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Radii of gyration and scattering curves of hollow bodies of homogeneous electron density: errata. By YUZURU HIRAGI and SHOJI IHARA, Institute for Chemical Research, Kyoto University, Gokasho, Uji 611, Kyoto-fu, Japan

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Abstract

Equations (15), (16), (17), (18), and (20) in the paper by Hiragi & Ihara [Acta Cryst. (1981), A37, 378-382] are incorrect. These equations should be as follows:

$$F = 4A^{2} C \left[\sum_{k=1}^{n} f\left(s_{1}, \varphi - \frac{2\pi}{n} k\right) \right] \Psi_{C},$$

$$f(s_{1}, \beta) = \left[s_{1}^{2} A^{2} \left(\tan^{2} \frac{\pi}{n} \sin^{2} \beta - \cos^{2} \beta \right) \right]^{-1}$$

$$\times \left\{ \exp(is_{1} A \cos \beta) \right.$$

$$\times \left[i \cot \beta \sin \left(s_{1} A \tan \frac{\pi}{n} \sin \beta \right) \right.$$

$$\left. - \tan \frac{\pi}{n} \cos \left(s_{1} A \tan \frac{\pi}{n} \sin \beta \right) \right] + \tan \frac{\pi}{n} \right\},$$
 (16)

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$$V = 2\pi ABC, \tag{17}$$

$$F = \frac{4\pi ABCJ_1(s_1, K)}{s_1 K} \Psi_C, \tag{18}$$

$$F = 4\pi ABC \frac{\sin(sL) - sL \cos(sL)}{(sL)^3}.$$
 (20)

Equations (15) and (16) in the original article lead to incorrect scattering intensity, whereas equations (17), (18), and (20) give the correct but unnormalized value. The figures in the article were calculated with the correct equations and hence need no alteration.

All information is given in the *Abstract*. The authors thank Dr P. Martel for pointing out the errors.

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Commission on Journals

Decisions taken at meetings in Ottawa, August 1981

The attention of authors planning to submit papers to Acta Crystallographica or Journal of Applied Crystallography is drawn to the following decisions taken by the Commission on Journals at meetings held in Ottawa, 14–16 August 1981. These and other revisions in editorial policy since 1978 will be published in a new version of Notes for Authors, which is presently in preparation.

International Symbols for Units

The Commission has recognized that, although multiples of 10^3 are the preferred prefixes in the SI System of Units, the centimetre is not prohibited by the SI system and therefore density and absorption coefficients may be given in units of g cm⁻³ and cm⁻¹ respectively, if authors so wish. In all other cases, however, authors are asked to use the recommended prefixes of decimal multiples and submultiples of the SI units rather than using ' $\times 10^n$ '.

Structural Papers

Estimated standard deviations for B_{eq} . The requirement of estimated standard deviations on equivalent values of the

Debye–Waller factor was reviewed. The Commission agreed that the significance of such estimated standard deviations may be ambiguous. In the case of high anisotropy, the estimated standard deviation is necessarily large although the individual anisotropic parameters may be well determined. In future, the presence of unusual anisotropy should be referred to in the text (including the maximum and minimum amplitudes and any nonpositive-definite coefficients found), or in the table of $B_{\rm eq}$ (by use of an asterisk), or illustrated by a plot of the atomic vibrational ellipsoids.

Calculated hydrogen-atom coordinates: Calculated hydrogen-atom coordinates will be published in future only at the Co-editor's discretion and if they are necessary to the understanding of the paper. They will otherwise be deposited.

Graphical chemical formulae: A graphical structural formula should always be given in the report of a structure determination of an organic or organometallic compound. The figure showing the atomic positions is not adequate for this purpose. However, a plot of the atomic vibrational ellipsoids can be used to illustrate atomic positions. Authors should ensure that such plots are of good contrast and quality. The numbering of atoms should be consistent throughout a paper and, as far as possible, correspond to the systematic name [Acta Cryst. (1982). B38, 700].

Least-squares planes: Least-squares planes and the deviations from them will only be published if they are referred to in the text of the paper and are significant in the consideration of the structure. They will otherwise be deposited.

Absorption correction: In a structural paper the absorption correction, if any, should always be described and the maximum and minimum corrections stated.

Melting point: In a structural paper the melting point of a compound should always be given if it is known.

Stereofigures: The requirement on stereofigures is one per structure unless the Co-editor and referees feel that more are necessary for the understanding of the structure described in the paper. These stereoviews must fit into a single column (80 mm wide). Authors are reminded that a nonstereo view (half a pair) is often an acceptable alternative to the stereo pair. In stereo pairs the relative sizes of the molecule and the whole figure should be such that when the figure is printed in a column of 80 mm, the individual atoms are easily distinguishable. The center-to-center separation in stereofigures must not exceed 55 mm.

In a charge density paper only one or two figures are required to illustrate the techniques or results described: any others will be deposited. The text should be adequate to give the remaining information.

Figures

Size: Illustrations should normally present information so that each figure or part of a figure can be printed in one column (80 mm width). Co-editors will need to be satisfied that the information density is high enough, if authors wish figures to be printed larger than this.

Half-tone illustrations: When a paper includes half-tone illustrations (photographs), particularly diffraction photographs, authors are asked to indicate on a photocopy which are the important parts of the figure, so that these may be given the correct emphasis when the paper is printed.

The attention of authors is also drawn to notices concerning stereofigures | Acta Cryst. (1978). B34, 3846|, dimensions of material for deposition | Acta Cryst. (1979). B35, 792, estimated standard deviations, SI units and anisotropic thermal parameters | Acta Cryst. (1979). B35, 1302, submission of connected computer output | Acta Cryst. (1979). B35, 2284-2285, chemical-connectivity relationships | Acta Cryst. (1980). B36, 1524, estimated standard deviations with a zero value for varied parameters Acta Cryst. (1980). B36, 2508, standards for the publication of powder pattern data [Acta Cryst. (1981). B37, 1161, deposition of macromolecular atomic coordinates and structure factors with the Protein Data Bank | Acta Cryst. (1981). B37, 1161; (1982). B38, 1050, submission of manuscripts based on powder diffraction profile fitting or refinement (Rietveld) methods: deposition of data [Acta Cryst. (1981). B37, 1162, format for papers to be published in Acta Crystallographic, Section C | Acta Cryst. (1982). B38, 699, and chemical formulae and nomenclature | Acta Cryst. (1982). B38, 700, in addition to the information given in Notes for Authors | Acta Cryst. (1978). A 34, 143–157|.

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Structure Reports

Volume 44B and Volume 46A of Structure Reports have recently been published. Volume 44B covers the literature for organic compounds for 1978, is bound in two parts (572 pages and 707 pages) and costs 374 Netherlands guilders for subscribers with standing orders. The full price for individual copies is 440 guilders but personal subscribers may buy a copy for their own use at 220 guilders. Volume 46A covers the literature for metals and inorganic compounds for 1980 (464 pages) and costs 153 Netherlands guilders for subscribers with standing orders. The full price for individual copies is 180 guilders but personal subscribers may buy a copy for their own use at 90 guilders. Orders for these publications may be placed direct with the publisher, D. Reidel Publishing Company, PO Box 17, 3300 AA Dordrecht, The Netherlands, or with any bookseller. Trade orders should be sent to Reidel.

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Molecular Structures and Dimensions

The International Union of Crystallography and the Cambridge Crystallographic Data Centre have published Volume 12 of the series, entitled *Bibliography* 1979–80, *Organic and Organometallic Crystal Structures*. It contains bibliographic information on 3836 structures published during 1979–1980. As in previous volumes the entries are arranged in 86 chemical classes and cover organic compounds, complexes and organometallic compounds. There are extensive indexes for authors, compound names and formulae.