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Manuscripts should be kept to minimum length, and, for clarity, each work should be subdivided into labeled sections, e.g., Introduction, Experimental, Results and Discussion, Conclusions and References.

2.1. Title Page

For the layout of the title page, a current issue of ACI should be consulted.

Attention is drawn to the following points:

a) The title of a manuscript, being of greatest importance for attracting readers" interest and for information retrieval, should clearly and accurately provide information on the content and emphasis of the work. The use of abbreviations, symbols, chemical formulae, and references in a title is strongly discouraged. First letters of nouns and adjectives are capitalized.

b) The authors" full first names, middle initials, and last names should be given, followed by the address(es) of the contributing laboratory or laboratories. The author to whom correspondence and/or inquiries should be directed should be indicated with an asterisk (*). Footnotes may be added to indicate the present mailing address(es) of the author(s). The corresponding author"s mailing address, phone number, fax number, and e-mail address should also be included.

2.2. Abstract

An abstract in English, independent of the language of the main text should be provided. The abstract, stating briefly the purpose of the research (if not clear from the title), the principal results, and major conclusions, should be self-explanatory and intelligible without reference to the text. References to structural formulae, Tables, Schemes, and Figures, by number, may be made in the abstract. For a typical contribution, an 80- to 200-word abstract is usually adequate.

2.3. Keywords

For all types of manuscripts, 3 - 5 keywords, which best characterize the paper, should be given. For guidance, consult Chemical Abstracts General Subject Index.

2.4. Introduction

The introduction (no heading) should state briefly, with relevant references, the purpose of the investigation and its relation to other work in the appropriate field. All relevant citations should be included. Preferred form of citation of a series of papers on the same subject are "clusters" (see 2.7.).

2.5. Experimental

In the experimental section materials, methods and procedures should be described in this order, in sufficient detail to enable other chemists to repeat the experiments. The instruments used as well as measurement conditions and corresponding physical units should appear in a paragraph at the beginning of the Experimental section. Description of standard techniques applicable throughout the work should follow the paragraph on instrumentation. Novel experimental procedures should be described in detail, but procedures already published should merely be referred to by literature citation. General reaction conditions should be given only once. Both weight amounts and molar equivalents of all reactants and weight amounts and percentage yields of products should be included. Whenever possible, elemental analyses should be provided for new compounds. However, the molecular formula may be determined from physical data (e.g., high-resolution MS) if evidence of purity is presented.

2.6. Results and Discussion

Usually, the results are presented first, followed by a discussion of their significance. Only strictly relevant results should be given. The section may be further divided by subheadings. Equations, tables and figures should be used to shorten the text and make it readily understandable. Data should not be presented in duplicate.

2.7. Conclusion

The main conclusions of the study may be presented in a short Conclusions section, which may stand alone or form a subsection of a Discussion or Results and Discussion section.

2.8. References

References should be numbered sequentially in the order they are cited in the text. The numbers should be set superscript, usually after punctuation marks. Titles of journals must be abbreviated according to Chemical Abstracts (cf. Chemical Abstracts Service Source Index, CASSI).

Attention is drawn to the following conventions:

a) Names of all authors of cited publications should be given. Use of "et al." in the list of references is not accepted.

b) Surnames of authors should be followed by a comma and precede forename initials. Each initial is followed by a period and separated from the next by a space (unless hyphenated). A comma follows the set of initials except for the first of only two authors.

Connectives should precede surnames, where appropriate; please distinguish whether or not they are capitalised (e.g. van or Van, el or El, d' or D'). Where a second part of a hyphenated forename (usually Japanese) has a lower-case style, only the first letter of the first part should be shown; e.g. Yamamoto, K., not Yamamoto, K.-i.,. Do not include jnr. or III etc. after authors names.

Hyphenated forenames should show full punctuation (i.e. Dubois, J. E., not Dubois, J E.). Give proper contractions of Russian letters (Ya., Yu., etc.).

c) The name of the journal cited should be given in italics and the journal volume numbers should be given in Bold (or the year, where there is no volume number). Note the required sequences: volume, page (year) for journals with a volume number; and year, page for journals with no volume number. Do not include lower case letters in Chem. Abs. citations, i.e. 89, 10852 (1978) not 89, 10852t (1978).1

d) Composite references may be used, instead of a series of individual ones.2 The use of the Latin terms ibid. and idem is not allowed, since these are not compatible with electronic information-retrieval systems.3 When a part of a composite reference is cited individually in the text, the parts of the composite reference may be specified by a), b), etc. 4a, 4b

Examples of references to book chapters, books, patents, computer programs, and Ph. D. Theses, are also given.

References

1. Braverman, S., Pechenick-Azizi T., Major, D. T., and Sprecher, M., Beta-halo-alpha,beta-unsaturated gamma-sultones, J. Org. Chem., 72, 6824 (2007).

2. Krässig, H. A., in "Cellulose Structure, Accessibility and Reactivity", M. B. Huglin, Ed., Gordon and Breach Science Publishers: Yverdon, 1992, Vol. 11, p. 6.

3. Dunitz, J. D., "X-Ray Analysis and the Structure of Organic Molecules", Verlag Helvetica Chimica Acta: Basel, and VCH: Weinheim, 1995.

4. Kamata, T. and Wasada, N., Jap. Pat., 2-204469, 1990, p. 381–384.

5. Sheldrick, G. M., SHELXL97, Program for the Refinement of Crystal Structures, University of Göttingen, Germany, 1997.

6. Peterson, B. R., Ph.D. Thesis, University of California, Los Angeles, 1994.

In the text, reference to author(s) of cited works should be made without giving initials, e.g., ". . . as shown by Kamata and Wasada15". If the reference carries the names of three or more authors it should be quoted as "Barbero et al.5", if Barbero is the first author, or as "Piscopo and co-workers1", if Piscopo is the senior author.

3.1. Typesetting

Special types of print should be used as follows:

- **Boldface**: headings, designated numbers of chemical compounds.
- *Italics*: subheadings, configurational prefixes (*(R)-, (S), cis-, trans-, etc.*), Latin words or abbreviations, trade names of chemical compounds (first letter should be capitalized), names of authors if mentioned in the text.
- SMALL CAPITAL: symbols of molar and normal concentrations (M and N), D and L, the names of the discoverer in the nomenclature of genera, species, or varieties.
- ***Boldface italic***: the italicized terms and prefixes in headings.

Use of hyphens

Hyphens should not be used for common two-word chemical composites, e.g. cation radical, radical anion, ion pair, hydroxy group, radical pair etc. However, composite adjectives should always be hyphenated, e.g. "the intimate ion-pair intermediate is one example of ion pairs that intervene"; "the transition state is as predicted by transition-state theory"; "the hydroxy group in this compound undergoes typical hydroxy-group reactions".

Series of words: if a series of words or compound names is given as a number of fore-terms and one stem-term, then the last complete word should be hyphenated accordingly, e.g. "methyl-, ethyl-, and nitro-benzene" (not nitrobenzene); "inter- and intra-molecular" (not intramolecular).

Spelling conventions

English (UK) should be used for word speeling.

3.2. Footnotes

Footnotes, i.e., explanations or comments on the text, should be kept to a minimum. Each one should be indicated in the manuscript by a superscripted special character, such as *, †, ‡. Each footnote should be typed at the bottom of the page of the manuscript in which it is first mentioned. Footnotes must not be included with the references.

3.3. Tables

Tables should be used only where the information is more effectively presented in tabular form than in the body of the text. Each table must be referred to in the text and given suitable captions. Column headings should be as short as possible but must define units unambiguously. When necessary, an abbreviated or symbolic column heading should be used and explained in the table-heading or in a footnote. Footnotes to tables should be labeled ^{a}, ^{b}, ^{c}, etc., and typed at the bottom of the table.

3.4. Structural Formulae, Schemes, and Figures

Use Arabic <u>not</u> Roman numerals to denote structure numbers; these should be typed as bold face both in the structure blocks and in the text, and *should always be enclosed in parentheses*.

Since only a few characters can be conveniently set above "arrows" in reaction sequences, longer descriptions of reagents, etc., should be numbered (i), (ii), ... and collected together at the foot of the block with the identifying number set above the appropriate "arrow".

Pay particular attention to the conventions adopted in publications for the presentation of structures, i.e. (**1**) not (I) and (**2**) not (II) are appropriate, as described below.

Thus, partial bonds (electron delocalization) are shown by broken lines ( ). Stereochemistry of bonds is shown by dark wedges for "in front of page" and broken ones (narrowing with distance from the observer) for "behind page" bonds. Hydrogen bonds are shown dotted (....). For a benzene ring, a Kekulé structure should be used and not a hexagon containing a circle. Small alkyl substituents are denoted by Me, Et, etc. (not CH_3, C_2H_5), Pr^{i}, Bu^{t} (with Roman superscripts italicised); *n* , *s* , *t* prefixes should be italicised (use of *tert* is discouraged).

Currently, the following chemical drawing packages are acceptable: ChemDraw up to version 11.0, or Isis/Draw up to version 2.5, ACD/ChemSketch up to version 11.0. For styles and drawing, follow this link: Chemicaldrawing

For authors using the *ChemDraw* program, the following preferences should be selected: bond spacing 15% of length, 8-pt *Helvetica* or *Arial* font for atom labels, 8-pt*Helvetica* or *Arial* font for captions, fixed length 14 pt (0.494 cm), bold width 2.0 pt (0.071 cm), line width 0.60 pt (0.021 cm), margin width 2.0 pt (0.071 cm), hash spacing 2.0 pt (0.071 cm). With appropriate margin settings, a maximum width of 12.5 cm should be created for structure blocks, schemes, and equations. Compound numbers should be in boldface type, but not atom labels or captions.

Figures that are subdivided into subfigures should have uniform designation with lower case letters, e. g. **1a** and **1b**.

Color reproduction of *Figures*, *Schemes* and/or formulae is possible. When any of the original graphics delivered with a manuscript are in color, it is assumed that the authors wish for them to be reproduced in color, unless otherwise specified in the cover letter. The authors must be prepared to bear the additional costs associated with color reproduction (the Editorial Office can provide an estimate of these charges upon request).

3.5. Chemical Equations and Physical or Mathematical Expressions

Chemical equations and physical or mathematical expressions should be numbered sequentially on the right-hand side with arabic numerals in parentheses. Physical quantities and variables that must be defined in the text should be written in italics. The symbols proposed by *IUPAC - cf. Pure Appl. Chem.,* **51**, 1 (1979) - are recommended. Fractional expressions should be written with a slash, *e.g., hv/kT*.

3.6. Nomenclature

All new compounds should be named in accordance with IUPAC rules. As an additional guideline, the Index Guide of Chemical Abstracts should be consulted. The use of ACD/Name (version 11.0) or ACD/Name Chemist Version are recommended.

Some special conventions peculiar to *Acta Chem. Iasi* are:

For common solvents, reagents, or other compounds, the molecular formulae or accepted abbreviations may be used: *e.g.*, $CHCl_3$, NaCl, $SOCl_2$, MeOH, DMF, DMSO, THF, Py. An *ad hoc* abbreviation may be used for a name or formula that occurs repeatedly. This has to be clearly defined, *e.g.*, tetrahydrocannabinol (THC).

Different alkyl or arylalkyl radicals should be designated with superscripted numbers: R^1, R^2, R^3, etc. (Subscripts are used only to denote stoichiometry.) Aryl radicals should be designated by Ar^1, Ar^2, etc., all others by X, Y, etc. (e.g., X = O, Y = NH_2, Z = Br).

Individual atoms should be referred to as C(2), N(5) (not C-2 and N-5), etc. For "hydrogen atom attached to carbon atom 4", etc., *ACI* prefers the notation H-C(4).

3.7. Units and Their Symbols

SI Units are to be used, especially in contributions dealing with physical chemistry.

3.8. Presentation of experimental data

A typical experimental procedure should be described as follow:

*To a soln of phosphapropadiene (**27**) (3.04 g, 0.01 mol) in anhyd THF (80 mL) under an inert gas atmophere a soln of triphenylphosphorane (4.28 g, 0.01 mol) in benzene (140 mL) was added dropwise at 0°C. After 3 h under stirring at room temperature the solvent was evaporated and the residue purified by column chromatography (silica gel, hexane); yield: 1.36 g (30%).*

Physical and spectroscopic data can be included in the experimental section or, in cases where a large number of compounds are prepared, presented in tables. Spectroscopic data should be presented according to the ACS Style Guide and be stated in the order and format shown in the following examples:

mp 241-234°C; $[\alpha]_D^{20}$ +25.4 (c 1.00, $CHCl_3$); R_f = 0.3 (hexanes-EtOAc, 5:1).

IR (KBr): 3245, 3120, 1720, 1690, 1535, 1460 cm^{-1}.

^1H NMR (400 MHz, CDCl3): δ = 2.44 (s, 3 H, CH_3), 2.79 (s, 3 H, $COCH_3$), 7.20 (d, J = 8.1 Hz, 1 H, H-7), 7.51 (d, J = 6.3 Hz, 1 H, H-8), 7.85 (s, 1 H, H-5), 17.75 (s, 1 H, OH).

^{13}C NMR (75 MHz, DMSO-*d6*): δ = 8.9, 30.3, 51.9, 66.2, 169.6, 178.8.

^{31}P NMR and other NMR nuclei likewise.

MS (EI, 70 eV): *m/z* (%) = 213.9 (90), 270.2 (100) $[M + H]^+$.

HRMS-FAB: *m/z* $[M + H]^+$ calcd for $C_{21}H_{38}N_4O_6S$: 475.5285; found: 475.5267.

UV/VIS (CH_2Cl_2): λ_{max} (log ε) = 236 (4.00), 278 (4.59), 284 (4.57), 329 nm (3.41); or UV (CH2Cl2): λ_{max} (e) = 268 (21900), 458 nm (68800).

Anal. Calcd for $C_{32}H_{50}BrP$: C, 70.44; H, 9.24. Found: C, 70.32; H, 9.43.

Product yields should be given in terms of g or mol as well as in % and it should be specified if this is for crude or pure product.

NMR: Always give coupling constants for well-resolved peaks. After each chemical shift, enter in parentheses multiplicity, coupling constants, number of protons, and assignment, in that order.

3.9. Special Instructions Concerning Contributions Containing X-Ray Crystal-Structure Results

All contributions which report the results of a crystal structure determination, even in a minor way, must adhere to the following instructions.

It is the results of crystal structure determinations that are of prime interest to readers of ACI. A detailed description of the experiment is not usually necessary and only the pertinent crystallographic data need to be summarized in the experimental section. However, the full crystallographic data must be deposited in one of the crystallographic databases [see (d) below] **before** the manuscript is

submitted. In addition, authors must validate their crystallographic data [see (c) below] and include the Validation Report with their manuscript. The manuscript will not be distributed to the referees until the database deposition numbers and Validation Reports for the reported crystal structures have been provided.

a) Information to be contained within the **Discussion Section**:

A labeled view of the molecule **with displacement ellipsoids, not arbitrary spheres**, will usually suffice, unless the authors specifically wish to discuss particular aspects of the structure or the experiment.

A brief description of the structure or any unusual features therein and a table of significant bond lengths, angles or torsion angles may be given, if appropriate to the discussion.

Full tables of refined atomic coordinates, bond lengths and angles, and related information will only be printed if *specifically* requested by the authors, and if the referees agree that the information is essential to the understanding of the discussion.

b) Information which must be contained within the **Experimental Part**:

A brief description of the procedures used for data collection, structure solution and refinement. For routine analyses this need not amount to more than a few sentences, but unusual parameters or procedures should be described. Crystallographic nomenclature and conventions should conform to the usage of *International Tables for Crystallography*. The following items should be given explicitly:

- Systematic name, *Chemical Abstracts* Reg. No. or other identifying name
- Source of material and solvent for crystallization
- Chemical formula
- Formula weight
- Crystal size
- Unit cell dimensions and volume with standard uncertainties
- Crystal system and space group
- Number of molecules or formula units per unit cell
- Diffractometer used
- Radiation and wavelength
- Temperature and pressure of measurement (if different from 298 K and 1 atm)
- Calculated density *Dx* (and measured density, *Dm*, if applicable)
- Linear absorption coefficient
- Method of measuring intensities
- Max. value of $(\sin\theta)/\lambda$ or θ reached in intensity measurements
- Type of absorption correction applied (if applicable) and max. and min. values of correction
- Decay correction (if applicable) with maximum decay value
- Method used to solve and refine structure including treatment of H-atoms
- Use of F or F2 magnitudes in least squares refinement
- Number of measured, independent and observed reflections
- Criterion for classifying reflections as observed [$I > n\sigma(I)$]
- Number of parameters refined

- Final values of R(F) for the I > nσ(I) reflections, wR (on F or F2) for all reflections used in the refinement, and S (*goodness-of-fit*)
- Max. positive and max. negative electron density in final Fourier synthesis.
- For polar structures, reason for choice of enantiomorph or method of testing absolute configuration
- All computer programs used

c) Validation of Crystallographic Data (to be done before submission of the manuscript)

In order to reduce the likelihood of incorrect or substandard crystal structures being reported, authors must test the validity of their crystal-structure determinations prior to submission of their manuscript. The CIF*) for each structure in the paper can be uploaded to the IUCr's CHECKCIF facility athttp://journals.iucr.org/services/cif/checking/checkform.html or validated locally with the program PLATON (downloadable from http://www.cryst.chem.uu.nl/platon/). Both of these validation methods generate a Validation Report. Authors should examine the Validation Reports to ensure that no serious oversight has occurred with their crystal structure determinations (*e.g.*, incorrect space group, seriously deficient data quality or structural model) and take appropriate corrective action when required. A copy of the final Validation Report for each structure in the paper must be submitted with the manuscript, and any unresolved serious validation issues should be commented upon.

* *Details concerning the Crystallographic Information File (CIF) format* are available from Acta Crystallogr., Sect. A **1991**, *47*, 655 or http://www.iucr.org/iucr-top/cif/index.html

d) Deposition of Crystallographic Data (to be completed before submission of the manuscript)

Prior to submission of a manuscript, all crystallographic data must be deposited electronically in CIF format with the appropriate crystallographic database so that the referees can access the data.

The crystallographic data for **organic and organometallic** compounds should be deposited with the Cambridge Crystallographic Data Centre (*CCDC*) (see:http://www.ccdc.cam.ac.uk). Send your data in CIF format (excluding structure factors) by e mail to deposit@ccdc.cam.ac.uk. The *CCDC* will provide the authors with one deposition number for each structure by return e-mail. These deposition numbers should be included as a footnote in the manuscript by using the following standard text:

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