

# Commercial Announcements

## X-Ray Fluorescence Software for Personal Computers

### NBSGSC

NBSGSC, a personal computer version of the National Bureau of Standards mainframe program, provides fundamental parameters X-ray fluorescence analysis with the COLA algorithm. Parameters include mass absorption coefficients, fluorescence yields, jump ratios, and line and edge wavelengths. Both measured or calculated source spectral distributions are selectable. Mass absorption coefficients are calculated from either the NBS Heinrich method or the Thin and Leroux method. Up to 25 analytes can be determined in up to 20 metal, oxide, or fused disk samples. Four different calibration curves are selectable. The program provides for known concentrations of unanalyzed elements. NBS updates and many other improvements are incorporated.

Utility programs and sample data files are included. Source code for user automation of data entry is included.

CALCO87 calculates theoretical alpha coefficients by means of fundamental parameters.

COMP87 applies the alpha coefficients from CALCO87 through the COLA algorithm to the calibration of standards and the determination of unknowns.

SDCC calculates infinite thickness or corrects thin-film intensities.

5¼" disks with documentation.

### Available Format

MS-DOS 2.0 or higher for IBM PC, PC-XT, PC-AT or compatible with 256K RAM and floppy and/or hard disk drives. No graphics necessary. Requires 8087 or 80287 coprocessor. Printer is optional.

The price is \$450.00.

### CORSET

CORSET, a personal computer version of Stephenson's mainframe program, provides quasi fundamental parameters X-ray fluorescence analysis by a most-efficient excitation energy algorithm that requires no source spectral distribution. The program applies necessary corrections for absorption and secondary fluorescence. The package contains programs to create, edit, and analyze data files. Sample data files are included. Up to 25 analytes under MS-DOS or 10 elements under Apple CP/M can be analyzed from a single composite standard, multiple composite standards, or multiple pure-element standards.

The data for standards and unknowns are contained in separate files. This enables the user to design the analytical task with great flexibility.

Under MS-DOS, the program accepts data and reports results in weight percent element, weight percent oxide, atomic percent element, and mole percent oxide formats. Under CP/M only, weight percent element is reported.

5¼" disk with documentation.

### Available Formats

1. MS-DOS 2.0 or higher for IBM PC, PC-XT, PC-AT or compatible with 256K RAM and floppy and/or hard disk

drives. No graphics necessary. Printer is optional. 8087 or 80287 coprocessor recommended.

2. Apple II CP/M for Apple II, II+, IIe, or IIc with Z-80 card, 80-column with lower case, 64K RAM and floppy and/or hard disk drives. Printer is optional.

The price for both versions is \$250.00.

### XRF4

XRF4, a personal computer version of H.E. Marr's BuMines IC 8712 program, reduces X-ray fluorescence data by means of popular empirical calibration models and flexible regression constraints in an off-line environment. The package contains programs to create, edit, and analyze data files. Sample data files are included. Up to 25 elements under MS-DOS or 6 elements under Apple DOS 3.3 or Apple CP/M can be analyzed for up to 50 samples.

Calibration models in XRF4 include straight line, multiple linear regression, self-absorption, Lucas-Tooth, Lachance-Traill, Rasberry-Heinrich, and Claisse-Quintin.

XRF4 offers to the user the flexibility of selection of all regression constraints and selection of model.

XRF4 is cyclic. At the end of each calculation the user can choose to print results, print coefficients, eliminate bad standards, change the model, change the element being regressed, or change constraints. XRF4 automatically identifies bad standards and offers the user the chance to eliminate them.

5¼" disk with documentation.

### Available Formats

1. MS-DOS 2.0 or higher for IBM PC, PC-XT, PC-AT or compatible with 256 K RAM and floppy and/or hard disk drives. No graphics necessary. Printer is optional.
2. Apple II CP/M for Apple II, II+, IIe, or IIc with Z-80 card, 80-column with lower case, 64K RAM and floppy and/or hard disk drives. Printer is optional.
3. Apple DOS 3.3 for Apple II+, IIe, or IIc with 48K RAM and floppy and/or hard disk drives. Printer is optional.

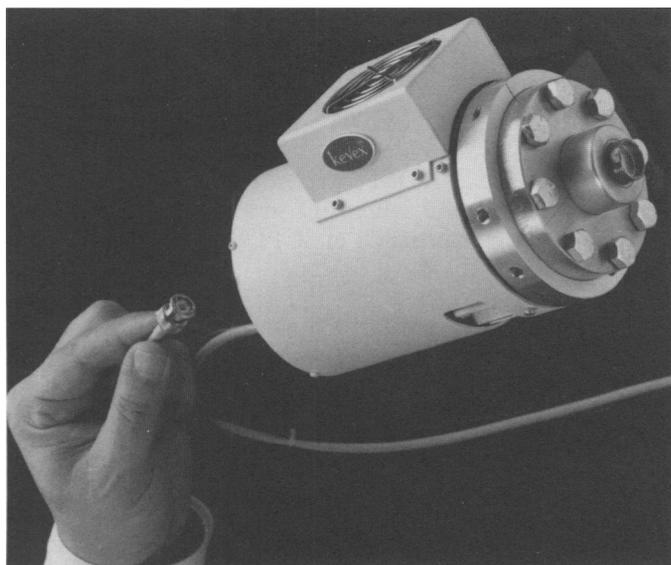
The price for all versions is \$150.00.

## New, Thermoelectrically-Cooled X-ray Detector (No Liquid Nitrogen)

Psi, the new X-ray detector from Kevex Corporation, eliminates the need for liquid nitrogen cooling in several materials analysis techniques. Psi provides the performance of a large LN<sub>2</sub>-cooled cryostat detector in a small, thermoelectrically-cooled package. Using Psi means basic improvements in the capabilities of several X-ray spectroscopy techniques.

Eliminating liquid nitrogen cooling means reduced size, reduced weight, reduced cost, and increased convenience. Increased ease of use, a wider range of applicability, and more mobility (portability) results for many types of analytical instruments.

X-ray spectroscopy techniques which will benefit include X-ray diffraction (XRD), energy dispersive X-ray fluorescence (EDXRF), wavelength dispersive XRF



(WDXRF), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and microprobe analysis. Some instrumentation will now be extended to process control, on-line/on-stream analysis, and warehouse/yard/field-portable analysis. Psi is also attracting interest in superconductivity materials and multi-layer thin films for near grazing incidence diffraction, total reflection X-ray fluorescence (TRXRF) and more traditional EDXRF composition and thickness studies.

The first implementations of this new technology are in products for X-ray diffraction (XRD) and wavelength dispersive X-ray fluorescence (WDXRF). In fact, several major manufacturers now offer Psi detectors on new automatic powder diffraction (APD) systems for XRD. Psi comes with mechanical and electronic interfaces that make it 100 percent compatible with existing APD systems, not just new ones.

The most important technical benefit of the Psi detector is that it captures the entire spectrum of energies from X-ray diffraction, scatter, and fluorescence information at every Bragg angle. The analyzer electronics can then select the "wanted" and reject the "unwanted" spectral window regions for processing.

In the older technology, scintillation and gas proportional detectors used crystal monochromators to reject "unwanted" X-rays before detection. They compensated for poor proportional detector resolution by diffracting only one band of wavelengths for analysis. For example, in the old approach to XRD a fixed monochromator limited structural study to diffraction of the X-ray tube K-alpha 1-2 doublet. Access was lost to the sample's K-beta and "white radiation" diffraction, Compton scatter, Rayleigh background and the complete X-ray fluorescence spectrum. In the old approach to XRF analysis, scanning monochromators limited materials chemistry studies to their Bragg bandwidth and reflection efficiency. Access was lost to the multi-element characteristic and scattered primary source spectrum.

XRD with Psi gives you 3 to 5 times faster throughput, 10 times better energy resolution, and the best diffraction

patterns you've ever seen. You even get clear  $K\alpha$  or  $K\beta$  scanning patterns from any diffraction tube anode. Teamed with the KeveX Spectrum Analyzer electronics, Psi gives you the complete sample spectrum — fully resolved. This means you choose your peaks, then optimize the spectral patterns to fit your application. It's an electronic monochromator.

We believe Psi detectors will rapidly replace monochromators and proportional detectors for most XRD and many XRF applications. Most of these X-ray applications also favor Psi in comparison with liquid nitrogen cooled intrinsic germanium ( $LN_2$ -IGe) and to curved or linear, position-sensitive proportional detectors.

In comparison with proportional detectors, expect Psi improvement factors for X-ray energy resolution of 8 to 20, detector capture efficiency of 2 to 4, and peak to background of 10 or more.

Compared to XRD monochromators, Psi achieves 2 to 4 times the counting efficiency, equivalent diffraction pattern peak resolution and up to a 5 times improvement in peak to background ratio.

Against  $LN_2$  cooled intrinsic germanium (IGe), Psi is clearly best in weight, size,  $LN_2$  replenishment cost and cooling convenience. The Psi vs.  $LN_2$ -IGe detector performance comparison is also clear. Energy resolution, peak to background, peak to tail, and count rate throughput favor silicon over germanium. All manufacturers, including those who supply to both X-ray and nuclear markets, use Si (Li) detectors for up to 40 KeV X-ray spectroscopy, and Ge (Li) or IGe for up to 3 MeV gamma ray spectroscopy.

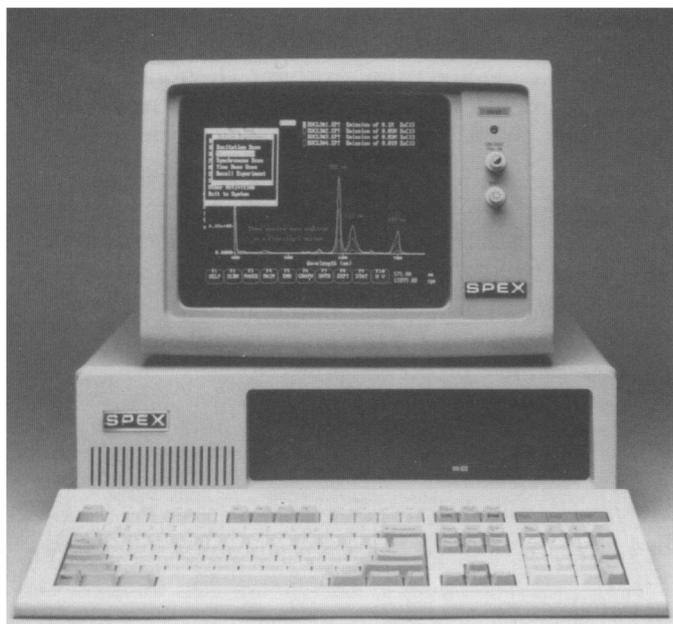
Psi is 4" in diameter by 6.5" long, and weighs < 7 pounds. Psi is compatible with an APD spectrometer's X-ray optics and mobility, without strain on its goniometer arm. The low power Peltier cooler stabilizes detector performance within 30 minutes of power up. It may be left on continuously, or turned off whenever necessary. The Psi cable set allows remote (up to 20 ft.) and convenient placement of all electronics.

**Technical Contact:** David Wherry, KeveX Corporation, 1101 Chess Drive, Foster City, CA 94404 (415)573-5866

## DM3000 Spectroscopy Computers Expand the Analytical Potential of SPEX Instrument Systems

The DM3000 series of spectroscopy computers has been introduced by SPEX Industries, Inc. to enhance the capabilities of all SPEX instrument systems. An exclusive new SPEX product line, the IBM compatible DM3000 series fully automates fluorescence, Raman or general spectrometric experiments via a dedicated hardware and software package.

XT or AT based depending on application, DM3000 models selectively incorporate hardware that encompasses high-voltage power supplies, scan controllers and data acquisition modules. All hardware is controlled by user-friendly, menu-driven SPEX software that includes experimental routines tailored to completely automate a



specific type of spectrometric analysis. Simple keystroke programming can also be used to create custom experimental methods, which may then be stored on disk to automate future work.

Data is displayed in as many as 16 colors on a thirteen-inch, high-resolution monitor. The system's dot-matrix graphics printer reproduces all displays with comprehensive file identification, and an optional multi-pen color plotter is available.

Headquartered at Edison, New Jersey, SPEX Industries has been supplying spectroscopists with state-of-the-art instrumentation for more than three decades. In addition to DM3000 spectroscopy computers, SPEX produces research spectrometers and spectrographs, filter fluorometers, spectrofluorometers, electro-optical and photoluminescence systems, cation measurement systems, and instruments for Raman spectroscopy.

**Contact:** Dean Maskevich, Marketing Communications Editor, SPEX Industries, Inc., Edison, N.J., U.S.A. (201) 549-7144.

## CD-ROM Search/Match System for Personal Computers

Materials Data, Inc. (MDI) announces the availability of Micro-ID/CD, search/match software that supports the newly released CD-ROM database from the JCPDS. Based on MDI's successful Micro-ID series of programs which permit rapid search/match of JCPDS subfiles (Micro-ID), full files (Micro-ID Plus), or a user's own databases (Micro-User), Micro-ID/CD is able to display images of matched phases in the complete JCPDS card format. These images include all information previously available only on card, book, or micro-fiche. Cell constants, space group and densities are just part of the new information which can be retrieved. Individual card images can also be easily printed for reports or laboratory use.

Micro-ID/CD operates on an XT, AT or compatible with a hard disk and requires a CD-ROM disk drive. The CD-ROM drive can be obtained from MDI or other sources.

Materials Data, Inc.  
P.O. Box 791  
Livermore, CA 94550  
(415) 449-1084

## PC Software and Systems

Responding to the needs of X-ray analysts, Criss Software is re-writing its XRF-11 package and other programs to run on the increasingly popular personal computers (XT and AT equivalents).

Delivery of the PC version of XRF-11 is planned for Fall 1987. The price will be \$4200, which includes the standard user license, programs, fundamental-parameters data files, media, documentation, shipping, telephone support service, and updates for one year.

Options will include selected PC systems and upgrades (XT- and AT-compatible), plus software for transferring data and results between the PC and other computers.

The new PC software development represents an addition, not a switch. Criss Software will continue to provide and support the highly successful versions of XRF-11 for Digital systems (for RT-11, RSX-11M, and VAX/VMS), which already have been supplied to laboratories in thirty-five countries.

Criss Software, Inc., 12204 Blaketen Street, Largo, MD 20772 USA (202) 249-7522.