Instructions for Preparing Manuscripts
for the *Journal of Physical and Chemical Reference Data*

Manuscript Submission The Editor welcomes appropriate manuscripts for consideration as Journal articles or monographs. **Please submit the proposed manuscript to:**

> **Editor, J. Phys. chem. Ref. Data, Bldg. 820, Room 103**
> **National Institute of Standards and Technology**
> **Gaithersburg, MD 20899-2310**
> **lnternet. jpcrd@nist.gov**

Typing Instructions Type all parts of the manuscript double-spaced on standard letter-size paper, single column one side only; see attached guidelines entitled "Typefaces for Symbols in Scientific Manuscripts". Submit a diskette of the manuscript in Microsoft Word, or REVTeX. A toolkit is available to assist in the preparation of manuscripts. World Wide Web: Point your browser to http://www.aip.org/epub/compuscripts.info.html. The Word author toolkit and the REVTeX macros are accessible from this point.

FIT: Available via anonymous ftp from ftp.aip.org. The Word author toolkit is available in the directory /ems. The REVTeX macros are available in the directory /pub/revtex.

Disk: Both the toolkit and the REVTeX macros are available on disk (specify Mac or IBM~DOS, Word). (e-mail: publish@aip.org).

Organization of Article The components of the article and their sequence should be as follows:

> Title
> Author(s)
> Affiliation
> Abstract (about 200 words)
> Key words (maximum 12, in alphabetical order, separated by semicolons)
> Contents
> List of Tables
> List of Figures
> Body of text (with numbered sections; include tables in the text where first mentioned, each on a separate page)
> Acknowledgments (financial support should be indicated here)
> References
> Appendices (if any)

Headings and Subheadings Headings and subheadings in the text should have a maximum of three levels and should be numbered as follows:

> 1.   (Main level)
> 1.1   (Second level)
> 1.1.1 (Third level)

The first numbered level is normally "1. Introduction" and the last is "References". When referring to numbered sections in the text use the form "..... .... ," except at the beginning of a sentence where "Section 1.1 .. ." is the correct form.

Mathematical Expressions Center equations on the page with numbers in parentheses at the right margin. Each equation should be numbered consecutively with Arabic numerals starting with "1." Identify any unusual symbols in the margin. Refer to equations in the text as Eq. (1), etc., except at the beginning of a sentence where "Equation (1)" should be used.

References The preferred style is to indicate literature references in the text by numerical superscripts, e.g., ... as discussed by Smith[3] in an earlier paper...

References should be numbered sequentially as they appear in the text. Reference citations at the end of the paper should have the following format:

> Periodical references: [7]R. W. Zwanzig, J. Chem. Phys. 32, 1173 (1960).

Books: [31]A. A Bondi, *Physical Properties of Molecular Crystals, Liquids, and Gases* (John Wiley and Sons, Inc., New York, 1968).
[48]J. Hilsenrath, Thermodynamic Properties of Gases, in *American Institute of Physics Handbook*, Second Edition, Dwight E. Gray, Coordinating Editor (McGraw-Hill Book Company, Inc., New York, 1963).
Reports: [72]R. S. Hager and E. C. Seltzer, Internal Conversion Tables, Part I, CALT-63-60, Pasadena, CA, June 1967.

An alternative style (sometimes called "British Style"), which is permitted for certain types of papers, is to indicate references by the first author's name and year of publication in parentheses, e.g.,

> ... was first observed by Phillips (1968)
> ... but other studies (Smith, 1975; Brown and Lee, 1961) have shown ...

In this case the reference list should be ordered alphabetically by the first author as follows:

> Erikson, G. W, 1977, J. Phys. Chem. Ref. Data 6, 831.
> Goldsmith, I.E., E. W. Weber, and T. W Hansch, 1978, Phys. Ref. Lett. 41, 1525.

Note the style of initials in multiple-author papers.
A third acceptable reference style is use of the reference squib. The squib format is yyABCIXYZ where yy is the year, ABC are the first three letters of the first author, XYZ are the first three letters of the second author. Should two or more papers appear with identical squibs, the first is designated as yy ABC(XYZ; the second by yyABCIXYZ2, the third by yyABCIXYZ3, etc. In this case the reference list should be ordered by year and then alphabetically by first author, e.g.,

> 9211N1CHE Jin, *Y,* Cheng, I., Varma-Nair, M., J..Phys. Chem. **96**, SISi (1992).
> 92KABIKOZ Kabo, 6. J., Kozyro, M. K., J. Chem. Thermodynam. **24**, 1(1992).
> 92KUL Kulshreshtha, S. K., 3. Phys. Chem. Solids **53**, 39 (1992).
> The editor should be consulted before a manuscript is prepared with any other style of citation.

Footnotes Footnotes should be used sparingly. When absolutely necessary, a footnote should be indicated by a letter superscript and typed at the bottom of the manuscript page on which it appears. Footnotes should be lettered consecutively through the entire manuscript, starting with "a".

Tables Tables should be typed on separate pages and the pages numbered such that the tables appear at approximately the right place in the manuscript: It is usually desirable to place very long tables at the end of the textual material.
Each table should have a concise heading which clearly indicates the contents. Avoid complicated column headings. Tables should be numbered consecutively with Arabic numerals. Footnotes to entries in the tables should be indicated by superscripts, a, b, c,..... and typed at the bottom of the table.
The table headings should be separated from column headings by a double horizontal line. A single horizontal line should be placed between the column headings and the body of the table and also at the end of the table. Vertical lines may be used if necessary to delineate columns clearly. Only the first letter of the first word in both table headings and column headings is capitalized.

Figures Include figures at the end of the manuscript with a list of figure captions typed (double-spaced) starting on a separate page. Number figures with Arabic numerals, starting with "1" and continue in sequence throughout the text. When referring to numbered figures in the text use the form ".... . Fig. 1...," except at the beginning of a sentence where "Figure 1..." is the correct form. See attached sheet on Preparation of Illustrations for more details.
Figures may be submitted as TIFF, Encapsulated Postscript (EPS), or PostScript (PS) files on the manuscript diskette(s) if they conform to the specifications above.

Units, Symbols, Terminology, and Chemical Nomenclature It is the policy of the *Journal of Physical and Chemical Reference Data* to follow the recommendations of recognized international bodies such as ISO, IUPAC, IUPAP, and CODATA unless there are strong grounds for making an exception. The most important sources of recommendations on symbols, terminology, and units are:

> Quantities and Units, ISO Standards Handbook, Third edition (1993).

> Quantities, Units and Symbols in Physical Chemistry, Second edition, IUPAC, Blackwell Scientific Publications, Oxford (1993).

Symbols, Units, and Nomenclature in Physics, IUPAP Document U. I. P.20 (1978).

Guide for the Use of the International System of Units (SI), B. N. Taylor, Natl. Inst Stand. Technol. Special. Publ. 811, 1995 Edition.

The International System of Units (SI) should always be employed unless the Editor has granted an exception.

The nomenclature practices of Chemical Abstracts should be followed. Authors preparing compound indices for their papers should consult the current CA Index Guide. It is highly desirable to include CAS Registry Numbers in tables that list chemical compounds.

Proofreading Authors are responsible for correcting errors in typeset proofs. Changes in typeset proofs should be limited to those that make the typeset proofs conform with the original manuscript.

Typefaces for Symbols in Scientific Manuscripts

Most word processing systems now in use are capable of producing lightface (that is, regular) or boldface letters of the Latin or Greek alphabets in both roman (upright) and italic (sloping) types. The understandability of typed and typeset scientific and technical publications is facilitated if symbols are in the correct typeface.

The typeface in which a symbol appears helps to define what the symbol represents. For example, irrespective of the typeface used in the surrounding text, "A" would be typed or typeset in

- italic type for the *scalar quantity* area: *A,*

- roman type for the *unit* ampere: A;

- italic boldface for the *vector quantity* vector potential: *A*.

More specifically, the three major categories of symbols found in scientific and technical publications should be typed or typeset in either italic or roman type, as follows:

- symbols for *quantities* and *variables:* italic;

- symbols for *units:* roman;

- symbols for *descriptive terms:* roman.

These rules imply that a subscript or superscript on a quantity symbol is in roman type if it is descriptive (for example, if it is a number or represents the name of a person or a particle); but it is in italic type if it represents a quantity, or is a variable such as x in E_x or an index such as i in $\Sigma_i x_i$ that represents a number. An index that represents a number is also called a "running number." The following four sections give examples of the proper typefaces for these three major categories.

Quantities and variables - italic

Symbols for quantities are italic, as are symbols for functions in general, for example, *f(x):*

t = 3 s	*t* time, s second	*T* =22 K	*T* temperature, K kelvin
r = 11 cm	*r* radius, cm centimeter	λ= 633 nm	λ wavelength, nm nanometer

Constants are usually physical quantities and thus their symbols are italic; however, in general, symbols used as subscripts and superscripts are roman if descriptive:

N_A Avogadro constant, A Avogadro   *R* molar gas constant

θ_D Debye temperature, D Debye

e elementary charge

Z atomic number

m_e *m* mass, e electron

Running numbers and symbols for variables in mathematical equations are italic, as are symbols for parameters such as *a* and *b* that may be considered constant in a given context:

$$y = \sum_{i=1}^{m} x_i z_i \qquad\qquad x^2 = ay^2 + bz^2$$

Symbols for vectors are boldface italic, symbols for tensors are sans-serif bold italic, and symbols for matrices are italic:

$A \cdot B = C$ (vectors) $\qquad\qquad T$ (tensors) $\qquad\qquad A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$ (matrices)

Symbols used as subscripts and superscripts are italic if they represent quantities or variables:

c_p p pressure $\qquad\qquad q_m$ *m* mass $\qquad\qquad \sigma_\Omega$ Ω solid angle $\qquad\qquad \omega_z$ z z coordinate

Units - roman

The symbols for units and SI prefixes are roman:

m	meter	g	gram	L	liter
cm	centimeter	µg	microgram	mL	milliliter

Descriptive terms - roman

Symbols representing purely descriptive terms (for example, the chemical elements) are roman, as are symbols representing mathematical constants that never change (for example, π) and symbols representing explicitly defined functions or well defined operators (for example, $\Gamma(x)$ or div):

Chemical elements:

Ar argon $\qquad\qquad$ B boron $\qquad\qquad$ C carbon

Mathematical constants, functions, and operators:

e	base of natural logarithms	Σx_i	Σ sum of
exp x	exp exponential of	$\log_a x$	$\log_a$ logarithm to the base a of
dx/dt	d lst derivative of	sin x	sin sine of

Symbols used as subscripts and superscripts are roman if descriptive:

$\varepsilon_0^{(ir)}$ $\qquad$ ir $\qquad$ irrational $\qquad\qquad$ E_k $\quad$ k $\qquad$ kinetic

V_m^l $\qquad$ m $\qquad$ molar, l liquid phase $\qquad$ μ_B $\quad$ B $\qquad$ Bohr

Sample equations showing correct type

$$F = \frac{q_1 q_2}{4\pi\varepsilon_0 r^2}$$

$\qquad\qquad F = ma \qquad\qquad pV = nRT$

$$\varphi_B = x_B V_{m,B}^{\cdot} / \Sigma x_A V_{m,A}^{'}$$

$\qquad E_a = R\ T^2\ d(\ln k)/dT \qquad c_1 = \lambda^{-5}/[exp(c2/\lambda T)-1]$

$$p_B = \lambda_B \lim_{\not p \to 0} (x_{\not p} / \lambda_B) \qquad\qquad \frac{F}{Q} = grad\ V$$

$$E = mc^2$$

Greek alphabet in roman and italic type

The following table shows the proper form, in both roman and italic type, of the upper-case and lower-case letters of the Greek alphabet.

Alpha	A	α	A	α
Beta	B	β	B	β
Gamma	Γ	γ	Γ	γ
Delta	Δ	δ	Δ	δ
Epsilon	E	E, ϵ	E	$E,\ \epsilon$
Zeta	Z	ζ	Z	ζ
Eta	H	η	H	η
Theta	Θ, θ [a]	θ, ϑ [a]	$\Theta,\ \theta$ [a]	θ, ϑ [a]
Iota	I	ι	I	ι
Kappa	K	κ, χ [b]	K	κ, χ [b]
Lambda	Λ	λ	Λ	λ
Mu	M	μ	M	μ
Nu	N	ν	N	ν
Xi	Ξ	ξ	Ξ	ξ
Omicron	O	o	O	o
Pi	Π	π,	Π	π,
Rho	P	ρ	P	ρ
Sigma	Σ	σ	Σ	σ
Tau	T	τ	T	τ
Upsilon	Υ	υ	Υ	υ
Phi	Φ	φ, ϕ	Φ	$\Phi,\ \phi$
Chi	X	χ	X	χ
Psi	Ψ	ψ	Ψ	ψ
Omega	Ω	ω	Ω	ω

[a] The International Organization for Standardization (ISO) gives only the first of the two letters *(tee* ISO International Standard ISO 310:1992).
[b] ~So gives these two letters in the reverse order (see ISO International Standard 150 31-0:1992).

INSTRUCTIONS TO AUTHORS: SUBMITTING ELECTRONIC GRAPHICS FILES

The American Institute of Physics is accepting electronic graphics files for production of author proofs and subsequent publication of articles.

If your electronic files are received after we have already processed the hardcopy illustrations, the electronic files will not be used. It is important that these procedures be followed precisely for the graphics files to be of use in the initial journal production process.

Although you are still required to send hard copies of your figures to the editorial office of the journal in which you are publishing, we strongly encourage you to send electronic graphics files to AlP to receive optimal quality. Send every figure in the article, in particular. halftones and combinations (line art + halftone). Computer-generated illustrations, when output to laser printers, produce a screen. These figures are the most problematic, because scanning screened output produces an unacceptable moiŕe pattern. Line art is less problematic for AlP, but is also accepted electronically, providing the line weights are sufficient (see *lnstructions for Preparation* of *Illustrations* on side 2 of this sheet).

Files should be sent to AlP as soon as you receive the letter of acceptance from the editorial office. Sending the files as soon as

you know the AlP code number (e.g., 00i704jap) will ensure that AlP will use your electronic graphics.

Before you send the files, please make sure that you have read and followed these instructions.

<div style="border:1px solid black">

ELECTRONIC GRAPHICS CHECKLIST:

* Article has been accepted for publication by the editorial office. Do not send electronic graphics prior to acceptance.
* Files are in acceptable formats (PS, EPS or TIFF).
* File settings are in accordance with AlP electronic submission requirements. Files are named according to AlP file naming conventions.
* Files have been checked for extraneous header information in the body of the file (for example, if you have received graphics files via Email, headers must be edited out).
* All figure files for the article have been FTP'ed to AlP.

</div>

ACCEPTABLE FORMATS:

AlP can accept PostScript, EPS (using either Anal or Times Roman fonts), or TIFF (lzw compressed) files. We cannot accept application files, e.g., Corel Draw, etc.

SETTINGS:

1. Size your illustrations according to your journal's specifications. Submit each illustration at the final size in which it will appear in the journal. The standard is 8.5-cm maximum width *(3-3/8″* or 20.5 picas) for one column.
2. Set the graphic for **600 dpi** resolution for line art, **264 dpi** for halftones (non-compressed), and **600 dpi** for combinations (line art + halftone).
3. Ensure that line weights will be **0.5 points** or greater in the final published size. **Line weights below 0.5 points will reproduce poorly.**
4. Save the files to grayscale (BIW), not color.

FILE NAMING CONVENTIONS:

Use the character alphanumeric AlP code number (included in the letter of acceptance you receive from the editorial office), and name the files as follows:

    (9-character AlP code No.][figure No.].(file format]

Example: 001 704japl Ps

FTP INSTRUCTIONS:

1. It is important that the files are not compressed. Do not use uuencode, BINHEX, zip, or any other compression utilities.
2. Make sure there is only ONE figure per file. Each figure file should include all parts of the figure. For example, if Figure 1 contains three parts (a, b, c), then all of the parts should be combined in a single file for Figure 1.
3. Delete extraneous header information (if necessary). The only data in the file should be the figure itself.
4. FTP to flp.aip.org Login as anonymous
   Password: Your full E-mail address
   cd/Ielecsubs
   For TIFF files only, type "bin" for binary transfer of files
   put *.*[file names]
   To logout, type "bye"
5. If you were unsuccessful in initially FTP'ing the files (due to a broken FTP connection, etc.). You should try to FTP them again. **IMPORTANT**: Use the following altered naming convention for resubmitting files. Since you will be unable to overwrite the first attempt, you should name your file as follows:

001704jap1.ps.2 (add the .2 extension)

USER SUPPORT:

If you have problems with FTP, or if you are unable to FTP your files effectively, please contact your System Administrator for more information or instructions on how to use FTP.

Questions regarding AlP electronic submission procedures may be sent to esubs@aip.org. These instructions may also be found on the AlP Physics Information Netsite at www.aip.org/epub/submitgraph.html.

INSTRUCTIONS TO AUTHORS:
PREPARATION OF HARDCOPY ILLUSTRATIONS FOR SCANNING

When preparing your hardcopy illustrations for submission, note that they will be scanned using a digital scanner and integrated with the text of the article, creating completely electronic pages. Please adhere to the following guidelines when preparing your hardcopy illustrations for submission:

Number figures in the order in which they appear in text. Label illustrations with their number, the name of the first author, and the journal, on the front of the figure well outside the image area.

Place only one figure per page. Place all parts of the same figure on one sheet of white bond paper, spaced 1/4 in. apart, using a glue stick or wax on the back of the illustration and leaving a 2-in. bottom margin. Label all figure parts with (a), (b), etc. Make sure each figure is straight on the page. *Photocopies of artwork are not acceptable.*

Prepare illustrations in the final published size, not oversized. Size your illustrations according to your journal's specifications. Submit each illustration at the final size in which it will appear in the journal. The standard is 8.5-cm maximum width (3-3/8" or 20.5 picas) for one column. This is especially important for screened or shaded illustrations; reduction of screened/shaded originals during the digitizing process introduces an unacceptable moiŕe pattern.

Do not use correction fluid or tape on illustrations. The scanner is extremely sensitive and reproduces all flaws (e.g., correction fluid, tape, smudges, dust). *Do not write on the back of the figure* because it will be picked up by the scanner.

Ensure a minimum of 8-point type size (2.8 mm high; 1/8" high) and 1-point line width within illustrations. Ensure that line weights will be 0.5 points or greater in the final published size. **Line weights below 0.5 points will reproduce poorly**. Avoid inconsistencies in lettering within individual figures, and from one figure to the next. Lettering and symbols cannot be handwritten. Avoid small open symbols that tend to fill in if any reduction is necessary.

Authors' laser-generated graphics are acceptable only if the lettering and lines are dark enough, and thick enough, to reproduce clearly, especially if reduction is required. Maximum black-white contrast is necessary. Choose a laser printer with the highest dot-per-inch (dpi) available (i.e.. the highest resolution possible). Remember that fine lines in laser-generated graphics tend to disappear upon reduction, even if the oversized original looks fine. To receive optimal quality, we strongly encourage you to send electronic graphics files to AlP, rather than laser output. In particular, halftones and combinations (line art + halftone) should be submitted electronically. Computer-generated illustrations output to laser printers produce a screen. These figures are the most problematic, because scanning screened output produces an unacceptable moiré pattern.

Submit continuous-tone photographs in final published size on white glossy or matte paper. Avoid glossy paper stock that is off-white, ivory, or colored because contrast within the illustration will be lost in reproduction. Print the photograph with more contrast than is desired in the final printed journal page. Avoid dull, textured paper stock, which will cause illustrations to lose contrast and detail when reproduced.

GLOSSARY OF GRAPHICS TERMS

Continuous-Tone (Contone) - A photographic image that contains gradient tones from black to white.

Halftone (HT) - The reproduction of continuous-tone artwork, such as a photograph, through a screen, which converts the image into dots of various sizes.

PostScript (PS) - A general purpose programming language with powerful graphics capabilities. Its primary application is to describe the appearance of text and images on printed or displayed pages.

Encapsulated PostScript (EPS) - A standard file format for importing and exporting PostScript language files among applications. EPS flies describe the appearance of a single page, and can contain any combination of text and graphics. Typically, the purpose of the EPS file is to be included, or "encapsulated" in another PS language.

Tagged Image File Format (TIFF) - A tagged-based universal graphics file format for storing and interchanging images. It is not a page description language.

Moire' - The undesirable screen pattern caused by scanning screened artwork, such as halftones. It is the interference pattern that usually occurs when two or more patterns superimpose.