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Summary of a Paper Presented at the Meeting of the International Mineralogical Association, Stanford University
Palo Alto, CA on July 18, 1986

Application of the 1986 JCPDS-ICDD Mineral Powder Diffraction File Computer Database to Mineralogical Problems

The 1986 update of the Mineral Powder Diffraction File (MPDF), Sets 1-35, is available for lease in computer readable form. Because it contains all of the information on the PDF card, queries of this database can include crystallographic and crystal chemical attributes, specific gravity, optical properties, etc., in addition to d-I data. Thus, the range of mineralogical problems that can be solved through application of the MPDF is greatly enlarged.

The database supplied by the JCPDS-ICDD adheres to a fixed format and is 10.5 Mb (132,000 80-column “cards”) in size. For efficient use it should be converted into a more compressed format, preferably through a data management system. Implementation of this database using the SAS Institute’s Statistical Analysis System on an IBM 3081 mainframe will be described. SAS INPUT statements provide conversion of the database fields to an internal storage format. The resulting SAS FILE is then searched on user-specified fields for desired ranges of values using logical relationships ranging from simple to sophisticated. Records matching the selection criteria become available to various SAS statistical and report procedures.

Examples of utilization of the MPDF database include:
(1) alphabetized sorts and creation of subfiles of minerals based on chemical, crystallographic and physical properties;
(2) statistical analysis of the MPDF for such characteristics as the "top 10 space groups" and the "most popular d-spacing for the strongest line in a pattern"; (3) delineation of minerals having particular properties (e.g. pyroelectricity) through selections of space group; (4) finding all minerals having a particular structure type (e.g. spinel) by selection of appropriate space group, Z and unit cell parameter range; (5) creation of a smaller searchable database that includes crystallographic data, physical properties and strong lines from the powder pattern.

A full paper based on this presentation will be the subject of a future article in Powder Diffraction.

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