



Fig. 2. Profile analysis of the TbAsO_4 magnetic 111 neutron diffraction peak measured at 0.4 K (data points). The analysis was performed by constraining the halfwidths of Gaussian functions according to the calibrated halfwidth characteristic of the diffractometer. The best fit (bold curve) ends with $R_{PF} = 2.3\%$ ($R_{PF}^{\text{stat}} = 1.6\%$) under the assumption of six curves (thin lines) representing three plus and minus satellite reflections each; a profile fit with only one Gaussian function results in $R_{PF} = 13.1\%$ (Kockelmann, 1989).

adapter. The program has been tested using a memory configuration of 640 kbyte and the operating system DOS 3.3. All necessary interface routines are implemented: driver for graphic display, mouse driver (Microsoft-compatible mouse) and plotter driver (HP-compatible plotter). The only input needed is the observed counting rates to be analysed. The appropriate angular scaling has to be defined by START, STEP, STOP information at the beginning of the data set. The refined parameter results are stored in a file PROFPRM, which additionally may contain U , V , W parameters to replace the program defaults.

Program specification: PROFAN-PC is dimensioned to handle data sets of up to 3275 data points. The data set has to be segmented into sections of up to 350 data points for performing the profile fitting. At maximum, 13 peak profiles containing three parameters each, i.e. 39 parameters, may be refined simultaneously.

A further version called XPROFAN-PC is provided to handle Pearson VII and pseudo-Voigt functions with four parameters each for an additional variation of Gaussian and Lorentzian profile contributions. XPROFAN-PC is limited to a maximum of 10 peak profiles and 40 parameters to be refined simultaneously.

Documentation and availability:

The source code of PROFAN-PC is available on a PC diskette. The program is delivered including a diffraction data file for an immediate handling and performance test. A detailed description of all handling facilities is provided. To apply for a copy of the program one of the authors should be contacted at the above address.

Keywords: Personal computer program, profile analysis, peak decomposition.

References

- Hamilton, W. C. (1964). *Statistics in Physical Science*. New York: Ronald Press.
- Jansen, E., Schäfer, W. & Will, G. (1988). *J. Appl. Cryst.* **21**, 228–239.
- Kockelmann, W. (1989). Diploma thesis, Mineralogica; Institute of Bonn Univ., Federal Republic of Germany.
- Rietveld, H. M. (1969). *J. Appl. Cryst.* **2**, 65–71.
- Schäfer, W. & Will, G. (1979). *J. Phys. Chem. Solids*, **40**, 239–245.
- Will, G., Jansen, E. & Schäfer, W. (1989). 12th European Crystallogr. Meet., Moscow, USSR, 20–29 August 1989.

Crystallographers

J. Appl. Cryst. (1990). **23**, 445

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

Professor **Frank C. Hawthorne**, Professor of Crystallography and Mineralogy at the University of Manitoba, has been elected a Fellow of the Royal Society of Canada. His work focuses on topological/graphical aspects of oxysalt minerals and their role in explaining mineral chemistry and behaviour in geological processes, and spectroscopic methods applied to mineral chemistry and characterization.

Professor **Arne Magnéli**, University of Stockholm, 1975–1978 IUCr President, has been awarded the Georges Chaudron Gold Medal by the French Society for High Temperatures and Refractories (Société des Hautes Températures et des Réfractaires).

Professor **A. McL. Mathieson**, Honorary Professor in the Department of Chemistry, La Trobe University, Bundoora, Victoria, Australia, received an honorary degree of DSc from the University of St Andrews, Scotland, on 6 July 1989.

New officers have been elected for the Society of Crystallographers in Australia. Professor **J. W. White**, Research School of Chemistry, Australian National University, Canberra, ACT, is the new President. Dr **A. H. White**, School of Chemistry, University of Western Australia, Nedlands, Western Australia, is Vice-President. Dr **G. A. Williams**, Australian Radiation Laboratory, Yallambie, Victoria, is Secretary and Dr **C. H. L. Kennard**, Department of Chemistry, University of Queensland, St Lucia, Queensland, is Treasurer.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

J. Appl. Cryst. (1990). **23**, 445–446

The Dorothy Hodgkin Prize of the British Crystallographic Association

In celebration of Professor Dorothy Hodgkin's 80th birthday, the British