

dard Weissenberg film, but for diffractometer data further counting would be required.

Although the estimated standard deviations for the film data obtained from the densitometer measurements are a useful guide in assessing the level of the random errors in the data, neither the 100 μm nor the 200 μm data-collection method gave a true measure of the errors. We conclude, therefore, that great emphasis should not be placed on these values in devising a weighting scheme to be used in the least-squares analysis of the data.

As a result of this work we have demonstrated that the diffractometer can be used for obtaining high-quality diffuse-scattering measurements in about the same time as the Weissenberg method (and quicker than using oscillation techniques as these require many separate exposures and unravelling of the diffraction patterns) and with about the same or better resolution. Normally the diffractometer is used by structural crystallographers for collecting only Bragg reflections and this must mean that a great deal of useful and informative diffuse scattering is missed. We hope that the present work will stimulate others to use their diffractometers at least to *look* for diffuse scattering as a routine part of their structural study. In some cases this may provide important clues to

the solution of the structure, particularly when normal refinement methods have failed.

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Standard crystallographic file structure – 84. By I. D. BROWN (SCFS Project Coordinator), *Institute for Materials Research, McMaster University, Hamilton, Ontario, Canada L8S 4M1*

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Abstract

The Commissions on Crystallographic Data and on Crystallographic Computing of the International Union of Crystallography have approved a revised version (SCFS-84) of the Standard Crystallographic File Structure reported in *Acta Cryst.* (1983), **A39**, 216-224. The major change involves the definition of new sections describing the space group (SG NAME) and atomic coordinates (ATOMS) to supersede those in the earlier standard (SPACE GROUP and ATOM respectively). A new section (BONDS) is defined and other sections are extended to include a wider range of data. Copies of SCFS-84 may be obtained from

the author or the Executive Secretary of the International Union of Crystallography.

The standard described in the *Abstract* has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42068 (33 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. Copies may also be obtained from the author.