(*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

spectroscopy and electron diffraction is described. Here it is shown how a combination of data from several methods can provide a solution when the individual methods cannot give a complete structure. Low-resolution microwave spectroscopy can often provide information about the conformational isomers present in the sample. This is valuable information in many GED studies, and Chapter 15 presents information about this method.

One chapter (Chapter 12) is devoted to the study of molecules with large vibrational amplitudes, while Chapter 8 shows how spectroscopic information can be obtained from electron diffraction. Conformational analysis is an important part of structural studies. Chapter 11 describes how conformational properties are obtained from electron diffraction and how thermodynamic properties like energy and entropy differences between conformers can be obtained by using GED data from several different temperatures.

Chapters 13 and 16 present two methods which are related to GED, namely EXAFS (extended X-ray absorption fine structure) and gas-phase X-ray diffraction. EXAFS can reveal the environment of a single element in a material and is primarily used with polycrystalline materials and with liquids, solutions and glasses. Gas-phase X-ray diffraction is today mostly used to investigate the electron distribution in atoms and molecules.

Part B is concerned with structural information obtained for selected classes of compounds. Boron and silicon compounds are treated in the first chapter. About 70% of the published structures are included and used to discuss problems and trends of stereochemical interest. In Chapter 2, more than 350 nitrogen and phosphorus compounds are reviewed, while oxygen and sulfur compounds are the subject of Chapter 3. The results for a large number of fluorine derivatives are discussed in Chapter 4, and comparisons between structural parameters of similar or analogous compounds are presented. Attempts are made to rationalize these parameters or trends on the basis of simple models such as polar effects or VSEPR theory. The structures and conformational equilibria in saturated (Chapter 5) and unsaturated (Chapter 6) organic molecules are thoroughly presented and several valuable tables of results are given. A separate chapter on benzene derivatives (Chapter 7) presents information on skeletal distortions of the benzene ring caused by substitution. Chapter 8 reviews the molecular structure of about 120 organometallic compounds determined by GED. Organic derivatives of main-group metals in groups 1, 2, 12, 13 (except boron) and 14 (except silicon) have been included. The last of the nine selected classes reviews the molecular structures of metal halides.

Part B is concluded by a chapter on the interaction of theoretical chemistry with GED, written by one of the leading experts on theoretical chemistry. Included is a description of how a molecular structure can be determined from quantum theory and how sufficient accuracy can be attained. Also presented is a description of how a molecular force field can be obtained from quantum theory, and the chapter is concluded with 'projections for the near future.'

Stereochemical Applications of Gas-Phase Electron Diffraction is a good presentation of a valuable technique. The combined use of GED and data from other sources has been well described. Structural information has been reviewed for several classes of compounds, and empirical trends and interpretation of structural variations have been presented. Most of these reviews stop at about 1985, so the editing and printing process seems to have taken somewhat of a long time. Even if the primary goal has been to present the GED method and possibilities to non-specialists, electron diffractionists will also undoubtedly make diligent use of the books, because of their breadth of information, which is otherwise spread over a large number of publications. The books should be of interest for everybody working with molecular structures and for users of molecular structural data. The books should be found on the shelves of all good chemistry libraries.

KOLBJØRN HAGEN

Department of Chemistry
University of Trondheim, AVH
N-7055 Dragvoll
Norway

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Book Received

The following book has been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Modern crystallography. IV. Physical properties of crystals. By L. A. SHUVALOV. Pp. xviii + 583. **Springer series in solid state sciences 37.** Berlin: Springer-Verlag, 1988. Price DM 198.00. A review of this book, by K. Simon, has been published in the September 1989 issue of *Acta Crystallographica,* Section A, page 659.