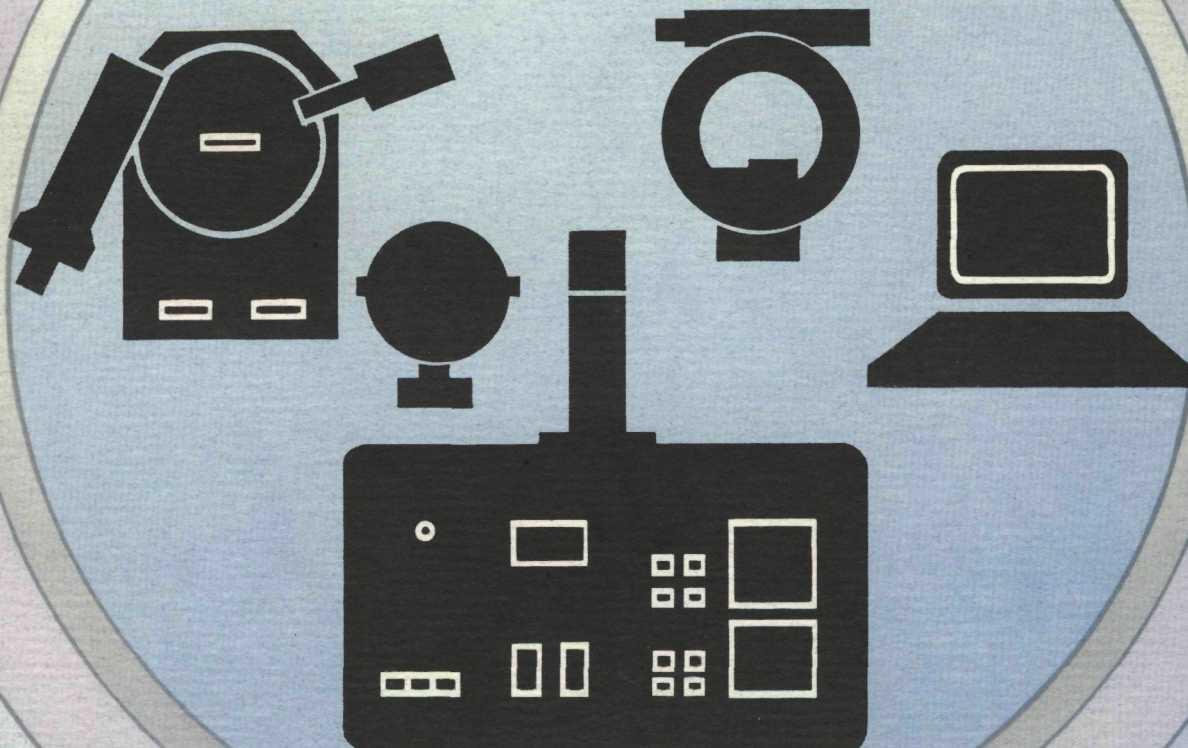
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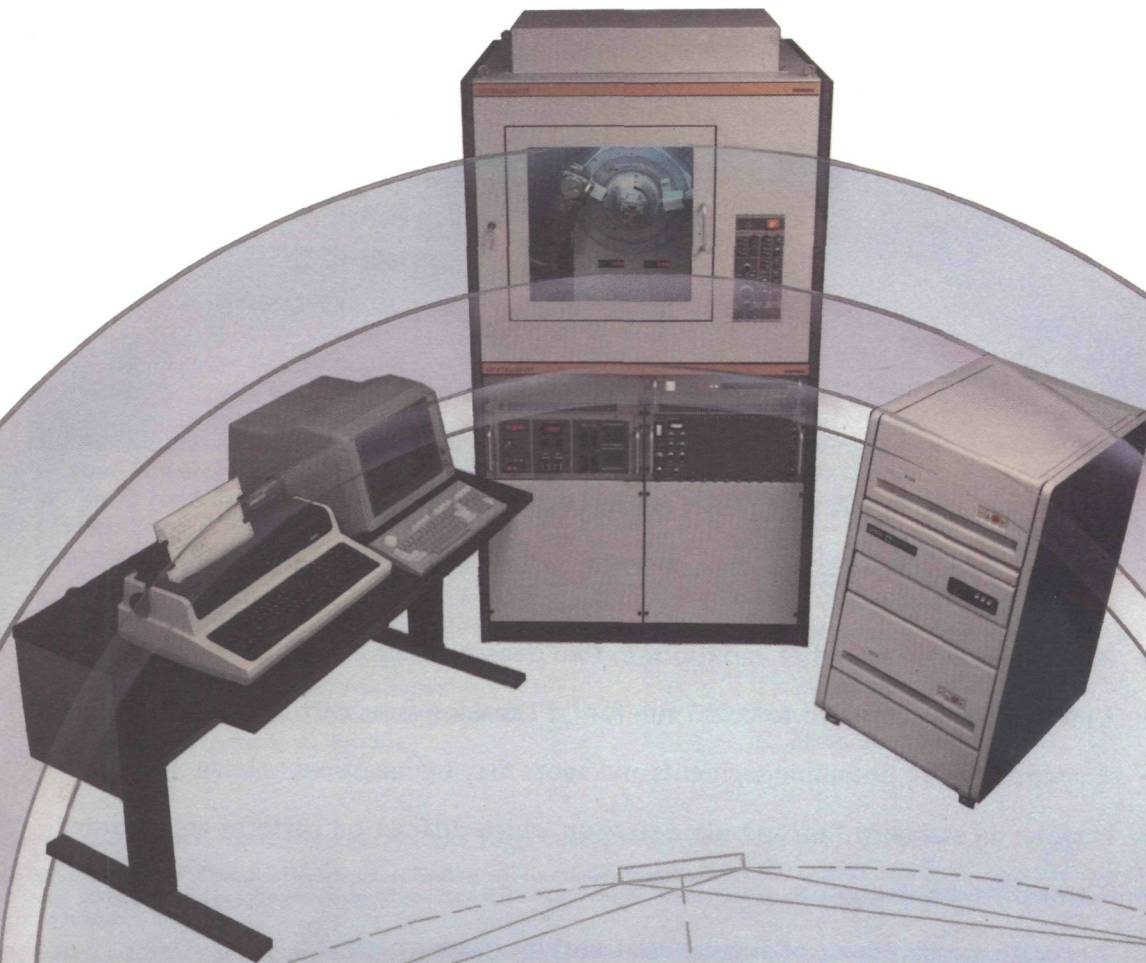
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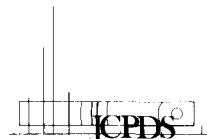
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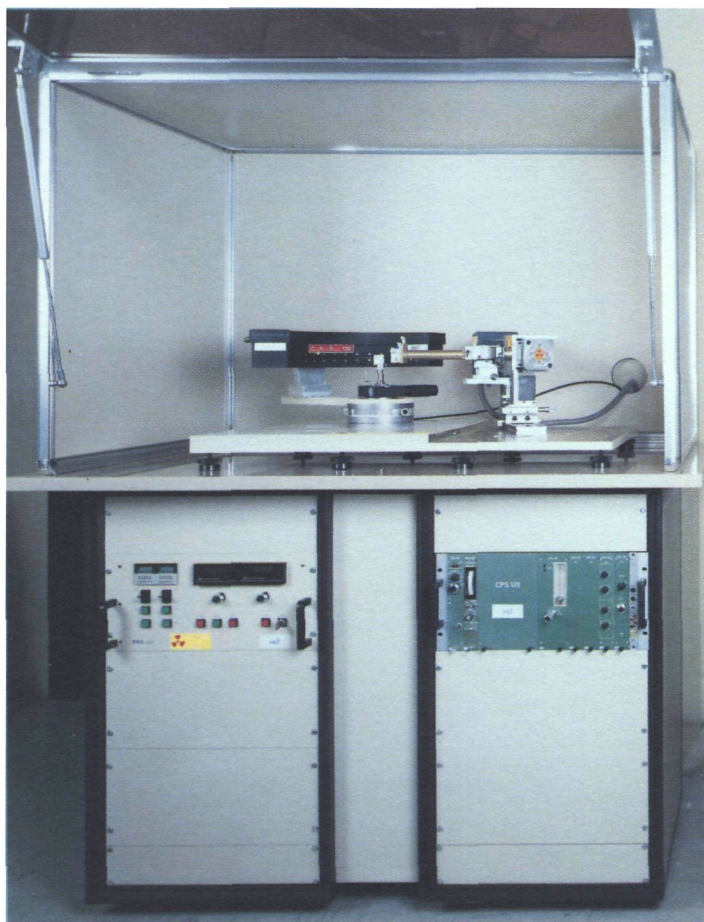
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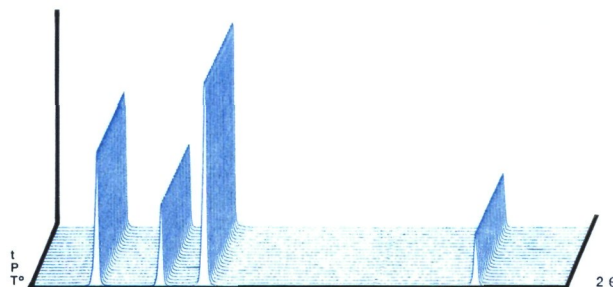
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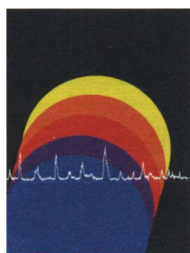
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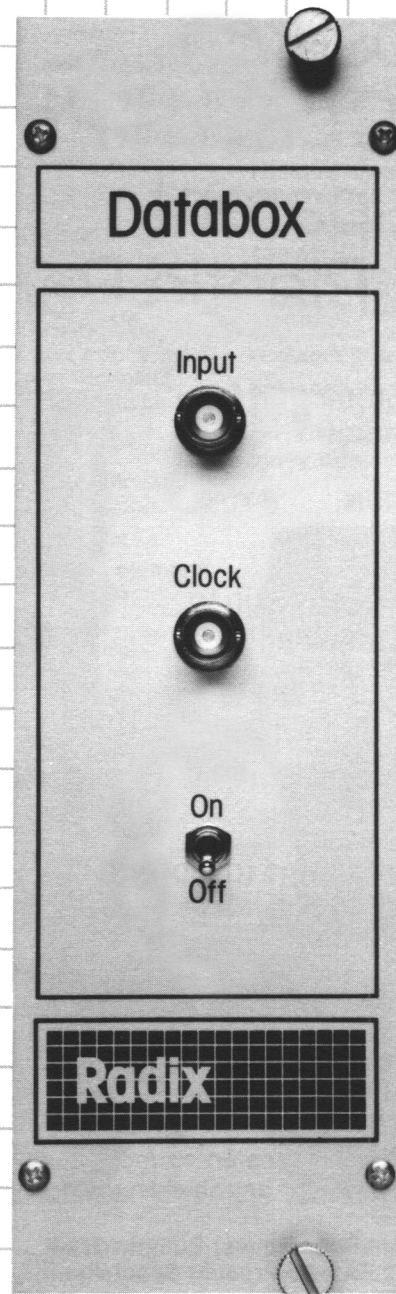
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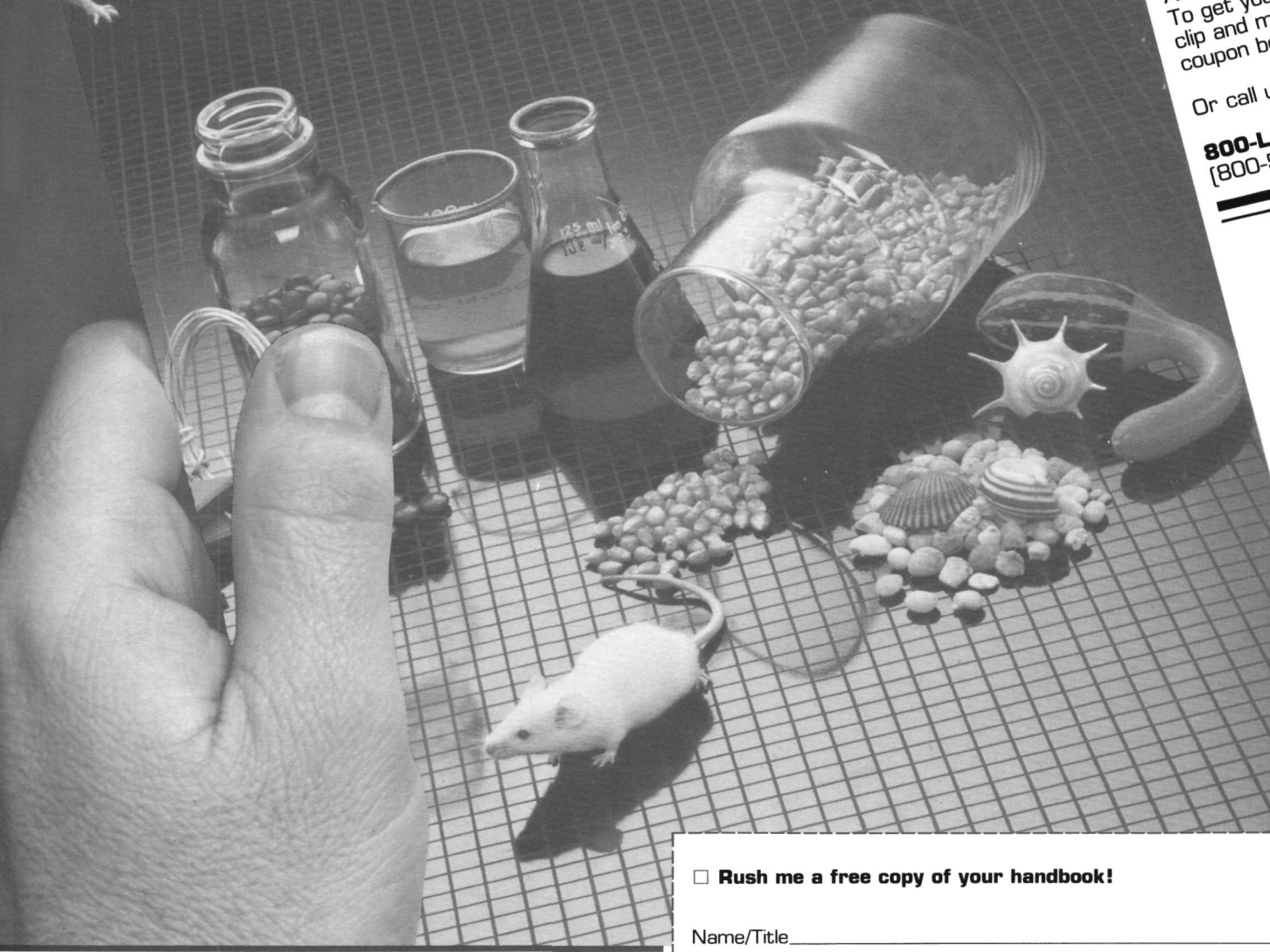
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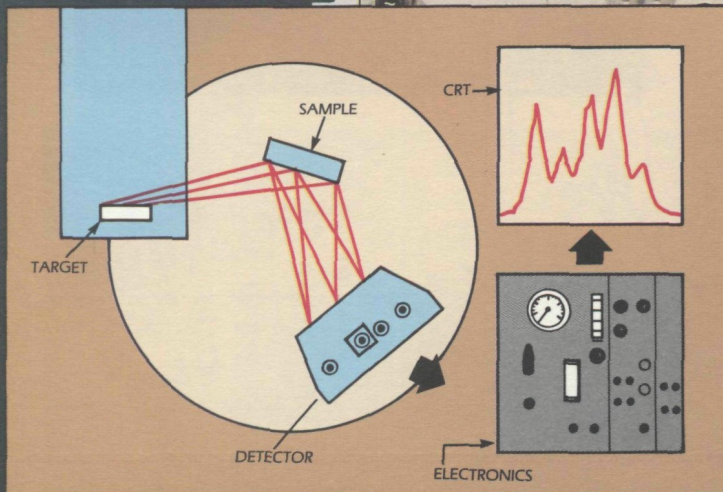
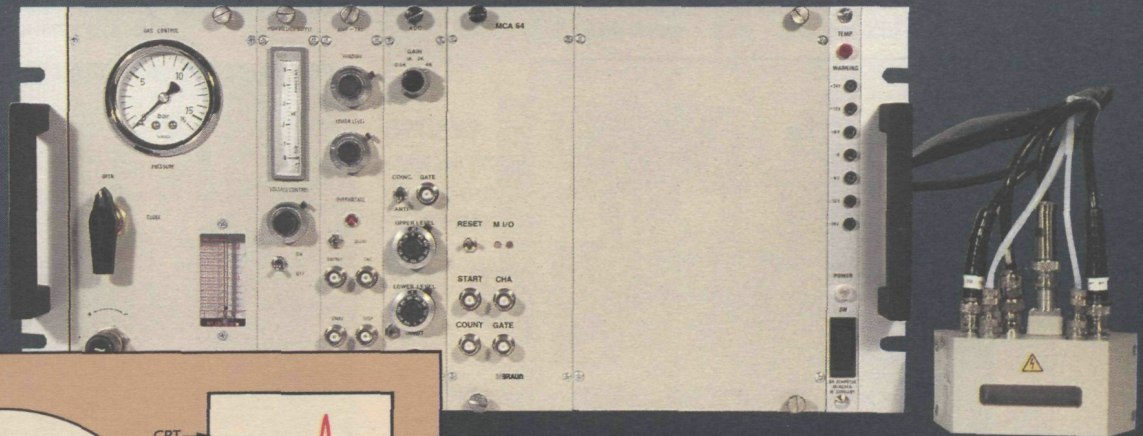
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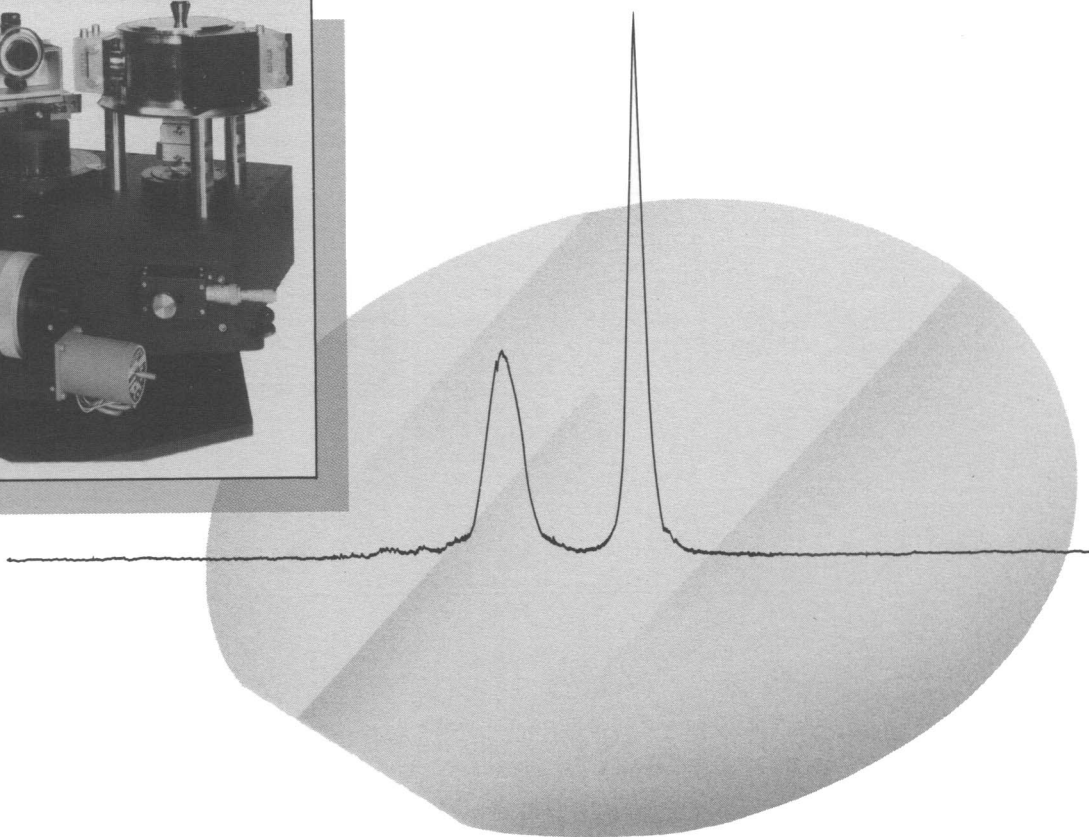
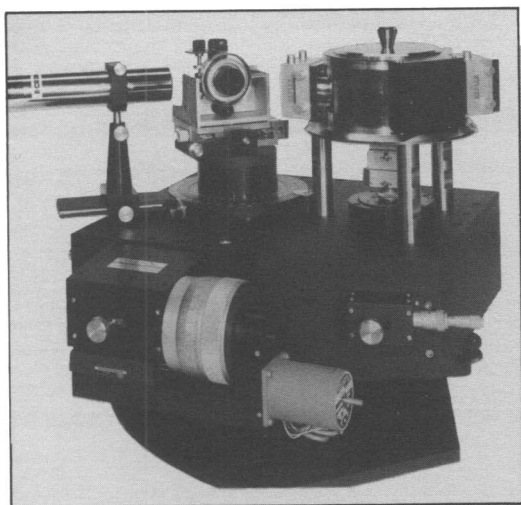
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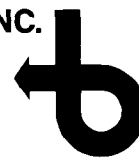
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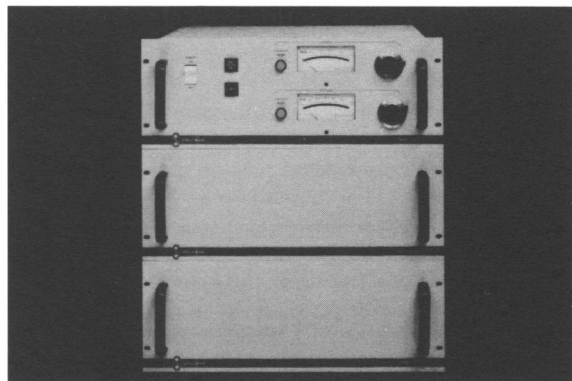
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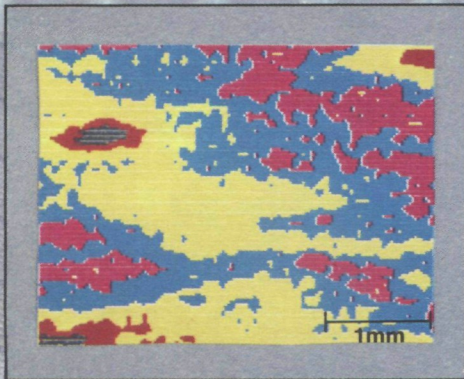
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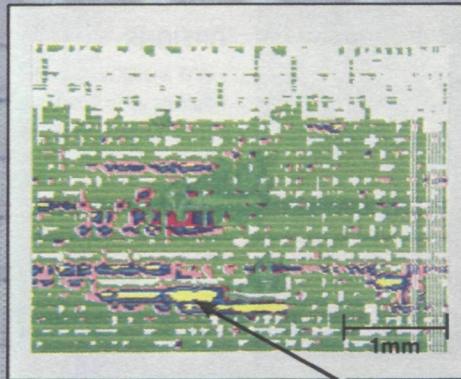
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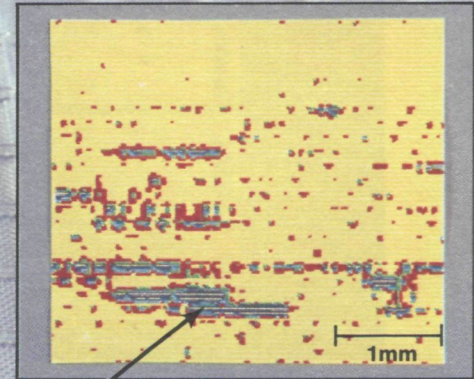


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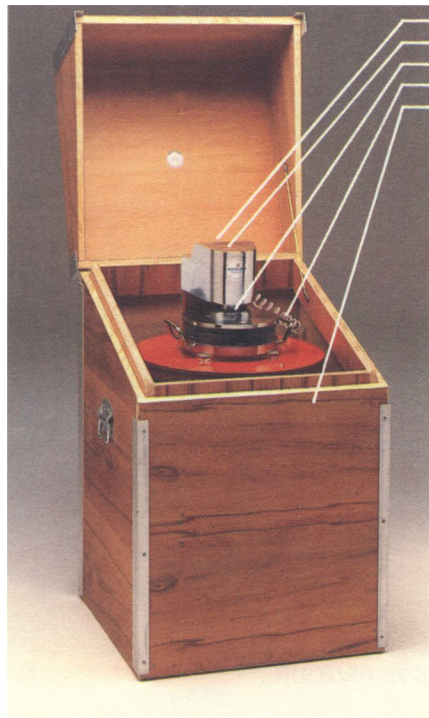


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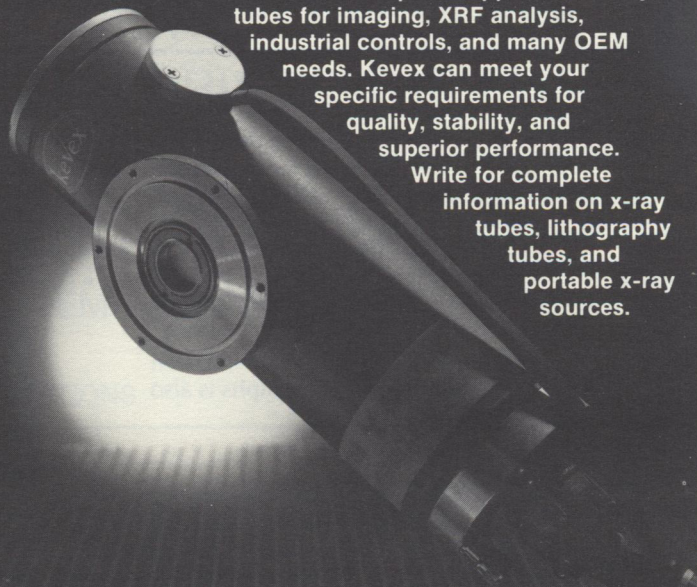
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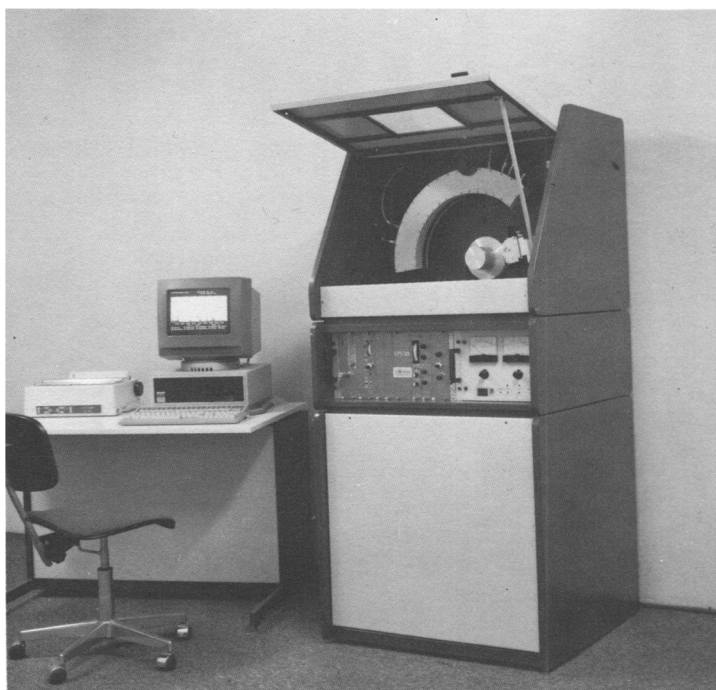


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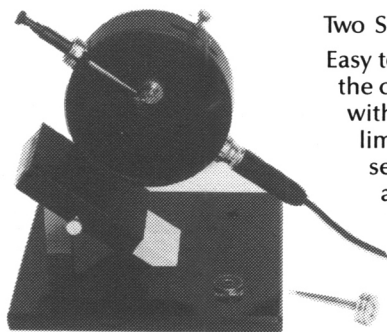
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PD17

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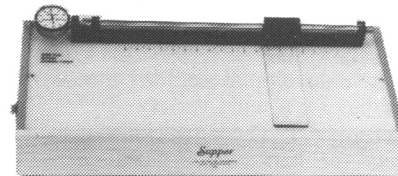
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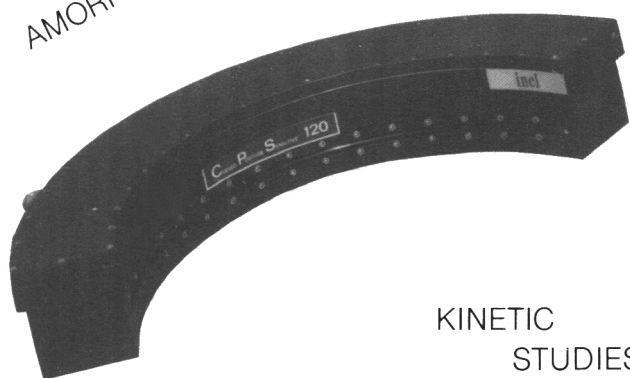
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PD18

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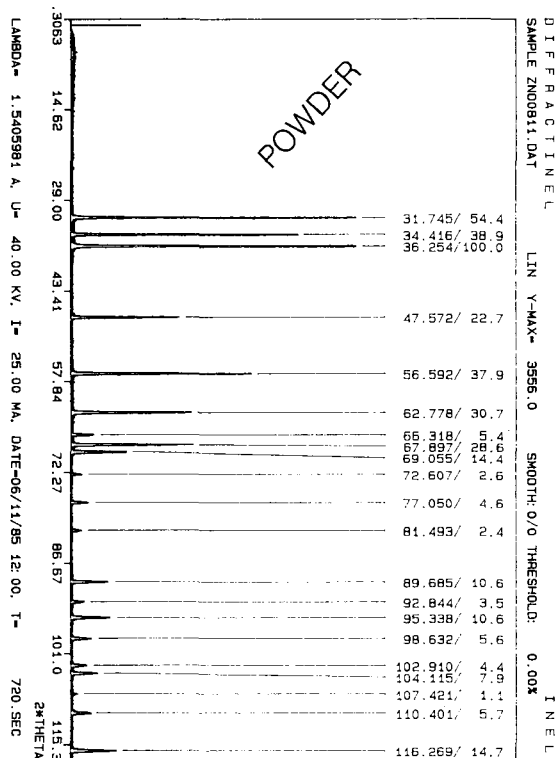
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PD19



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PD20

Guest Editorial

Help Wanted!

The number of known crystalline organic phases far outnumbers that of inorganic phases. However, organic phases are poorly represented in the Powder Diffraction File, numbering only about 12,500 of the 48,000 patterns in the current file. Historically, fewer scientists have prepared and published powder diffraction patterns of organic phases than those who have published patterns of mineral, metal, alloy, ceramic, and other inorganic phases. Undoubtedly, the smaller number of scientists using powder diffraction for organic materials is due, in part, to the development of analytical methods such as infrared spectroscopy and gas chromatography/mass spectrometry and the publication of collections of data for these methods. Powder diffraction not only can be an important analytical technique for confirming identification by these methods, but it can also be used to uniquely identify which polymorph is present for those compounds which form more than one crystalline phase.

The usefulness of the Organic and Organometallic File of the Powder Diffraction File has been hindered by two major problems: the relatively small number of reference patterns available, and the lack of access to patterns in the File using information from other analytical techniques. Most of the diffraction patterns in the Organic and Organometallic File have come from two types of sources: data which have appeared in the open literature and data which have been contributed by X-ray diffractionists directly to the Powder Diffraction File. Due to this reliance on published data and contributions, coverage of many common and useful areas has been very spotty, further limiting the usefulness of X-ray diffraction for organic analysis. Currently, reliance on data in the open literature produces few new patterns for the Powder Diffraction File because many journals no longer publish long tables of data such as X-ray diffraction patterns due to the rise in publishing costs in recent years.

In order to increase the number of useful organic patterns in the File, the International Centre for Diffraction Data has particularly emphasized organics in its calls for proposals for its Grant-in-Aid program the last few years. More projects are still needed in this area. Grants-in-Aid can be awarded either for preparation of powder diffraction patterns or for preparation of materials suitable for preparing such patterns. Projects in special areas such as polymers, forensic areas such as drugs and pigments, and common organic phases are of particular interest, but other classes will also be considered.

To provide access to patterns in the file using information from other analytical techniques, the Organic Subcommittee has actively promoted the classification of the patterns

in the Organic and Organometallic File according to functional groups. At this time, about 20% of the file has been classified by functional groups. This monumental work, which has been done almost entirely by one person, has now progressed to the point where a trial index has been prepared. Initial evaluations of the trial index have shown that it is possible to locate phases using information available from other analytical techniques (functional groups from infrared, elemental information from X-ray fluorescence or energy dispersive spectrometry, and combinations of these), or to determine how many phases having a particular functional group (e.g., tertiary amine), a combination of functional groups (e.g. a benzene ring with one or more halogens), or a broader class (e.g., morphine and its derivatives) are present in the File. However, much remains to be done in classifying the remaining 80% of the patterns in the file and testing trial indexes. The Organic Subcommittee needs more people who can help in this effort, either on a volunteer basis or, perhaps, with a limited amount of support.

Many diffractionists who analyze organic materials have little knowledge of organic nomenclature or structures. Most organic chemists know little or nothing about powder diffraction. This editorial is an appeal for those reading this journal to participate in these efforts to improve the Organic and Organometallic File. If you do diffraction work with organics or organometallics, consider submitting patterns of phases which are not currently in the File or which are poorly represented in the File, applying for a Grant-in-Aid to prepare patterns or to prepare material suitable for diffraction pattern generation, or volunteering to help with the work in the Organic Subcommittee in classifying and testing indexes based on functional groups. If you know someone in your department, university or industry who could contribute to the improvement of the Organic and Organometallic File, please find that person and suggest participation in one of the above ways. The Organic File has the potential to be far more useful than it is today. That usefulness can be realized by contributions of data and ideas by you and your colleagues.

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JCPDS – International Centre for Diffraction Data