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International Union of Crystallography

Commission on Electron Diffraction.

Guide for the Publication of Experimental Gas-Phase Electron Diffraction Data and Derived Structural Results in the Primary Literature*

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This report contains general recommendations for the guidance of authors, referees, and editors on the reporting of electron diffraction data and derived structures. They are intended to facilitate reliable evaluation, ease of comparison with other data, and the retrieval of information if later reanalysis becomes desirable in the light of new theories or experiments.

Introduction

This report is concerned with the presentation of structural investigations by electron diffraction. Its aim is to make results obtained by specialists more accessible to those in other disciplines and, at the same time, to increase the potential value of the original data to other specialists if subsequent events warrant reinvestigation. The needs of compilers and correlators of information will also be benefited by attention to these considerations. Only if enough information is provided to allow readers to appraise the precision and accuracy of the work, and only if reasonably uniform standards of reporting the results are adhered to, can all ends be met.

This report is an abbreviated version of a document approved by the Commission on Electron Diffraction of the International Union of Crystallography in August, 1975. For its general recommendations the original document quoted extensively from the *Guide for Publication of Experimental Data and Derived Numerical Results in the Primary Literature* prepared for CODATA and UNESCO in 1973 by the CODATA Task Group on Publication in the Primary Literature (1973). The present report concentrates on specialized problems encountered in the field of gas-phase electron diffraction, certain aspects of which have been referred to in review papers in the field (Akishin, Rambidi & Spiridonov, 1967; Bartell, 1971; Bastiansen, Seip & Boggs, 1971; Bauer, 1970; Beagley, 1973; Davis, 1971; Haaland, Vilkov, Khaikin, Yokozeki & Bauer, 1975; Hilderbrandt & Bonham, 1971; Karle, 1973; Kuchitsu, 1972*a*, *b*; Robiette, 1973; Seip, 1973). Literature citations are illustrative, not exhaustive.

* This report is based on a draft written in 1973 by the Gas-Diffraction subcommittee of the IUCr Commission on Electron Diffraction in consultation with workers in a majority of the existing laboratories of electron diffraction. The present version incorporates suggestions received during discussions of the *Guide* in scheduled open sessions at the Austin Symposium on Molecular Structure, Austin, Texas, March, 1974; the Second European Crystallographic Meeting in Keszthely, Hungary, August, 1974; and the Tenth International Congress of Crystallography in Amsterdam, August, 1975; and by correspondence from interested IUCr members.

While an adequate documentation of experiment and interpretation is vital, so also, in the avalanche of scientific literature we must contend with, is brevity and conciseness. Possible ways to achieve both ends are as follows. It would be desirable to develop a compact style of reporting essential details that vary from analysis to analysis. Standard equipment and procedures in a given laboratory that have been described clearly in readily available journals or accessible depository services may be documented simply by citing the appropriate references. Workers in every laboratory have an obligation to provide this information, as outlined in the following sections and to revise it every few years when substantial changes are made. Special procedures and certain data that are important for a critical evaluation of results but not of general interest to readers should be summarized and placed in a suitable depository service or published as microfilm together with the article.

More and more highly specialized computer routines are being used to process data, to convert it to molecular parameters, to compute the effects of a host of influences such as electron density shifts, distortions of diffracted waves, molecular vibrations, *etc.*, and to interpret derived structures in terms of quantum-chemical or other models. References to important computer packages employed and their sources should be given.

Structural investigations by gas-phase electron diffraction differ so much in complexity and in aim that it is impractical to recommend rigid rules for the reporting of procedures and presentation of results. Investigations in which low precision suffices need not be documented as minutely as those in which high precision is claimed. In the following are presented recommendations intended to be helpful in the preparation of a full paper. This guide may not fit all cases, and future developments may necessitate modifications. However, it is our hope that authors will deviate from the recommendations only after careful consideration.

I. Experimental apparatus and procedures

An adequate description of the experimental procedures used to obtain the numerical results should be made available. The major points to be considered are:

A. *Sample*

The source, verification of purity, and relevant handling procedures should be stated. When temperatures or reactivities are such that several species may be present, information concerning the vapor phase composition should be cited. The sample pressure should always be recorded when possible.

B. *Reference to the diffraction unit used*

If the detail of the unit has been published previously, a simple citation may suffice. If not, all relevant details must be given.

C. *Uncertainty in the s-scale*

The accuracy of measurement and means by which that accuracy is checked and maintained should be described.

D. *Nozzle and sample temperature*

The nozzle and reservoir temperatures are straightforward and should be reported. There is as yet no consensus on the effective temperatures of various internal molecular motions after the free expansion of the gas jet to the electron beam. Suitable caution in expressing the sample temperature seems advisable. The sample temperature at the electron beam depends upon (and, in principle, can be calculated from) the sample pressure, the nozzle dimensions, the distance of the electron beam from the nozzle lip, and the electron beam diameter. In all studies in which temperature is important, it is imperative that the above experimental quantities be given. Routinely the nozzle-beam dimensions should be made available.

E. *Sector calibration (if used)*

Some laboratories do and some do not calibrate the shapes of the sectors they use. It is important that an explicit statement be given about whether a calibration has been made, what means have been used, and what accuracy is achieved. A purely optical measurement with a standard traveling microscope may not be sufficient for the calibration of the inner range of a sector. For example, if the traveling microscope has a precision of 2×10^{-4} cm and if a two parts per thousand precision in the sector opening is desired, the smallest radius of an r^3 sector that can be measured optically with the requisite accuracy is 1·1 cm for a sector with $r_{max} = 4{\cdot}4$ cm and 1·8 cm for a sector with $r_{max} = 8{\cdot}8$ cm.

F. *Intensity measurement*

The precision but not accuracy of the intensity measurements will be revealed, in part, in the least-squares residuals to be discussed later. Reference should be made to the calibration of the measuring device, both with respect to scattering angle and with respect to intensity value. Some laboratories favor establishing intensity measurement with reference to some standard molecule such as benzene. If photographic recording is used, the assumption of a linear density–exposure relation may distort derived amplitudes of vibration (or, in some cases, it may even interfere with the determination of structure). Whether plates are spun, oscillated (over what amplitude), or read with a linear scan should be stated.

G. *Number of measurements*

The number of independent data points used should be given (but see II*D* and III*D* below). If photographic recording is used, the numbers of plates for each camera geometry should be stated.

II. Treatment of diffraction data

In operations to transform observed intensity values into a form convenient for comparison with theoretical expressions, the major points to be enumerated are:

A. *Leveling procedure*

If intensities are leveled, converted to an $s^4I(s)$ basis, or otherwise modified prior to determination of the background function, the requisite scattering factors or assumptions about electron distributions, polarization corrections, *etc.*, should be identified.

B. *Extraneous scattering corrections*

Significant excursions of the background of leveled intensities from a flat, horizontal line should be noted. They may signify extraneous scattering (an additive effect), variation of plate sensitivity (a multiplicative effect) or inaccurate scattering factors. The manner of compensation can influence derived molecular parameters and needs to be known if later reanalyses of data are made.

C. *Background function*

The derivation of this important function (analytical or hand drawn) should be stated. It would be good practice to report the effective number of shape parameters implicit in the background if it has non-uniform derivatives.

D. *Interpolation of data*

The procedures used to interpolate and/or smooth data points and the means of determining data correlations should be referred to (see III*D* below).

III. Derivation of structural parameters

(Akishin, Rambidi & Spiridonov, 1967; Bartell, 1971; Bastiansen, Fritsch & Hedberg, 1964; Bauer, 1970; Beagley, Cruickshank, Hewitt & Haaland, 1967; Corbet, Dallinga, Oltmans & Toneman, 1964; Harshbarger, Lee, Porter & Bauer, 1969; Hedberg & Iwasaki, 1964; Iwasaki, Fritsch & Hedberg, 1964; Karle, 1973).

The principal points requiring attention are:

A. *Equations relating intensities to molecular quantities*

An explicit reference should be made to the electron scattering formulae used including scattering factors or electron distribution functions, polarization corrections, dynamic corrections, *etc.* Note that the functions adopted in structure refinements may not be the same as those employed in the leveling of data.

B. *Auxiliary information*

The values of force constants, rotational constants, or related quantities used in analyzing data should be given and their origin should be cited. Such quantities may enter the analysis in (1) computation of non-varied amplitudes of vibration; (2) computation of shrinkage corrections; (3) estimation of asymmetry parameters in internuclear distribution peaks; (4) searching for plausible models of refinement *via* the Westheimer–Hendrickson 'molecular mechanics' approach; (5) adopting spectroscopic quantities such as rotational constants as constraints or merging them with diffraction intensities in the matrix of observations; (6) correcting spectroscopic quantities in (5) to be compatible with vibrational averages derived by diffraction.

C. Geometry adjustments

A discussion of the range of structural models tried must be given with statements: (1) whether symmetry constraints or other simplifications were imposed (*e.g.*, assumptions of local C_{3v} symmetry for a CF_3 group). All such constraints should be stated explicitly. (2) Whether multiple minima in least-squares solutions were searched for or encountered (false, deceptive minima are encountered in molecules as simple as SeO_2F_2). (3) Whether a static model with broadened peaks or a superposition of models distributed along various internal coordinates was taken.

D. Analysis of uncertainties

Estimates of the precision and probable accuracy should be given. It is essential to describe the various sources of uncertainty with a clear separation between measurement imprecisions, numerical analysis deviations, and possible systematic biases. The methods and assumptions made in the statistical analyses should be indicated including the weighting scheme and the inference of random errors and data correlations. Discussions of sources of experimental errors are given in several references, including Akishin, Rambidi & Spiridonov (1967); Bartell (1971); Bastiansen, Seip & Boggs (1971); Bauer (1970); Beagley (1973); Davis (1971); Harshbarger, Lee, Porter & Bauer (1969); Hilderbrandt & Bonham (1971); Karle (1973); Kuchitsu (1972*a*, *b*); Robiette (1973); Seip (1973); Vilkov (1964). Statistical analyses are outlined in several places including Bartell (1971); Bartell & Yow (1973); Bastiansen, Fritsch & Hedberg (1964); Hamilton (1964); Hedberg & Iwasaki (1964); Iwasaki, Fritsch & Hedberg (1964); MacGregor & Bohn (1971); Morino, Kuchitsu & Murata (1965); Murata & Morino (1966); Seip & Stølevik (1972); Seip, Strand & Stølevik (1969); Vilkov & Sadova (1967). One useful indicator that should *always* be determined and reported in diffraction studies is the 'index of pattern contrast' or 'index of resolution' defined as the ratio of $[I_{\rm molec}(s)/I_{\rm backgr}(s)]_{\rm obs}$ to $[I_{\rm molec}(s)/I_{\rm backgr}(s)]_{\rm calc}$ best characterizing the adjustable scale factor for the molecular intensity in the strong part of the pattern. Values much lower than unity indicate a washed-out pattern or imperfect intensity calibration. In complex molecules with overlapping internuclear distances it may be prudent to investigate couplings between systematic errors in intensities and derived parameters over and above simple scale-factor errors (Bartell & Yow, 1973).

E. The meaning of the parameters determined

The physical significance of the lengths, angles, and amplitudes of vibration deduced is implicit in the form of the equation adopted to relate observations to derived quantities. The complexity of the possible range of corrections (see III*A*, III*B*, and IV*B*) makes it necessary to identify explicitly the meaning of the final values reported insofar as possible. Many of the problems encountered are discussed in Iijima (1972); Kuchitsu (1968); Kuchitsu & Cyvin (1972); Rambidi & Ezhov (1968); and Sutton (1965).

IV. Presentation of results

The most important considerations are:

A. Conventional symbols, terminology, and units

It is suggested that authors follow wherever feasible the recommendations of the international system of units (SI) (IUPAP Commission for Symbols, Units, and Nomenclature 1965; *Le Systéme International d'Unités* (*SI*), 1970; McGlashan, 1970; *Rules for the Use of Units of the International Systems...*, 1969) and the symbols and nomenclature approved by the various international unions (e.g., CODATA, 1973; International Union of Crystallography, 1973; IUPAC Commission on Thermodynamics and Thermochemistry, 1972; Triple Commission for Spectroscopy, 1963). The Commission on Electron Diffraction, however, accepts the IUCr recommendation to crystallographers (IUCr, 1973) that, in reporting structures, the ångstrom unit is preferred to an SI unit. If SI units are not adopted, the CODATA Task Group (CODATA, 1973) recommends footnotes such as 'Throughout this paper Torr = (101·325/760) kPa, and Å = 100 pm'.

B. Specialized symbols

In the field of electron diffraction no universally accepted notation has emerged, and the diversity of (continually evolving) procedures extant makes it unprofitable to try to impose a standard notation in such quantities as reduced intensity functions and radial distribution functions. It is desirable, however, to have a consensus on meanings of symbols for well defined molecular parameters since so many different types of averages are of concern in structural chemistry that the risk of confusion is great in the absence of standardization. Most of the following symbols are in widespread use and seem clear and concise enough to be adopted (Kuchitsu, 1968; Kuchitsu & Cyvin, 1972; Sutton, 1965).

(1) *Internuclear distances of special importance in electron diffraction*:

r_g Thermal average value of internuclear distance.

r_a Thermal average value of internuclear distance evaluated with an r^{-1} weight factor in the averaging. See IV*B*(4) below for relation to diffraction pattern.

r_z, r_α^0 Distance between average nuclear positions in ground vibrational state (r_z often refers to spectroscopic and r_α^0 to diffraction determinations).

r_α Distance between average nuclear positions at thermal equilibrium.

r_e Distance between equilibrium nuclear positions (structure at minimum potential energy).

If the above set of alternative parameters seems redundant and needlessly esoteric it should be noted that each member serves a useful role and, unless the associated distinctions are made and understood, it is impossible to publish fundamentally significant and precise structure results based on electron diffraction (or any other) studies. The parameters r_e, r_α, and r_z enjoy the property of corresponding to distances between points representing atoms in a geometrically self-consistent structure capable of representation by Cartesian coordinates. The true mean distance r_g and the natural diffraction distance r_a do not share this property, in general, owing to vibrational effects. But r_e, the theorists' preferred quantity, is seldom accessible (though plausible estimates can often be made), and r_α (and r_z) are misleadingly far from physical average internuclear distances to be optimally useful for consumption by nonspecialists who may seek to relate distances to interatomic forces, *etc.* One possible compromise is a structure (sometimes called an r_y structure) in which *bond* lengths are assigned their r_g values and bond angles and torsion angles are given the values in an r_α structure. In such an 'r_y' structure, which can always be expressed in Cartesian coordinates in the case of acyclic molecules, internuclear distances differ from true mean distances only by relatively small 'Bastiansen–Morino shrinkage corrections'. A disadvantage of the r_y convention is that its basis is less fundamental in that it requires an arbitrary distinction between bonded and nonbonded distances. Furthermore, in the case of those cyclic molecules whose ring angles can be altered by a totally symmetric stretching deformation, the r_y structure cannot be precisely self-consistent (except by accident).

(2) *Bond angles*:

No special notation has arisen and none seems necessary at this time. It is well to mention, however, that angles deduced solely from r_g or r_a distances without shrinkage corrections in general cannot correspond exactly to angles in a geometrically self-consistent structure, and the difference between r_g-based angles and the self-consistent r_α and r_e angles may far exceed experimental uncertainties. When amplitudes of vibration are very large, the physical meaning of bond angles may be obscure, particularly in the case of quasilinear or quasiplanar molecules. Due caution in reporting should be exercised in these cases.

(3) *Amplitudes of vibration*:

These are commonly designated by the symbols l or u, either of which is acceptable. For purposes of illustration we follow Cyvin (1968) and write l:

l_g represents $[\int(r-r_g)^2\,P(r)\mathrm{d}r]^{1/2}$

l_e represents $[\int(r-r_e)^2\,P(r)\mathrm{d}r]^{1/2}$

l_m represents the effective amplitude found by identifying the vibrational modulation of the molecular intensity curve with the damping factor $\exp(-l_m^2 s^2/2)$.

(4) *Interference patterns*:

s The scattering variable $(4\pi/\lambda)\sin(\varphi/2)$ where φ is the scattering angle.

κ A parameter, characteristic of the asymmetry in an internuclear distribution peak, showing up in the argument of the associated sinusoidal interference features as $\sin\{s[r_a-\kappa s^2+\mathrm{O}(s^4)]\}$.

$f(s)$, $\eta(s)$ Complex atomic scattering factor for electrons where $f(s)=|f(s)|\exp i\eta(s)$, assuming that atoms are spherical. Notation for corrections for atoms in molecular environments is not yet standardized.

C. *Mode of presentation of the results*

The CODATA Task Group (CODATA, 1973) recommends, as a general principle, that results be reported in a form as free from interpretation as possible (*i.e.* as close as is practical to experimentally observed quantities). These results should be reported in such a manner that the degree of experimental randomness can be assessed. The reader should be able to recover enough of the experimental data so that he can reanalyze them in terms of different hypotheses. Graphical and analytical representations of important results, although convenient for the reader, are not acceptable substitutes for tabular presentation of accurate experimental results.

D. *Quantities to be reported in standard structure analyses*

Publication of the following tabular and graphical information is recommended:

(1) *Tables*

(*a*) *Digital values of leveled total intensities* (*molecular plus background*) ***and*** *the background used by the author.* Alternatively, the molecular intensities might be substituted for the leveled total intensities (while retaining a report of the background). Molecular intensities are less 'primary' than total intensities but are more convenient to analyze. These vital data should *always* be made available in work meriting publication in standard professional journals but may be deposited as supplementary material rather than as a tabulation in the journal article itself. It would be desirable to report indices of resolution for the various camera geometries here *as well as in the text.*

(*b*) *Bond distances, bond angles, and their uncertainties.* The meaning of the uncertainties must be specified in the tables as well as in the abstract and it is recommended that 2σ or 3σ be reported since they are more appropriate quantities than σ for consumption by non-specialists. Present methods of estimating σ are unreliable because errors are not statistically distributed in conventional diffraction analyses. It is to be hoped that progress will be made in error analyses.

The table should refer to a description of the principal systematic errors as well as random errors, either by direct inclusion, in a footnote of the table, or by an explicit reference in the table to the part of the text or other publication where the errors are discussed. The discussion should include how *known* systematic errors are corrected and how the magnitudes of poorly known systematic errors are estimated and included in the final uncertainties.

(*c*) *Mean square amplitudes.* The temperature should be specified insofar as is possible.

(*d*) *Error matrix or correlation matrix for derived parameters* (Hamilton, 1964). The correlation matrix with elements ϱ_{ij} is more immediately diagnostic of potential troubles in the analysis (if correlations are high) than is the error matrix. The full error matrix with elements $\varrho_{ij}\sigma_i\sigma_j$ is needed to calculate regression lines. The regression slope $\varrho_{ij}\sigma_i/\sigma_j$ may be valuable in allowing a quick estimation of $\Delta\theta_i/\Delta\theta_j$ where $\Delta\theta_i$ is the expected change in parameter θ_i from its least-squares value if subsequent information indicates that parameter θ_j should be changed from its least-squares value by $\Delta\theta_j$.

A good compromise between convenience and space is to tabulate the row matrix with elements σ_i and to tabulate immediately beneath it the correlation matrix. In some cases the correlation matrix is too large to warrant publication and a useful compromise might be to list only the elements with values exceeding, say, 0·5.

Some authors may wish to present a table of atomic coordinates to make it convenient for readers to calculate nonbonded distances, dependent angles, moments of inertia, *etc.* Interpretational difficulties (see IV*B*), however, mar the utility of such a table.

(2) *Figures*

(*a*) *Radial distribution curve.* In many cases these curves and their residuals (the differences between experimental and calculated curves) provide insights not readily apparent in intensity curves. They should be labeled with clear indications of the assignments of the prominent features.

(*b*) *Molecular intensity curves.* It may be useful, particularly when the tabulated intensities are not published in the article itself, to illustrate the molecular intensity curves, including the residuals. These should never be considered as a replacement of the tabular information in IV*D*(1*a*) above, however, for such figures are not easily subjected to reanalysis.

Some authors may wish to present figures showing experimental and theoretical intensities for separate plates or separate camera geometries. In addition, figures may compare residuals with experimental uncertainties obtained by computing values from each plate separately. Such plots may often be helpful.

Abbreviated check-list for electron diffraction publications

I. *Experimental apparatus and procedures*
- *A*. Sample (source, purity, pressure)
- *B*. Apparatus (description)
- *C*. Uncertainty in the *s*-scale
- *D*. Nozzle specifications and sample temperature
- *E*. Sector calibration
- *F*. Intensity measurement
- *G*. Number of independent measurements

II. *Treatment of diffraction data*
- *A*. Leveling scheme (description if used)
- *B*. Extraneous scattering corrections (description if used)
- *C*. Background function (method of derivation, number of implicit shape parameters)
- *D*. Interpolation of data (procedures, smoothing involved, correlations in interpolated data)

III. *Derivation of structural parameters*
- *A*. Equations (scattering formulae, scattering factors)
- *B*. Auxiliary information (force constants, rotational constants, asymmetry parameters, *etc*.)
- *C*. Geometry adjustments
  1. Symmetry constraints imposed
  2. Whether multiple solutions searched for or encountered
  3. Method to represent peak broadenings
- *D*. Analysis of uncertainties (how done)

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