Preparation of Manuscripts

(Revised January 2003)

Preparation of Manuscripts. The manuscript should be typewritten, *double spaced* throughout, including tables and footnotes, on 22 × 28 cm ($8^1/_2$ × 11 in.) (or A4) paper of good quality. Clear, sharp copies made by a permanent duplication process are acceptable. If a word processor is used in the preparation of the manuscript, a printer which produces *high quality, easily readable* copy must be used. Authors should consult recent issues of this journal, *The ACS Style Guide* (available from Oxford University Press, Order Department, 201 Evans Rd., Cary, NC 27513), and the journal web site (http://pubs.acs.org) as a guide to format for typing, headings, etc. All pages of a manuscript should be numbered consecutively, including tables. The latter should be grouped at the end of the manuscript. Authors should indicate, by text or marginal notations in the typescript, where the figures and tables are to be inserted.

For all authors, the given name (*not* the initial), initial(s) of the middle name(s), and the last name should be given for complete identification. Authors are asked to provide their e-mail addresses and fax numbers along with postal addresses.

Only manuscripts written in English can be considered. Authors who are not fully familiar with idiomatic English are requested to seek expert assistance in preparing the manuscript *before* submitting it to the editorial office.

Because the journal uses a graphic table of contents format, each manuscript submission should be accompanied by a two-page table of contents entry. **On one page should be the title of the contribution, the complete list of authors, and the summary (all double-spaced).** The summary must be brief, two sentences at most; the *absolute* limit is 75 words. This page should be labeled "for table of contents use only". The summary should bring the key findings of the study being reported, stressing the novel features. **The chosen graphic should be on the second page.** It should be large and clear enough to be photoreducible to either a 1.75 in. square or 4 in. wide by 1 in. high rectangle and remain legible. This requires also the selection of appropriate type size for any labels, formulas, or numbers that are used.

The following are examples of items that are suitable for the graphic to be used: a structure (ORTEP, PLUTO, ball and stick, line drawing); one or more formulas; an equation or a brief reaction scheme; a graph. Most often, a line drawing is best for clear, readily comprehensible presentation of a structure. In general, spectra and tables of data are not acceptable since they do not reproduce well after photoreduction.

The table of contents entry (2 copies) should be provided on separate pages. It should *not* be incorporated in the manuscript.

Nomenclature. All nomenclature used in manuscripts submitted to this journal should be consistently clear and unambiguous and should conform as closely as possible with current American usage. Insofar as possible, authors should use systematic names similar to those used by *Chemical Abstracts* and the International Union of Pure and Applied Chemistry. Authors are referred to the following publications on nomenclature: (a) *Nomenclature of Inorganic Chemistry, Definitive Rules*; IUPAC 1990; Blackwell: Oxford, U.K., 1990. (b) *Nomenclature of Organic Chemistry, Sections A−F and H*; IUPAC 1979; Pergamon Press: Oxford, U.K., 1979. (c) *A Guide to IUPAC Nomenclature of Organic Compounds*; IUPAC 1993; Blackwell: Oxford, U.K., 1993; (d) Ring Systems Handbook; American Chemical Society: Columbus, OH, 1988. (e) "Chemical Substance Index Names", *Chemical Abstracts Index Guide*; American Chemical Society: Columbus, OH, 1988. (f) *Inorganic Chemical Nomenclature*: *Principles and Practice*; American Chemical Society: Washington, DC, 1990. For CA nomenclature advice, consult the Manager of Nomenclature Services, Chemical Abstracts Service, P.O. Box 3012, Columbus, OH 43210-0012. A name generation service is available for a fee through CAS Client Services, 2540 Olentangy River Road, P.O. Box 3343, Columbus, OH 43210-0334; Telephone: (614) 447-3870; Telefax: (614) 447-3747; or e-mail: answers@cas.org.

Rigid and consistent conformance to these recommendations is not possible in organometallic chemistry because they conflict on certain details. The nomenclature employed in a manuscript at minimum should accurately state the stoichiometric composition of a compound. Whenever possible, the topology of the compound should be indicated in the nomenclature. For most compounds this can be accomplished by a consistent application of *hapto* nomenclature with superscript numbers indicating bonding ligand atoms. Thus η^5-cyclopentadienyl has five carbon ligand atoms and η-cyclopentadienyl has an indeterminate number of ligating atoms. Cage and cluster compounds, especially boron cage compounds, may be named and numbered following the recommendations of the references cited above or may be named with the more recent notation developed by Casey, Evans, and Powell (*Inorg. Chem.* **1981**, *20*, 1333). The cage numbering is the same in all references; the Casey et al. reference extends cage and cluster numbering to a much greater number of structures. Names derived by application of these recommendations should be given in the first place the compound is mentioned, especially in titles. In the text it is preferable to use names of simple substances instead of formulas (e.g., "nitrogen atmosphere" rather than "N_2 atmosphere"). However, formulas for all but well-known substances should be given in a paper. Abbreviations may be used in nomenclature *after* the complete name has been given in a paper. Common abbreviations should not be used with an unconventional meaning (e.g., Me is not an acceptable abbreviation for metal) and element symbols are not to be used in the context of an abbreviation with another meaning.

Common organic group abbreviations may be used: Me, Et, Pr, *n*-Bu, *i*-Bu, *s*-Bu, *t*-Bu, Ph (but *not* ϕ), but they should be applied consistently throughout the manuscript. For instance, Me and CH_3 should not be used interchangeably in the manuscript. Use Cp only for C_5H_5, not for substituted cyclopentadienyl groups.

Note that TMS is the abbreviation for tetramethylsilane; it should *not* be used for the trimethylsilyl (Me_3Si) group.

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Abbreviations. Letters used to represent quantities in mathematical expressions should be underscored or printed in italic type to indicate that they are to be printed in italics. Greek or unusual characters should be written plainly or should be explained by annotations. Simple fractions should be written with a slant line so that only a single line of type is required. All subscripts and superscripts should be carefully made and placed. The preferred forms for a few of the more commonly used abbreviations are %, °C, K, cm, L, mL, μL, g, mg, equiv, Hz, nm, ppm, A, s, min, h, bp, mp, TLC, VPC (or GC), NMR, IR, UV, eq. Note that these are used in ACS journals without periods.

The dimensions should be specified for all numerical quantities. In agreement with international convention, all rate constants should use seconds as the unit of time. The energies of infrared peaks should be expressed in wavenumbers (cm^{-1} or μm^{-1}). Chemical shift data should be expressed on a ppm basis and the standard used should be specified. Symbols in mathematical equations must be defined.

Tables. Tables should be numbered consecutively with Arabic numbers and should be grouped at the end of the manuscript. Footnotes in tables should be given a letter designation and cited in the table by superscript letters. The sequence of letters should proceed by line rather than by column. If a footnote is cited both in the text and in a table, insert a lettered footnote in the table to refer to the numbered footnote in the text. Each table should be provided with a descriptive heading, which, together with the individual column headings, should make the table, as nearly as possible, self-explanatory. In setting up tabulations, authors are requested to keep in mind the type area of the journal page ($\sim$18 $\times$ $\sim$25 cm) and the column width ($\sim$8 cm or 50 elite characters) and to make tables conform to the limitations of these dimensions. Arrangements that leave many columns partially filled or that contain much blank space should be avoided. Abbreviations and *linear* chemical formulas should be used in headings and columns of tables or in the body of tables; *structural* formulas should not be used in column headings or in the body of tables but may be used in the main heading.

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margin width	1.6 pt (0.056 cm, 0.0222 in.)
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(2) As text settings select:

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size	10 pt

(3) Under the preferences choose:

units	points
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Paper: US Letter
Scale: 100%

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High-resolution mass spectrometric molecular weights may be provided in lieu of elemental analyses in some cases, especially for routine intermediates in a synthetic scheme. Such data must, however, be accompanied by independent evidence of purity. Exclusions from these requirements may be permitted in special cases. These include, but are not restricted to, the following: (a) compounds that are unstable at room temperature or that would have decomposed by the time they were received by an external analytical laboratory; (b) compounds that are oils from which solvent cannot be removed completely or solids which tenaciously retain fractional amounts of solvent; (c) compounds that are formed in only very low yield, so that only a few milligrams are available; (d) compounds that are members of a group of similar compounds for which several members already have been analyzed.

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Product Yields. Yields of products obtained in reactions which are reported should be given in terms of g or mol as well as in %. If it is not obvious, it should be stated on what reagent the % yield is based. It should be made clear whether the yields reported are of crude product (specify purity, if possible) or of pure product. If yields are obtained by gas chromatography, details of the yield determination should be provided.

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ABSTRACT. It is sufficient to state in the abstract that the structure of a given compound has been determined by X-ray diffraction. Crystal data should not be given in the abstract.

EXPERIMENTAL SECTION. The description of the data collection and structural analysis should be as brief as possible for routine structure determinations. The required crystal data should be summarized in tabular form and include the following information: (a) chemical

formula, source of material and habit; (b) lattice constants, wavelength assumed in their calculation, temperature at which they were measured; radiation used in intensity measurement; type of filter or monochromator; (c) space group (method of distinguishing between groups with the same absences); (d) crystal dimensions in Å units (not pm), μ, range of absorption (or transmission) factors; method of correcting for absorption; (e) type of diffractometer, diffraction geometry, conditions for collecting reflections (i.e., 2θ range and sign(s) for hkl data collected); (f) number of reflections measured, number of independent reflections, agreement between equivalent reflections when multiple forms of the data have been collected; (g) final R factors (weighted and unweighted). A brief outline of the method used for the structure solution should be given. Computer programs and source of atomic scattering factors and anomalous dispersion ($\Delta f'$ and $\Delta f''$) should be appropriately referenced. Tests for the chirality of a noncentrosymmetric crystal (assuming that anomalous scattering is included) and corrections for extinction should be included when appropriate. Designation of atoms refined with anisotropic thermal parameters, treatment of hydrogen atoms, and geometrical constraints should be described.

STRUCTURAL RESULTS. In addition to the discussion of the structure, a *selected* list of pertinent bond lengths in Å units (not pm) and angles should be provided in tabular form. All remaining structural information will be deposited as Supporting Information and includes: (a) the final values of all *refined* atomic coordinates; (b) all calculated atomic coordinates; (c) all anisotropic thermal parameters, as either U_{ij}'s or B_{ij}'s; (d) a complete list of bond lengths in Å and angles; (e) least-squares planes and atomic deviations therefrom; (f) important intermolecular contacts; (g) unit cell and packing diagrams. Deposited material must be suitable for scanning with clean, unbroken alphanumeric characters.

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FIGURES. One computer-generated figure should show the labeling of atoms and the reported thermal vibration ellipsoids (preferably anisotropic). Stereoviews are permitted but must be provided at the correct magnification (about 50−55 mm or $2^1/_8$ in. between image centers).

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   (d) Experimental Section, written in the past tense (optionally, the Experimental Section may precede the Results and Discussion section(s))
   (e) Supporting Information Available paragraph, if applicable
   (f) References (labeled a, b, c, ... if more than one citation under a reference number)
   (g) Schemes, tables (with titles), and figures (with captions)
5. Supporting Information
   (a) Title page (list title and authors and SUPPORTING INFORMATION)
   (b) Text and/or tables, which should have clear titles. Give compound formulas and numbers in titles
6. Submission
   (a) Two copies of table of contents entry
   (b) Four copies each of the manuscript and Supporting Information, of which at least one copy should be printed on only one side of the paper