

Australian Journal of Chemistry

Notice to Authors 2011

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Australian Journal of Chemistry – an International Journal for Chemical Science is a general chemistry journal with a broad readership; 80 % of the journal's subscribers are outside Australia. Each manuscript should include a general introduction that allows all readers to appreciate the significance and general context of the work, and a conclusion, where possible future directions may also be noted. All manuscripts should be submitted as a single file containing schemes, figures, and tables embedded in the text.

The covering letter should contain a justification explaining the novelty and significance of the work to the general chemical community. The covering letter should also contain a statement that the manuscript has not been published elsewhere, and is being submitted exclusively to the *Australian Journal of Chemistry*.

Manuscripts should be submitted using the Online Submission and Peer Review system **OSPREY**, found at the journal's homepage. Please include the name, address, fax and telephone numbers, and email address of the corresponding author. A signed and completed Licence to Publish form should accompany the manuscript or be faxed (to +61 3 9662 7611) or emailed soon after submission.

A Table of Contents entry must also be provided for the online Graphical Abstract and RSS feed. The entry should contain an appropriate image and a short (approximately 50 words) summary written for interested non-experts to encourage further exploration of the paper. The image does not need to appear in the article and should capture the essence of the work. Please ensure that any text within the image is readable, that the image is a maximum size of 9 cm wide × 4 cm high, and that it is submitted as a 96 dpi JPEG file. For examples of our Graphical Abstracts please refer to the latest online Table of Contents or RSS feed. In addition, the names and contact details of five potential referees should be supplied.

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 communication, in which case a reprint should be provided. A full paper will not be published if all relevant

experimental details have already been published as Supporting Information in a communication elsewhere or in the *Australian Journal of Chemistry*. Evidence must be given that substantial new material is submitted. 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 (and/or Computational Methods) sections.

Communications: Communications are short reports of urgent 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 should be included. Adequate experimental details, including full characterization of new compounds, should be given as supporting information in the Accessory Publication. The submission should be accompanied by a brief statement explaining why urgent publication is merited.

Reviews: Review articles are usually not more than 10 printed pages and should give a critical overview of a subject of high current interest in chemical science. Authors are encouraged to take a stance and lead the reader through the field. Overall a review should take us forward and show where a field is heading. The introduction should arouse the reader's interest, describing the background, significance, and development of the field, and should be comprehensible to a broad audience. The main part of the review should be a comprehensive but critical analysis of recent (last three to five years) developments, current problems, and future directions. The review should conclude with a summary of the highlights (pointing out their significance) and unsolved problems. A passport photo and a short biography (ca. 100 words) should be submitted with the manuscript.

Highlight: Highlight 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 general reader. A short abstract (maximum 100 words) should be provided at the start of the manuscript. A strong introduction describing the

significance of the work and the reason for recent heightened interest should be followed by a clear and succinct presentation of important results, without the extensive technical details required for an original article or the extensive history required for a Review. 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.

Focus: Focus articles are brief (one or two published pages) accounts 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 (with graphics) 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 (can be separate)
- Conclusion
- Experimental (and/or Computational Methods)
- 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. Email 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, the present address should be indicated in a footnote.

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* (Wiley-VCH: Weinheim, 1989) 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 numbered 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.

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 provided here. Compound names (rather than numbers) should be given wherever possible. Physical data should be arranged, where possible, as follows: physical data (melting/boiling point – optical rotation) — spectroscopic data (IR – UV-vis – ¹H NMR – ¹³C NMR – mass spectrometry) — chemical data (combustion — elemental analysis). 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. The names of new compounds should appear in italics where they are first mentioned in the Experimental section. Elemental analyses should be presented as Anal. Calc. for C₁₃H₁₃NO₄: C 63.14, H 5.30, N 5.67. Found: C 62.99, H 5.32, N 5.65 % (a tolerance of 0.4 % is usually acceptable). NMR data should be presented in the order chemical shift (multiplicity, coupling constant(s), integration, assignment). Coupling constants *J* should be given where appropriate. Indicate the machine frequency if non-routine, e.g. δ_H (500 MHz, CDCl₃) 4.07 (q, *J* 7.5, 2H, CH₂CH₃).

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. In such cases, copies of ¹H and ¹³C NMR spectra must be provided as an Accessory Publication. HPLC or GLPC chromatograms and low-resolution mass spectra under conditions that minimize fragmentation may be useful as additional evidence of purity. Supplementary spectra and spectral assignments, e.g. 2D NMR spectra that are not needed for the general understanding of the text, may also be published in the Accessory Publication.

Reports of experiments conducted with microwave reactors must document the manufacturer and model of the reactor and indicate whether sealed or open reaction vessels were used. The method used to monitor the temperature of the reaction mixture, and the temperature–time profile, must also be included. Papers describing syntheses with domestic (kitchen) microwave ovens are not encouraged.

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

^AE. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, A. J. Thor, *Quantities, Units and Symbols in Physical Chemistry*, 3rd edn **2007** (RSC: Cambridge).

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

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

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 CH₂Cl₂ (250 mL) and water (250 mL). The phases were separated and the aqueous layer was extracted with CH₂Cl₂ (3 × 200 mL). The combined organic phases were dried (MgSO₄), 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). $[\alpha]_{\text{D}}^{20}$ 1.57 (*c* 0.3 in MeOH). 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} 4.07 (q, *J* 7.5, 2H, CH₂CH₃), 3.63 (m, 2H), 3.39 (t, *J* 7.5, 3H, CH₂CH₃), 7.51 (complex m, 4H, ArH), 5.47 (s, 2H, ArCH₂). 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⁺), 209 (19, [M – C₃H₇O₂]⁺), 196 (61), 167 (48), 91 (90), 61 (100). Anal. Calc. for C₁₈H₁₈O₃: C 76.56, H 6.43. Found: C 76.85, H 6.41 %.

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 authors are required to run the *checkCIF* Program (<http://checkcif.iucr.org/>) and submit the output as supporting information for assessment by the referees. The crystallographic information file (cif) should also be submitted with the manuscript as supporting information for assessment by referees, but it will not be published.

Tables of relevant bond lengths and angles not needed in the general discussion but of interest to the specialist may be published in the Accessory Publication, but the full crystallographic data will not be published (e.g. atomic coordinates and anisotropic displacement parameters), as it will be available from the CCDC. The manuscript to be published should contain a standard description of the crystal data and structure refinement in the Experimental section. This includes the chemical formula, formula mass, 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. An *ORTEP* (or similar) diagram should be incorporated in the text. Important bond lengths and angles may be included in a table or in the figure or figure caption. If the structure is peripheral to the subject of the

paper, it should be published in the Accessory Publication. Additional views or details of the structure(s), crystal packing, etc., may, when relevant, be published in the Accessory Publication.

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 Publication, 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) and absolute energies of all calculated structures should be provided in the Accessory Publication. Where applicable, imaginary frequencies and IRC calculations 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).

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. Tables should be prepared for single-column format whenever feasible. 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 [D₈]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, <i>J</i> 4.8) | 9.96 (1H, s) |

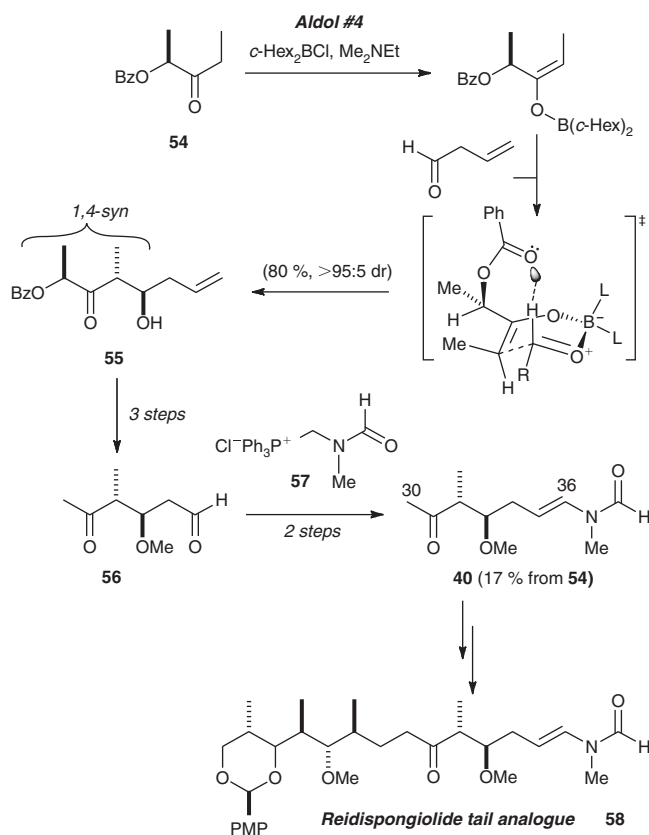
^ANot found.

^BSpectra for compound **9** showed some decomposition.

Graphics: Figures, Schemes, and Charts should be of sufficient quality to allow direct reproduction. They should be prepared for single-column format (85 mm width) whenever possible. Double-column figures are acceptable where necessary, but attention should be paid to economical use of space. 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 ensure the resolution is at least 300 dpi and for colour images use RGB with the highest resolution possible. For colour images in the print version, authors will be asked to help contribute towards the costs associated with colour printing. Authors may wish to choose to have their colour figures produced in

^DThe 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).

^EAb 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>.



colour in the online version of their paper, free of charge, and black and white in the print version.

All illustrations should have titles, even if there is no caption.

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 ChemDraw or ChemBioDraw in the style shown here, namely using standard bond angles and fixed bond lengths (wherever possible) of 0.5 cm/0.2 inches, line width 0.02 cm, bold width 0.07 cm. In general, atom labels should be Helvetica 10 pt and compound numbers Helvetica bold 10 pt.

Accessory Publications: Supporting material of a detailed nature, which is not essential in the printed paper but may be useful to other workers, may be submitted with the manuscript (see Syntheses, Crystallographic data and Computational results). Such material will be made available on the web, and a note to this effect should be included at the end of the paper (before the Acknowledgements section).

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

References should be in the Vancouver style. Please ensure references are embedded within the manuscript and not in a referencing software program such as EndNote or ProCite. 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^[5,17–20]

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- [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).
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(b) *Fluoroquinolone Antibiotics* (Eds A. R. Ronald, D. E. Low) **2003** (Birkhäuser: Basel).
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- [20] L. A. Marshall, K. E. Steiner, G. A. Schieser, *U. S. Patent 4 889 858* **1989**.

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A covering letter must accompany the submission and should include the name, address, fax and telephone numbers, and email address of the corresponding author. The letter must contain a statement explaining the novelty and importance of the work and justifying its consideration for publication in the journal, that the manuscript has not been published elsewhere, and that it is being submitted exclusively to the *Australian Journal of Chemistry*. Five potential referees must be proposed. A completed Licence to Publish form (which you will be asked to download from the website as part of the submission process) should be faxed (+61 3 9662 7611) scanned and submitted electronically (email: osprey.ajc@csiro.au) as soon as possible after submission. The manuscript number (e.g. CH09xxx) must be included on the form.

Authors are advised to read recent issues of the journal to note details of the scope of papers, headings, tables, illustrations, style, and general form. Observance of these and the following details will shorten the time between submission and publication. Poorly prepared and unnecessarily lengthy manuscripts have less chance of being accepted.

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Revised Manuscript: Please include a detailed explanation of your responses to the referees' comments and also submit a copy of the revised manuscript with the changes highlighted.

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