2. It should be noted that a number of peaks overlapped with Al peaks from the sample holder and could not be used in the refinement. In view of possible correlation effects, significance tests on b_{Cs} were carried out as described by Hamilton (1965). The confidence intervals at the 95 and 99% levels were found to be $\pm 0{\cdot}015$ and $\pm 0{\cdot}022 \times 10^{-12}$ cm respectively, and the final value of b_{Cs} has therefore been chosen as $0{\cdot}55 \pm 0{\cdot}02 \times 10^{-12}$ cm.

At 4·2°K, the observed temperature factors may be equated directly to the zero-point energy parameter $6h^2/4km\theta$ in the Debye–Waller expression, which yields θ values of 94 and 225°K for Cs and Cl, respectively. The Debye temperature of CsCl has been reported as 159°K from elastic measurements (Fedorov, 1968) or 166°K from specific heat measurements (*International Tables for X-ray Crystallography,* 1962).

The value of $0{\cdot}55 \times 10^{-12}$ cm for b_{Cs} is radically different from the value of $0{\cdot}75 \pm 0{\cdot}02 \times 10^{-12}$ cm recently reported by Zivadinovic & Prelesnik (1966), who also worked with CsCl. It is, however, in excellent agreement with values obtained by refinement of intensity data from some $\mathrm{CsMX_3}$ compounds (Table 3), and within experimental error agrees with the value of $0{\cdot}49 \times 10^{-12}$ cm found by Shull & Wollan (1951). It is perhaps significant that Zivadinovic & Prelesnik's figure was derived in a different way, namely from measurements of the intensities of strong reflections of the type $h+k+l=2n$ only, which were then placed on an absolute basis by means of a nickel standard. This procedure requires fairly substantial absorption corrections, which must be determined experimentally. It is to be noted that an amplitude of $0{\cdot}75 \times 10^{-12}$ cm would result in an intensity ratio of about 2% for the first two peaks, while the observed ratio in their published pattern is clearly about 10%. No details of the amount of half-wavelength contamination were given, but for neutrons of 1·03 Å wavelength it is unlikely that this can account for more than a small fraction of this difference. Moreover, rough intensity calculations based on several peaks of this pattern do in fact yield a value of about $0{\cdot}5 \times 10^{-12}$ cm. It is not clear why the use of an external standard should give such a different result.

Table 3. *Values of* b_{Cs} *obtained from least-squares refinement of neutron powder data from various* Cs *compounds*

Standard errors are given in parentheses. Other scattering amplitudes taken from the Neutron Diffraction Commission (1969) compilation.

Compound	b_{Cs} ($\times 10^{12}$ cm)
CsCl	0·549 (7)
$\mathrm{CsNiCl_3}$	0·551 (15)
$\mathrm{CsCoBr_3}$	0·569 (23)
$\mathrm{CsMnBr_3}$	0·546 (8)

References

COPLEY, J. R. D. (1970). *Acta Cryst.* **A26**, 376.
FEDOROV, F. I. (1968). *Theory of Elastic Waves in Crystals*, p. 356. New York: Plenum Press.
HAMILTON, W. C. (1965). *Acta Cryst.* **18**, 502.
International Tables for X-ray Crystallography (1962). Vol. III, p. 240. Birmingham: Kynoch Press.
KOESTER, L. (1967). *Z. Phys.* **198**, 187.
MERIEL, P. (1970). *C. R. Acad. Sci. Paris*, **B270**, 560.
Neutron Diffraction Commission (1969). *Acta Cryst.* **A25**, 391.
SHULL, C. G. & WOLLAN, E. O. (1951). *Phys. Rev.* **81**, 527.
WANG, F. F. Y. & COX, D. E. (1970). *Acta Cryst.* **A26**, 377.
ZIVADINOVIC, M. S. & PRELESNIK, B. V. (1966). *Acta Cryst.* **20**, 315.

Acta Cryst. (1971). **A27**, 495

Supplement to the powder intensity project of the IUCr.

By M. LINKOAHO, E. RANTAVUORI and U. KORHONEN,
Laboratory of Physics, Helsinki University of Technology, Otaniemi, Finland

(*Received* 16 *March* 1971)

It is concluded that an accuracy of ±1% can be attained, at least relatively, in powder intensity measurements.

The results of the *Powder Intensity Project* of the International Union of Crystallography (Jennings, 1969) show that 'integrated intensities may not be relied on to better than 5%, even on a relative basis' and 'it does appear that the absolute measurements do not show markedly more range than the relative measurements'. In order to obtain some explanation of the discrepancies in these results the respondents were asked to answer a detailed questionnaire considering the method and the treatment of the results of their measurements. Only three laboratories were, however, able to give a thorough clarification. For that reason these participants obviously form a definite group. In this report we shall consider further results obtained in these laboratories.

Paakkari, Suortti & Inkinen (1970) have published a thorough report, where they have described the research work performed in connexion with the project. The details of their experimental arrangement have been studied very carefully. Table 3 of their report shows new absolute values of $10^4 f^2/\mu$ for the nickel sample SC. These results are shown in Table 1 column 3, normalized (the original values are in parenthesis) so that the sum of the reflexions is the same as Jennings' results for sample SL, which are in column 2.

We have, in our laboratory, devoted considerable effort to the measurements of the polarization factor (k) of our quartz monochromator. We have repeatedly measured integrated intensities from both powder specimens and from a perfect Ge crystal with and without monochromator. Our final result was $k=0{\cdot}90 \pm 0{\cdot}02$. This value is near to that expected for a perfect crystal, $k=\cos 2\theta_M = 0{\cdot}89$, but differs from our previous result used in the project. Table 1 shows our corrected results (for sample SJ) compared with other

Table 1. *The new results* $10^4f^2/\mu$ *obtained for the samples SC and SJ of the International Powder Intensity Project compared with the results of Jennings for the sample SL*

The range of these values is shown together with the total range in the project. The values in parenthesis refer to the absolute measurements.

1	2	3	4	5	6
	Jennings (1969)	Paakkari *et al.* (1970)	Present work	Range	Total range
hkl	SL	SC	SJ	%	%
111	6271	6317 (6344)	6324 (6512)	0·8 (3·8)	4·1 (5·9)
200	5905	5841 (5866)	5865 (6040)	1·1 (2·9)	3·2 (5·7)
220	3173	3172 (3186)	3207 (3303)	1·1 (4·0)	3·9 (9·0)
311	2132	2129 (2138)	2114 (2177)	0·8 (2·1)	5·7 (12·2)
222	1880	1870 (1878)	1878 (1934)	0·5 (2·9)	7·2 (11·8)
400	1281	1312 (1318)	1254 (1291)	4·5 (2·8)	9·1 (13·3)

measurements. Owing to this correction, our absolute values (in parenthesis) appeared to be on an average 2·5% higher than those of Jennings (1969) and Paakkari *et al.* (1970). We have not, however, remeasured the intensity of the primary beam. Column 5 gives the range of the results in columns 2–4 and column 6 shows the whole range obtained in the project (excluding SO). In calculating the values in column 6 we have used the normalized values of Jennings's report.

Table 1 shows clearly that the results obtained in three laboratories for the Ni samples SL, SC and SJ are in good agreement, in contradistinction to the general situation. It should be pointed out that although the integrated intensities of each of the first three reflexions for every specimen in the project were originally within 0·5% of each other, the remeasurements of Jennings (*cf.* Paakkari *et al.*, 1969, p. 20) indicated deviations up to 1% between the samples SC and SL. The results of Jennings (sample SL, column 2) have been obtained with an incident-beam monochromator and a wide receiving slit, the results of Paakkari *et al.* (sample SC, column 3) with an incident-beam monochromator and a narrow receiving slit and, finally, our measurements (column 4) have been performed using a diffracted-beam monochromator and a narrow slit. The polarization factor of the monochromator has been measured by 90 degree scattering (Jennings), by a Bormann crystal (Paakkari *et al.*) and by Miyake's method (this work). Further the TDS corrections have been applied in different ways. Thus the measuring methods are different. We conclude, therefore, that the agreement between these results reflects an accuracy and care of comparable degree in the measurements of these laboratories. We conclude further that the 'magical' level of 1% in accuracy of the powder intensity measurements is attainable, at least on a relative basis.

References

Jennings, L. D. (1969). *Acta Cryst.* A**25**, 217.

Paakkari, T., Suortti, P. & Inkinen, O. (1970). *Ann. Acad. Sci. Fenn.* Ser. A VI, No. 345.

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 (J. N. King, International Union of Crystallography, 13 *White Friars, Chester CH*1 1*NZ, England).*

Sir Lawrence Bragg
1890–1971

Sir Lawrence Bragg, F.R.S., Professor Emeritus and formerly Director of the Royal Institution, died on 1 July 1971. Sir Lawrence, in conjunction with his father Sir William Bragg, carried out the earliest crystal structure determinations by X-ray spectrometry, receiving for this work the Nobel Prize for Physics in 1915. It was as a result of these investigations that it first became possible to obtain absolute values of lattice parameters. Sir Lawrence and his school thereafter developed the quantitative aspects of X-ray diffraction techniques and worked out large numbers of more complicated crystal structures, especially those of silicate minerals. Sir Lawrence took a leading part in the formation of the International Union of Crystallography in 1947, and he became its first President.

A full obituary will be published later.

Seminar on Low Energy Electron Diffraction
Washington, D. C., U.S.A., 27–28 April 1972

The Sixth LEED Seminar will take place on 27–28 April 1972 in Washington, D.C. The Seminar is a Topical Conference of the American Physical Society, sponsored by the Division of Electron and Atomic Physics. The program will include contributed and invited papers dealing primarily with basic processes and phenomena of LEED. Topics of special interest are: new developments in LEED theory and comparisons with experiment, innovations in experimental technique, and the analysis of data.

Abstracts for contributed papers may be no more than 200 words in length and should conform to the format standards of the Bulletin of the American Physical Society. They should be received not later than 4 February 1972. Abstracts and requests for information should be mailed to: Dr Ray Kaplan, Code 6479, Naval Research Laboratory, Washington, D.C., 20390, U.S.A.