HEEG, M. R. (1987). *Acta Cryst.* C43, 2017–2018.
JEFFREY, G. A., POPLE, J. A., BINKLEY, J. S. & VISHVESHWARA, S. (1978). *J. Am. Chem. Soc.* **100**, 373–379.
JEFFREY, G. A. & YATES, J. H. (1979). *Carbohydr. Res.* **74**, 319–322.
JOHNSON, C. K. (1971). *ORTEP*II. Report ORNL-3794, revised. Oak Ridge National Laboratory, Tennessee, USA.
LEMIEUX, R. U., EARL, R. A., JAMES, K. & NAGABHUSHAN, T. L. (1973). *Can. J. Chem.* **51**, 19–26.
LEMIEUX, R. U., JAMES, K. & NAGABHUSHAN, T. L. (1973). *Can. J. Chem.* **51**, 27–32.
LEMIEUX, R. U., JAMES, K., NAGABHUSHAN, T. L. & ITO, Y. (1973). *Can. J. Chem.* **51**, 33–41.
LUGER, P. & BÜLOW, R. (1983). *J. Appl. Cryst.* **16**, 431–432.
MILJKOVIĆ, M., GRIGORIJEVIĆ, M., SATOH, T. & MILJKOVIĆ, D. (1974). *J. Org. Chem.* **39**, 1379–1384.
PALMER, H. T. & PALMER, R. A. (1976). *Acta Cryst.* B**32**, 377–380.
PÉREZ, S., ST-PIERRE, J. & MARCHESSAULT, R. H. (1978). *Can. J. Chem.* **56**, 2866–2871.
SHELDRICK, G. M. (1986). *SHELXS*86. Program for crystal structure determination. Univ. of Göttingen, Federal Republic of Germany.
SMIATACZ, Z. & MYSZKA, H. (1989). *Carbohydr. Res.* In the press.
SMIATACZ, Z., MYSZKA, H. & CIUNIK, Z. (1988). *Carbohydr. Res.* **172**, 171–182.
SMIATACZ, Z., SZWEDA, R. & DREWNIAK, J. (1985). *Carbohydr. Res.* **143**, 151–159.
SUNDARALINGAM, M. (1968). *Biopolymers*, **6**, 189–213.
TOURE, P. S., LAPASSET, J., BOYER, B. & LAMATY, G. (1979). *Acta Cryst.* B**35**, 2790–2792.
ZACHARIASEN, W. H. (1963). *Acta Cryst.* **16**, 1139–1144.
ZACHARIASEN, W. H. (1967). *Acta Cryst.* **23**, 558–564.

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Commission on Biological Macromolecules

Policy on Publication and the Deposition of Data from Crystallographic Studies of Biological Macromolecules

I. *Preamble*

1. Crystallographic analyses of protein, nucleic-acid and virus structures produce an extraordinary amount of information, and these results are widely recognized as having unique value. Available information transcends that which can be recorded in usual scientific publications, and the Protein Data Bank is often used as a supplementary repository for such results. As in all science, it is imperative that sufficient information be made available so that the structural results can be reproduced and verified.

2. The importance of preserving the fundamental data and results from diffraction studies is recognized alike by producers and users of this information. There are, however, concerns that results from the early stages of analysis will be inaccurate in detail and that investigators should have the opportunity to complete the analysis and interpretation of their data. On the other hand, an open-ended protection of authors' interests conflicts with the general scientific good and it creates the risk that valuable data will be lost forever. Accordingly, the deposition policy promulgated below stipulates immediate deposition of atomic coordinates and diffraction data supporting publications on structure, but it provides for the possibility of a specified delay in the release of this information for public use.

II. *Policy*

1. The Commission on Biological Macromolecules of the International Union of Crystallography endorses a deposition policy for crystallographic studies to permit independent verification of the results and to preserve the primary data for future use. Scientific publications reporting results from crystallographic determinations of macromolecular structure should be accompanied by a deposition of atomic coordinates and structure-factor information at a level appropriate to the description given in the paper.

Specific provisions of the policy are elaborated below:

(*a*) *Provisions for atomic coordinates.* Two different levels of description arise with respect to the coordinates of macromolecular structures. In the case of chain-tracing descriptions, the α-carbon coordinates for proteins or phosphorus positions for nucleic acids are appropriate for deposition. If the interpretation presented depends on atomic details as shown in figures of side chains or numbers derived from atomic coordinates, then the full coordinate list should be deposited. Atomic displacement parameters (*B* values) and occupancy factors that are part of a model should also be deposited. Investigators might choose to flag regions of a structure that are judged to be particularly unreliable or subject to revision.

(*b*) *Provisions for diffraction data.* Native structure-factor magnitudes should be deposited to the limit of Bragg spacings stated in the paper. The deposition of additional data used in phase determination (heavy-atom isomorph data, Bijvoet mates, multiple wavelength measurements, *etc.*) is also encouraged. In the case of structure reports that do not involve atomic models (*e.g.* low-resolution studies) both structure amplitudes and phases used in Fourier syntheses that are reported should be deposited.

(*c*) *Provision for publications in methodology.* The policy applies to reports on structural results. Those papers that describe purely advances in methodology are exempt from this policy even if diffraction data or structural results were required for their development.

(*d*) *Provision for manner of deposition.* The Protein Data Bank at Brookhaven National Laboratory is recognized by the Commission on Biological Macromolecules of the International Union of Crystallography as the appropriate repository for results from macromolecular crystallography. Accordingly, data should be deposited in machine form as instructed by the Protein Data Bank.

(*e*) *Provision for delayed release.* It is the intention of this policy that the deposition of data associated with a scientific publication should occur concurrently with publication of the article. Nevertheless, provision is allowed for the authors to request a delay in the release of the deposited data. For deposited coordinates this delay is not to exceed one year from the date of publication. For deposited structure factors, the requested delay can be up to four years from the date of publication.

(*f*) *Provision for enforcement.* The provisions of this policy require inclusion in the publication of a statement to the effect that 'the atomic coordinates and structure factor data described here have been deposited in the Protein Data Bank at Brookhaven'.

III. *Journals*

The Commission recommends that this policy be communicated to all the relevant scientific journals and that they be urged to adopt its provisions.

IV. *User obligations*

1. The Commission hopes that the practice of depositing coordinates used in structural description will be extended to publications based on spectroscopic data (*e.g.* nuclear magnetic resonance, EXAFS) and from theoretical and modelling studies.

2. Users of deposited data should cite the primary references, as well as the Protein Data Bank, when making use of the data.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. O. Gould, Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, Scotland). As far as practicable books will be reviewed in a country different from that of publication.

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Stereochemical applications of gas-phase electron diffraction. Edited by I. HARGITTAI and M. HARGITTAI. Part A: **The electron diffraction technique.** Pp. xviii + 563. Part B: **Structural information for selected classes of compounds.** Pp. xviii + 511. Weinheim, New York: VCH Verlag, 1988. Price DM 375, US$210 per volume.

The first part of this book describes the development and the present capabilities of gas-phase electron diffraction (GED). Several contributions also deal with the combined applications of GED with other techniques. The second part contains structural results for nine different classes of compounds.

According to the editors, the main function of these books is to present modern gas electron diffraction to the nonspecialist and to answer questions such as: Which compounds are suitable for stereochemical analysis by electron diffraction and which are not? What are the limitations of the size of a molecule for such analysis? How reliable are the parameters determined, and how reliable are the error limits given in the original work? In which direction is the technique developing? What are the advantages of using GED compared with other techniques? These questions and others are addressed in 26 chapters written by 38 authors who are either working with GED or in fields closely related to GED.

Part A starts with a survey of the GED technique. Following a short description of the historical development, it presents the fundamental theoretical expressions and gives a short description of the structural analysis. It provides a good introduction for those who are utilizing information from GED, but are not themselves using the technique.

The next chapter gives the status of electron scattering theory with respect to accuracy of structure analysis. It identifies the effects believed to be primarily responsible for systematic residuals seen in conventionally measured GED intensities, such as asphericity of atoms in molecules, anharmonicity of molecular vibrations and the breakdown of the kinematic or quasi-kinematic approximations.

Chapter 3 describes the experimental and theoretical aspects of small-angle electron scattering by gas molecules. These studies may be used to examine the quality of the molecular wavefunctions. GED can also provide information on electron density distribution in molecules and this is the subject of Chapter 4, while Chapter 5 is a description of the temperature dependence of GED parameters, both theoretical and experimental.

Chapter 6 gives a description of an electron diffraction experiment. The Hungarian electron diffraction group has developed several special gas nozzles, and the descriptions of these nozzles will be valuable for those already working with GED. Also included is a description of simultaneous mass spectrometric and GED measurements, which may be used when high-temperature vapours, free radicals or reaction products are studied.

The joint use of GED and high-resolution spectroscopic data is discussed in Chapter 7. These combined data can improve the precision and accuracy of the structural parameters determined. Use of data from other sources together with GED data is probably the most important development in the GED method since the introduction of least-squares analysis about 25 years ago. Chapter 9 describes the use of quantum-chemical calculations together with GED in what has become known as MOCED (molecular-orbital-constrained electron diffraction), while Chapter 10 discusses how self-consistent molecular models can be obtained from a combination of GED, microwave and infrared data together with theoretical calculations. In Chapter 14, the combined use of liquid-crystal NMR