Aust. J. Chem. **2004**, *57*, 3–6

Australian Journal of Chemistry

Notice to Authors 2004

Scope

Australian Journal of Chemistry—an International Journal for Chemical Science publishes research papers from all fields of chemical science, encompassing synthesis, structure, new materials, macromolecules and polymers, supramolecular chemistry, analytical and environmental chemistry, natural products, biological chemistry, nanotechnology, and surface chemistry.

The *Australian Journal of Chemistry* is a general chemistry journal with a broad readership (80% of the journal's subscribers are outside Australia), and each manuscript should include a general introduction that allows all readers to appreciate the significance and general context of the work, along with a final paragraph summarizing the conclusions that can be drawn, and noting possible future directions.

The journal appears 12 times per year in print and on the web (www.publish.csiro.au/journals/ajc), the web version being updated more frequently and containing information on papers in press.

Submission of Manuscripts—Overview

All manuscripts for the *Australian Journal of Chemistry* should be submitted as a single file containing text, tables, and graphics, with an accompanying justification and a short text (50–100 words) explaining the significance of the manuscript to the general chemical community. The submission process is found below.

Manuscript Categories

Full Papers: Full papers are complete reports of original research results that have not previously been published, except in the form of a preliminary communication (reprints or preprints should be provided). A short abstract (maximum 100 words) should be provided at the start of the manuscript. The paper should be divided into Introduction, Results and Discussion, Conclusion, and Experimental sections.

Short Communications, Rapid Communications: Short communications are brief reports of preliminary research findings, and should not exceed 2000 words and three graphics. A short abstract (50–100 words) should be provided at the start of the manuscript. The text should not otherwise be broken up into sections; however, an introductory paragraph should provide a general context for the work, explaining its significance, and indicating why it should be of interest to chemists in other areas, while the final paragraph should summarize the major conclusions that can be drawn, pointing to possible future directions. A short Experimental section may be included. Reports of exceptional importance and interest may be submitted as Rapid Communications, and should be accompanied by a brief statement explaining why urgent publication is merited.

Reviews: Review articles should give a general overview of a subject of current interest in chemical science. The introduction should arouse the reader's interest, describing the background, significance, and development of the field, and should be able to be understood by a broad audience. The main part of the review should be a comprehensive summary of recent (last three to five years) developments, and should provide a starting point in the specialist literature. The review should conclude with a summary of the highlights (pointing out their significance), unsolved problems, and possible future directions. The manuscript should be 5000–8000 words in length and contain 10–15 graphics. A passport photo and a short biography (approximately 100 words) should be submitted with the manuscript.

Current Chemistry: Current Chemistry articles summarize recent developments in a new or developing field of chemistry, and are intended to serve as an introduction to the field for the generalist reader. A short abstract (maximum 100 words) should be provided at the start of the manuscript. A strong introduction describing the significance of and motivation behind the work should be followed by a clear and succinct presentation of important results, without the extensive technical details required for an original article. The conclusion should highlight the significance of the findings, and point to possible future directions. All of this should be presented in a manuscript of up to 2000 words and three graphics.

Focus: Focus articles are brief (one published page) accounts by a postdoctorate or postgraduate reporting on a new reagent, technique (e.g. particle or film preparation), or analytical/imaging method (microscopy, spectroscopy, etc.). The article consists of one to two paragraphs that introduce the reagent/technique and discuss its significance, how it is prepared/used, and why it represents an advance on previous reagents/methods. This is followed by single-paragraph summaries of recent reports of its usage. A brief biography (approximately 60 words) and a photo of the author should be submitted with the article. The total length of the article should not be greater than 600 words.

Manuscript Preparation

Order: The sections of a manuscript should appear in the following order:

- Title, Authors and Addresses, Abstract
- Introduction
- Results and Discussion
- Conclusion
- Experimental
- References

The Experimental section may, when necessary, appear in the body of the manuscript.

Title: The title should be succinct and no longer than ten words. The title should capture important keywords.

Authors and Addresses: The full names of all authors contributing to the work should be included, along with their complete postal addresses. Fax number(s) and e-mail address(es) of the contact author(s) must be included. The addresses listed should be the institution(s) where the work was conducted; if this is different from the present address, this should be included in a footnote. Authors of multi-authored papers may wish to assign relative values to their contributions, or to indicate that two or more authors contributed equally to a paper, which can be done in a note at the end of the address field on the paper.

Abstract: This should state concisely the scope of the work and the principal findings in no more than 150 words. Abstracts are not published for Focus articles.

Text: Every manuscript (except Focus articles) should contain introductory and concluding paragraphs written in a general style that will allow the main points to be appreciated by a broad audience of readers across the chemical sciences. Robert Schoenfeld's *The Chemists' English* may be useful to intending authors. A good rule is: use clear language that drives your story forward. Authors not fully fluent in the finer points of English are urged to consult native English-speaking colleagues before submitting manuscripts. Please define acronyms on their first appearance except ones commonly understood by all chemists (such as NMR and UV-vis); when in doubt include a definition. Relevant compounds should be labelled numerically, consecutively, and in boldface.

Introduction: This should provide a general context for the work, explaining its significance, and indicating why it should be of interest to chemists in other areas.

Conclusion: This should summarize the major conclusions that can be drawn, pointing out their significance, and alluding to possible future directions.

Keywords: Up to five keywords should be provided.

Symbols, units, and nomenclature should conform to the recommendations of the International Union of Pure and Applied Chemistry. SI units should be used for physical quantities (see IUPAC recommendations on these in the Green Book*, e.g. s for second, min for minute, etc.). If other units must be used, their first appearance in a paper should be followed by a footnote or parenthesis giving the conversion factor. Both IUPAC and *Chemical Abstracts* nomenclature are acceptable. Refer to the Blue Book† and the Red Book‡ for a guide to IUPAC nomenclature.

Syntheses should be clearly documented and logically presented, as shown in the example below. Physical data should be arranged, where possible, as follows: physical data (melting/boiling point – optical rotation)—chemical data (combustion – elemental analysis)—spectroscopic data (IR – UV-vis – ^{1}H NMR – ^{13}C NMR – mass spectrometry). Spectral peaks should be listed as they read from left to right in the spectrum. The order should at least be consistent within the manuscript. New compounds should appear in italics where they are first mentioned in the Experimental section. Elemental analyses may be presented as either (Found: C 63.1, H 5.4. $C_{13}H_{13}NO_4$ requires C 63.2, H 5.3%) or (Found: C 63.1, H 5.4. Calc. for $C_{13}H_{13}NO_4$: C 63.2, H 5.3%). If a molecular mass is to be included add (Found: C 63.1, H 5.4, M^+ 352. $C_{13}H_{13}NO_4$ requires C 63.2, H 5.3%, M^+ 352). NMR data should be presented in the order integration – multiplicity – coupling constant(s) – characterization.

Adequate evidence to establish identity and purity of new compounds should be provided. An accurate mass measurement of a molecular ion is acceptable as evidence for chemical composition provided that independent evidence for sample purity is given. Low-resolution MS data under conditions that minimize fragmentation are acceptable. If there is a specific need to distinguish alternative formulas with the same molecular mass (within one amu), then high-resolution MS data are necessary. Where such data are not available, the ^{13}C NMR and (or) ^{1}H NMR spectra of certain compounds, or other evidence, may be acceptable provided that these alternatives are convincing to the referees and Editor, and that evidence (e.g. ^{1}H NMR, ^{13}C NMR, HPLC, GLPC, etc.) is supplied as Accessory Material.

9-[(2-Methoxyethoxy)methoxy]anthracene 7

Anthrone **13** (10.0 g, 51.5 mmol) was added in one portion to a magnetically stirred suspension of NaH (2.28 g, 95.0 mmol) in dry THF (250 mL) maintained at 0°C (ice bath) under a nitrogen atmosphere. Stirring was continued for 1 h at 0°C, after which time MEMCl (8.8 mL, 77.1 mmol) was added dropwise. Stirring was continued at about 18°C for a further 5 h and the resulting yellow suspension was re-chilled (ice bath) and then treated with water (250 mL) (CAUTION!). The reaction mixture was concentrated under reduced pressure to remove the THF and the residue partitioned between DCM (250 mL) and water (250 mL). The phases were separated and the aqueous layer was extracted with DCM (3×200 mL). The combined organic phases were dried ($MgSO_4$), filtered, and concentrated under reduced pressure to give a light-orange oil. This material was subjected to flash chromatography (silica; 1 : 4 EtOAc/hexane elution) to afford, after concentration of the appropriate fractions (R_F 0.5), a dark yellow oil that crystallized upon standing.

Recrystallization (hexane) of this material afforded the *title compound* **7** (13.6 g, 93%) as white needles, mp 62–63°C (lit.[19] 62°C). $[\alpha]_D^{20}$ 1.57 (*c* 0.3 in MeOH). (Found: C 76.9, H 6.4%. $C_{18}H_{18}O_3$ requires C 76.6, H 6.4%.) ν_{max} (KBr)/cm^{-1} 2920, 2873, 1344, 1277, 1176, 1110, 1052, 1028, 935. λ_{max}/nm (ε/M^{-1} cm^{-1}) 320 (5000). δ_H 8.32 (2H, m,

* I. Mills, T. Cvitas, K. Homann, N. Kallay, K. Kuchitsu, *Quantities, Units and Symbols in Physical Chemistry 2nd edn* **1993** (Blackwell: Oxford).

† R. Panico, W. H. Powell, J.-C. Richer (Eds), *A Guide to IUPAC Nomenclature of Organic Compounds* **1993** (Blackwell: Oxford).

‡ G. J. Leigh (Ed.), *Nomenclature of Inorganic Chemistry* **1990** (Blackwell: Oxford).

H4 and H6), 8.25 (1H, s, H2), 8.02–7.96 (2H, complex m, H1′ and H5′), 7.51–7.42 (4H, complex m, ArH), 5.47 (2H, s, $ArCH_2$), 4.07 (2H, q, CH_2CH_3), 3.63 (2H, m), 3.39 (3H, s, CH_2CH_3). δ_C 132.3, 128.3, 125.5, 125.3, 124.9, 122.7, 122.6, 100.1, 71.8, 69.8, 59.1 (one signal obscured by overlapping). m/z (ESI) 284 (44%, $M^{+\bullet}$), 209 (19, $[M - C_3H_7O_2^{\bullet}]^+$), 196 (61), 167 (48), 91 (90), 61 (100).

Crystallographic data should broadly conform to the recommendations of the International Union of Crystallography. Prior to manuscript submission, the author should deposit data for organic and metal-organic structures with the Cambridge Crystallographic Data Centre.[§] The data will be assigned one CCDC deposition number per structure, which should be quoted in the manuscript. The crystallographic information (.cif) file will not be published; however, it should be submitted with the manuscript for assessment by referees, and will be made available as Accessory Material on the web.

The manuscript to be published should contain a description of the essential features of the structure, including an ORTEP (or similar) diagram, and important bond lengths and angles (which could be included in the figure caption). Brief details of the data collection and structure analysis should be provided in the Experimental section, and should include the chemical formula, formula weight, crystal system, space group, crystal colour and dimensions of crystal, unit cell parameters (with standard uncertainties), data collection temperature, number of formula units in the unit cell, linear absorption coefficient, range of transmission factors, wavelength of radiation, 2θ range, number of measured and independent reflections, number of reflections included in the refinement, goodness of fit, and final R values.

Computational results should aim to follow the IUPAC guidelines for reporting the results of calculations.** Sufficient detail should be provided, within the manuscript or in the Accessory Materials, to enable readers to reproduce the calculations. Necessary detail includes, for example, force-field parameters and/or equations, or references thereto, defining the model. Results describing electronic structure calculations should provide the geometries (Cartesian coordinates or Z-matrices) of all stationary points whose relative energies are given in the manuscript; absolute energies computed at these geometries should be provided in the Accessory Materials. Where applicable, imaginary frequencies should be reported to identify stable structures and transition states.

Equations and Mathematics: Equations should be numbered sequentially. Please avoid double sub- or superscripts. We recommend following the formats outlined in the Green Book (upright for constants (e, π, i), italic for variables, bold italic for vectors and matrices).

Acknowledgements: As brief as possible, and to appear before the references.

References should be in the Vancouver style. In-text references are presented numerically, superscript in square brackets, after any punctuation. Citations should appear in numerical order throughout the text, consistent with the reference list at the end of the main text body. The reference list should also have reference numbers in square brackets. Initials are listed before surnames. The penultimate and final name in the list should be separated by a comma, the final name should be followed by a comma. The journal title should be italicized, followed by the year of publication in boldface, the volume number in italics, and the page number upright. Books follow the order authors – title – editors – year, volume, chapter, page – publisher. Computer programs, and patents follow essentially the same order with logical substitutions. Reference to internal publications, conference proceedings, and web pages should be avoided. For example,[5,17–19]

[5] J. H. Burroughes, D. C. C. Bradley, A. R. Brown, M. K. Mackay, R. H. Friend, P. L. Burn, *Nature* **1990**, *347*, 539.
[17] A. B. Bloggs, C. D. Smith, in *Pigments in Nature* (Ed. M. E. Brown) **1996**, Vol. 6, Ch. 8, pp. 98–102 (Pergamon: Chicago, IL).
[18] *Xtal ver. 3.4* (Eds S. R. Hall, D. J. du Boulay, R. Olthof-Hazekamp) **2001** (University of Western Australia: Perth).
[19] L. A. Marshall, K. E. Steiner, G. A. Schieser, *U.S. Patent 4 889 858* **1989**.

Tables: Table numbers are designated by Arabic numerals. Tables consist of three horizontal rules, with box headings centred over each column. Material in body of table is usually justified on the left-hand side. Numerical data are usually justified on the decimal point. Footnote references within tables are superior capital letters. Footnotes appear at the bottom of the table, in the same size text as the body of the table. A simple example follows:

Table 1. Selected NMR chemical shifts [ppm] for the fungal pigments 1, 3, 8, and 9

NMR spectra were recorded in [D_8]THF at 400 MHz

Fungal pigment	Chemical shift δ		
	H1	H3	H5
1	5.65 (3H, s)	2.22 (2H, m)	—[A]
3	5.65 (3H, s)	2.26–2.43 (2H, m)	10.10 (1H, s)
8	5.73 (3H, br s)	2.34 (2H, m)	9.89 (1H, br s)
9[B]	5.65 (3H, m)	2.10 (2H, d, *J* 4.8)	9.96 (1H, s)

[A] Not found.
[B] Spectra for compound **9** showed some decomposition.

Graphics: Figures, Schemes, and Diagrams should be of sufficient quality to allow direct reproduction. Single-column (85 mm) width is preferred; double-column figures are acceptable where necessary. Numbers, letters, and symbols should be of the correct size to be 1.8 mm (8 pt) high after reduction. Images with grey tones or colour should be provided as high quality originals, and as electronic files in (ideally) TIFF, EPS, or PDF format with the highest resolution possible (at least 300 dpi). For scanned photographs

[§] The data (without structure factors) should be sent by email to deposit@ccdc.cam.ac.uk as an ASCII file, preferably in CIF format. The CIF file must be validated before deposition using *Checkcif*, available at the IUCR website (www.iucr.org). Hard copy data should be sent to CCDC, 12 Union Road, Cambridge, CB2 1EZ, England. A checklist of data items for deposition can be obtained from the CCDC Home Page on the World Wide Web (http://www.ccdc.cam.ac.uk/) or by e-mail (to fileserv@ccdc.cam.ac.uk with the one-line message: send me checklist).

** Ab initio electronic structure calculations: J. E. Boggs, *Pure Appl. Chem.* **1998**, *70*, 1015; http://www.iupac.org/reports/1998/7004boggs/index.html. Force-field calculations: D. J. Raber, W. C. Guida, *Pure Appl. Chem.* **1998**, *70*, 2047; http://www.iupac.org/reports/1998/7010raber/index.html.

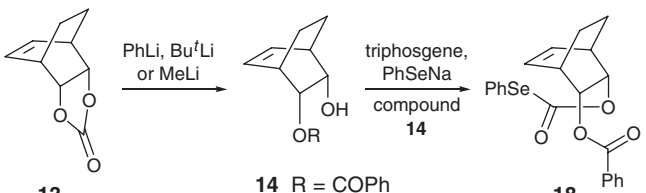
ensure the resolution is at least 300 dpi and for colour images use RGB with the highest resolution possible. Image quality may be improved between the initial (for refereeing) and final (for publishing) manuscripts. For colour images in the print version, authors will be asked to help contribute towards the costs associated with colour printing.

All illustrations should have titles, even if there is no caption. Simple molecular structures that the author deems to be neither Figures nor Schemes should be labelled as Diagrams, and should be referred to as such in the text.

In ORTEP or similar diagrams, (selected) atoms should be labelled and the labelling consistent with all other atom numbering system used in the manuscript.

Symbols representing variables or physical quantities should be in italics.

Chemical structures should be produced using preferably *ChemDraw* in the style shown below, namely using a fixed bond length (wherever possible) of 0.407 cm/0.1694 inches. In general, the text should be Arial 7 pt and compound labels Arial 8 pt.



14 R = COPh
15 R = COBu^t
16 R = COMe
17 R = H

Accessory Materials: Supplementary material of a detailed nature, which is not essential in the printed paper but may be useful to other workers, may be lodged with the Editor if submitted with the manuscript for inspection by the referees. Such material will be made available from our website and a note to this effect should be included in the paper.

Submission of Manuscripts

Initial Submission: Submission of manuscripts by e-mail is recommended in order to accelerate and simplify the refereeing process. Each manuscript should be prepared as a single file containing the text, tables, and graphic materials, and should be submitted in both Word (.doc) and PDF (.pdf) format. Each manuscript should be accompanied by a letter including a statement of justification that outlines why the work should be considered for publication in the journal. The letter must disclose any proprietary, financial, professional, or personal interests that may influence positions presented in, or the review of, the manuscript. Authors are encouraged to provide several names of potential referees, and may also request that certain persons not be invited to review the manuscript. A graphic and short text (50 words or less) for the Table of Contents are also very welcome. Papers reporting X-ray crystal structures should be accompanied by the crystallographic data (.cif) files and matching CCDC deposition numbers. A properly completed copyright form[††] should also be submitted with each manuscript.

Submission checklist:

- A single Word file containing text, tables, and graphic materials
- A PDF version of the same file
- Letter including statement of justification for publication
- Names of potential referees
- Entry for Table of Contents
- Necessary Accessory Materials as appropriate
- Completed copyright form

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Revised Manuscript: Include a brief note of your responses to the referees' comments. Substantial changes should be highlighted. At this point the graphics can be properly drafted to publication standard.

Proofs: Proofs will be sent to the corresponding author(s) in two rounds, the first to check the text, the second to approve the layout.

Reprints: The corresponding author(s) will be sent a PDF of their paper on publication.

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