

Commission on Crystallographic Apparatus

An international project for the calibration of absolute intensities in small-angle X-ray scattering

The importance of absolute intensity measurements in small-angle X-ray experiments has been recognized for many years, and a wide variety of methods have been reported for achieving such calibrations (Luzzati, 1960; Gerold, 1961; Kratky & Wawra, 1963; Damaschun & Müller, 1965; Kratky, Pilz & Schmitz, 1966). Apart from a comparison by Weinberg (1963) of the foil-attenuation method with the gas-scattering method and a comparison by Shaffer (1964) and Shaffer & Beeman (1970) of the data for zero-angle scattering for several gases, there has been no attempt to compare the many techniques. The problem of precision in measurements of absolute intensity, and the need for a comparison of the different techniques for a common standard sample, were discussed at the recent Second International Conference on Small-Angle Scattering of X-rays held in Graz, Austria, in August, 1970. The results of these discussions may be summarized as follows:

I. An international project should be established with the aims of (1) testing the precision of reproducibility and the comparative accuracy of the various calibration techniques in current use, and (2) clarifying the areas of difficulty in absolute intensity calibration.

II. There shall be no attempt to nominate a single absolute intensity calibration technique. Each participating laboratory will use its own preferred technique to carry out measurements on a set of standard specimens to be provided by the project organizer.

III. The secondary standards would be (1) chemically, thermally, and physically stable, (2) unaffected by long exposures to X-rays, (3) easily transported, and (4) easily handled. On the basis of these criteria, liquid samples were eliminated from consideration. Three solid samples were agreed upon as suitable standards: (1) glassy carbon, (2) polyethylene, and (3) cellulose acetate. Each specimen would be mounted in a specimen holder suitable for use in almost all small-angle scattering geometries.

IV. The project organizer would have the responsibility for (1) designing the specimen holders, (2) preparing the instructions to participants, (3) maintaining and distributing the standards, and (4) collecting and comparing the data.

Each participating laboratory will receive for calibration one of each of the three standard samples from the project organizer. The same three samples will be distributed sequentially to all participants in order to assist in separating technique errors from specimen errors. Detailed instructions regarding the kind and quantity of data required to make the comparison of results from different laboratories meaningful will be provided. Basically, data will be required that fully characterize (1) the geometry of the small-angle collimation system, (2) the X-ray generator and the focal spot, (3) the X-ray wavelength and monochromatization, and (4) the X-ray detection system. These data will be recorded on forms provided. Detailed descriptions of the calibration techniques and all raw data will be recorded. Equations and sample calculations for the data reduction must be shown, including the method of collimation corrections if any is used. The final result – the absolute differential X-ray scattering cross section for each sample – will be used to compare the results from the different laboratories. The data from participants will be analyzed with the assistance of L. B. Shaffer and a report prepared for publication. Complete anonymity of all participants will be maintained.

The standard samples and their mounts and the detailed instructions for participation are now being prepared and checked. All interested researchers are encouraged to communicate with the project organizer (address below) for further details.

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References

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 SHAFFER, L. B. (1964). *Absolute X-ray Scattering Cross-Sections of Liquids and Solutions*. Ph.D. thesis, Univ. of Wisconsin.
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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 CH1 1NZ, England).

American Crystallographic Association

Ad hoc Committee on Small-Angle X-ray Scattering

A computerized international mailing list is being prepared of all researchers who are active or interested in small-angle X-ray or neutron scattering. This list will be used by the ACA, the IUCr, or other qualified professional organiza-

tions exclusively for dissemination of information of interest to the field (*e.g.* announcements of forthcoming small-angle meetings, workshops, *etc.*). The list will be coded both geographically and by field of interest in order that selective mailing lists can be prepared.

All persons who wish to be included in this compilation should send a post card, with the information indicated below, to Robert W. Hendricks, Metals

and Ceramics Division, Oak Ridge National Laboratory, P. O. Box X, Oak Ridge, Tennessee 37830, U.S.A. The information required is (1) name and title, (2) complete mailing address, (3) membership in crystallographic organizations, and (4) field of interest (choose up to 3): (a) All areas of SAS, (b) inorganic materials, (c) polymers, (d) biological, (e) liquids and solutions, (f) critical phenomena, (g) neutron SAS, (h) theory, (i) other.

Crystallographers

We regret to have to record the death on 1 April 1971 of Professor Dame **Kathleen Lonsdale**, who was Professor of Chemistry and Head of the Department of Crystallography, University College, London from 1949 to 1968. Her many contributions to crystallography included her work as General Editor of *International Tables for X-ray Crystallography*. She was one of the first women to be elected Fellow of the Royal Society and the first woman President of the British Association for the Advancement of Science. As President of the International Union of Crystallography she chaired the sessions of the Seventh General Assembly in Moscow, 1966. A full obituary is to be published in *Acta Crystallographica*, Section A.

Dr **J. V. Silverton**, formerly at Georgetown University, has accepted a post in the Laboratory of Chemistry, NHLI, National Institutes of Health, Bethesda, Maryland, U.S.A.

Professor **C. A. Taylor** has been appointed a Vice-President of the (U.K.) Institute of Physics with special responsibilities for education. Professor Taylor is Professor of Physics at University College, Cardiff, Wales and is Chairman of the I.U.Cr. Committee on Crystallographic Teaching.

Dr. **Eric J. Gabe** has left the Mines Branch to become a Research Officer of the Chemistry Division, National Research Council, Ottawa, Canada.

Professor **D. W. J. Cruickshank** has been appointed Deputy Principal of the University of Manchester Institute of Science and Technology for the two-year period 1971–73. Professor Cruickshank is the General Secretary and Treasurer of the I.U.Cr. and also continues his teaching duties as a professor of chemistry.

Professor **Dorothy C. Hodgkin** has received one of the highest honors the U.S.A. National Academy of Sciences can bestow, that of election as a foreign associate. A professor of chemistry at Oxford University, Chancellor of Bristol University, and Nobel laureate, Dr Hodgkin is a member of the I.U.Cr. Executive Committee.

Dr **Roberto Colella** will join the Physics Department of Purdue University, Lafayette, Indiana, U.S.A., as an assistant professor in September. He has been at the Catholic University, Washington, D.C. for the past year.

Professor **Chatar Singh**, once at Cambridge and now at the School of Physics and Mathematics, University of Penang, Malaysia, is developing a strong crystallography program with the participation of Dr **Turid Pedersen**, formerly of Melbourne.