Computer Program Abstracts

The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a Computer Program Abstract will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 *of the June* 1985 *issue of the Journal* [*J. Appl. Cryst.* (1986), **18**, 189–190].

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JOGGING – programs to add, shape, smooth and differentiate X-ray absorption spectra.

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The crystallographic problem: To prepare a theoretical analysis or simply follow the small changes in the X-ray absorption near-edge structures, it is easier to work with the second derivative (Poumellec, Marucco & Touzelin, 1987). Its use is often limited by noise in the absorption spectra and many people prefer to use the first derivative. In order to decrease the noise, users record several identical spectra and compute the mean value of absorption for each energy step. This method is efficient but is not correct because an erratic variation of 0·1 eV in the magnitude of the energy is commonly encountered owing to the mechanics of the monochromator. At the same time, changes in the incident intensity occur due to thermal variations of the apparatus.

Method of solution: Instead of computing the mean value step by step, merging of the almost identical spectra is preferred. A shift in intensity is commonly encountered between two successive spectra and therefore *JOGGING* analyses the nature of the difference. The first spectrum is taken as a reference and the relative difference between it and the next is calculated. If the incident intensity has varied, a constant relative difference is obtained. If two spectra give the absorption of a sample for different positions, a relative difference proportional to the reference absorption is obtained. If a hole is present in a sample, it yields a non-linear effect. *JOGGING* takes into account the first two cases and subtracts a mean difference expressed as $a + b\mu(E)$ (where a and b are constants) in order to collect a new file. The second derivative is not obtained in the conventional way by the finite difference method but by regression of a second-degree polynomial. A mean-square fit is performed on a set of experimental points within an energy window typically 3 eV wide and moved over the whole energy range. The derivative of the second-degree polynomial supplies the derivative of the absorption spectrum at the same time that smoothing is performed.

Software environment: An Apple IIE version is written in Applesoft Basic and uses an overlay structure in order not to exceed the 6144 bytes available for the code. The overlay structure was created by insertion into the DOS memory space of a procedure saving pointers to the variables before loading each overlay file. No graphics library is necessary for the Apple IIE. An IBM PC version is written in Fortran of R. M. Farland Corp. and uses the GRAFMATIC library of Microcompatibles Inc. Alternative graphics libraries could easily be implemented since the screen plotting is confined to a single subroutine.

Hardware environment: The program was initially implemented on a Tandy model II then on an Apple IIE and now runs on IBM PC/XT compatibles. To take full advantage of the interactive mode, the microcomputer should have some graphics facilities.

Program specification: *JOGGING* is an interaction program for a microcomputer performing all elementary procedures required for the shaping process of X-ray absorption spectra: baseline correction (polynomial), standardization (maximum–minimum, at fixed energy or by EXAFS extrapolation) and glitch suppression. The spectrum is displayed in interactive high-resolution graphics mode at each stage of the shaping process and a screen copy facility is included. The program listing contains 950 lines.

Documentation: The program is provided with some instructions for use in both machine-readable and printed form.

Availability: The program source code and its associated documentation are available from the authors. Two $5\frac{1}{4}$ inch floppy disks are required. For the IBM PC version, the Fortran source graphics subroutine is provided but requires the GRAPHICS library available from Microcompatibles Inc.

Keywords: EXAFS, XANES, X-ray absorption, data analysis.

Reference

Poumellec, B., Marucco, J.-F. & Touzelin, B. (1987). *Phys. Rev. B*, **35**, 2284–2294.

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LOGO DESIGN CONTEST

Prize: US$1000 in IUCr publications or US$600 in cash, as chosen by the winner

Entries are invited for the design of a LOGO for the International Union of Crystallography.

Conditions

(1) All designs must be received by the

IUCr Logo Committee,
c/o Professor Kaarle Kurki-Suonio,
Department of Physics,
University of Helsinki,
Siltavuorenpenger 20 D,
SF-00170 Helsinki,
Finland
Telephone 358 0 650211,
Telex 122229 nuphu sf, Telefax 358 0 656591

on, or before, the closing date of 15 July 1988.

(2) The selection of the winning logo will be the responsibility of the IUCr Logo Committee subject to approval by the Executive Committee. The winning entrant will be informed directly and the winner's name will be published in *Acta Crystallographica* and *Journal of Applied Crystallography*.

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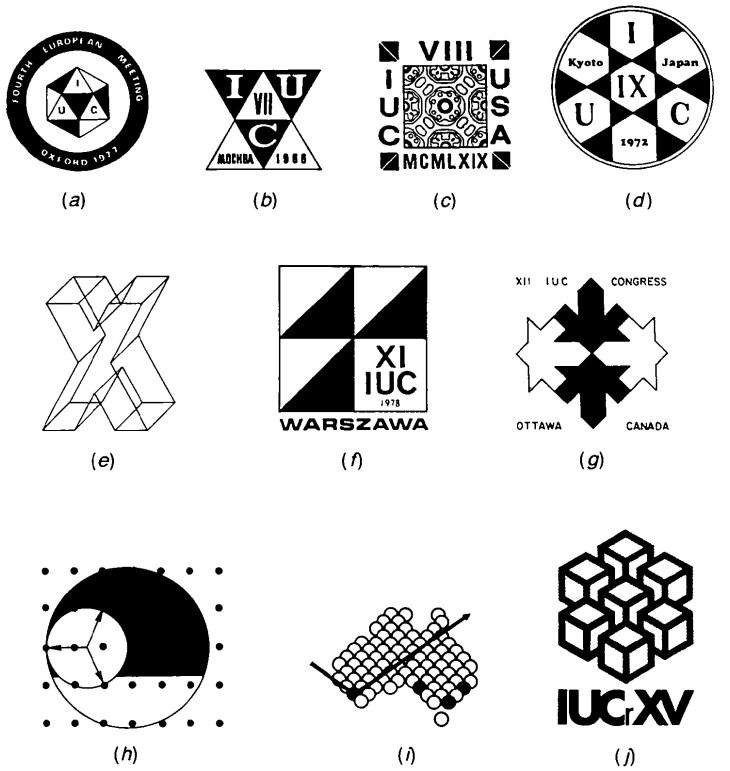

(*a*) (*b*) (*c*) (*d*) (*e*) (*f*) (*g*) (*h*) (*i*) (*j*)

Fig. 1. Some logos for crystallographic conferences. (*a*) Fourth European Crystallographic Meeting, Oxford, England, 30 August–3 September 1977. (*b*) IUCr VII, Moscow, USSR, 12–19 July 1966. (*c*) IUCr VIII, Stony Brook, USA, 13–21 August 1969. (*d*) IUCr IX, Kyoto, Japan, 26 August–7 September 1972. (*e*) IUCr X, Amsterdam, The Netherlands, 7–15 August 1975. (*f*) IUCr XI, Warsaw, Poland, 3–12 August 1978. (*g*) IUCr XII, Ottawa, Canada, 16–25 August 1981. (*h*) IUCr XIII, Hamburg, Federal Republic of Germany, 9–18 August 1984. (*i*) IUCr XIV, Perth, Australia, 12–20 August 1987. (*j*) IUCr XV, Bordeaux, France, 19–28 July 1990.

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