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Remarks on a suggestion by Lee. By JERRY DONOHUE, *Department of Chemistry and Laboratory for Research on the Structure of Matter, University of Pennsylvania, Philadelphia, Pennsylvania* 19104 *U.S.A.*

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A crystal structure should not be refined in a space group of unnecessarily low symmetry.

Lee (1971) has suggested that 'in cases where the space group is not absolutely certain, from a structural point of view it is safest (and cannot be wrong) to assume the lower symmetry'. I wish to point out that *no* space group is absolutely certain. Accordingly, if Lee's suggestion is carried to its logical conclusion all structures should be refined in *P*1. Unfortunately, the least-squares method cannot then be used, for if a set of parameters corresponding to a higher symmetry is refined in *P*1, catastrophic results will ensue (see Ermer & Dunitz, 1970). Nor can the Fourier method be used, for it has been shown by Cochran (1948) and Cruickshank (1952) that this method is equivalent to least squares with a particular set of weights. *Sic transit gloria diffractionis.*

A prudent way out of this dilemma would be to use Occam's razor and refine on the assumption of *higher* symmetry. If the resulting agreement with experiment is satisfactory then the assumption must have been correct, but if not, incorrect.

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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 organizations 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 adress, (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*) criterial phenomena, (*g*) neutron SAS, (*h*) theory, (*i*) other.

International Union of Crystallography 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-radiation, (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 reductions 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 analysed 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 at the following address for further details:

Robert W. Hendricks
Metals and Ceramics Division
Oak Ridge National Laboratory
P. O. Box X
Tennessee 37830
U.S.A.

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