CARBOHYDRATE RESEARCH
INSTRUCTIONS FOR AUTHORS 2009

INTRODUCTION

Carbohydrate Research publishes reports of original research in the following areas of carbohydrate science: action of enzymes, analytical chemistry, biochemistry (biosynthesis, degradation, structural and functional biochemistry, conformation, molecular recognition, enzyme mechanisms, carbohydrate-processing enzymes, including glycosidases and glycosyltransferases), chemical synthesis, isolation of natural products, physicochemical studies, reactions and their mechanisms, the study of structures and stereochemistry, and technological aspects.

Papers on polysaccharides should have a "molecular" characterization component; a paper on new or modified polysaccharides should include structural information in addition to the usual studies of rheological properties and the like. A paper on a new, naturally occurring polysaccharide should include structural information, preferably detailed analysis of monosaccharide components and linkage sequence.

Papers devoted wholly or partly to X-ray crystallographic studies, or to computational aspects (molecular mechanics or molecular orbital calculations, simulations via molecular dynamics), will be considered if they meet certain criteria. For computational papers the requirements are that the methods used be specified in sufficient detail to permit replication of the results, and that the conclusions be shown to have relevance to experimental observations — the authors' own data or data from the literature. Specific directions for the presentation of X-ray data are given below under "Results and discussion".

Types of Papers

Contributions to *Carbohydrate Research* may be in the form of the following article types:
Full Papers - these should be substantial completed pieces of original research that are of significance and which, in addition, are presented clearly and concisely.
Notes - these are concise but complete descriptions of an investigation of a limited scope that will not be included in a later paper.
Mini-Reviews - these are critical reports reviewing important research in that field. While manuscripts usually are submitted at the invitation of Editors, contributions can be made by interested individuals if they contact an Editor to ensure that a suggested topic is both suitable and not already in process. Mini-reviews are often solicited for a Special Issue on a particular topic.

BEFORE YOU BEGIN

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submission for the review process, these source files are needed for further processing after acceptance. All correspondence, including notification of the Editor's decision and requests for revision, takes place by e-mail and via the author's homepage, removing the need for a hard-copy paper trail.

Referees
Please submit, with the manuscript, the names and addresses of 3-6 potential referees.

PREPARATION

Language
Please write your text in good English (American or British usage is accepted, but not a mixture of these). Use decimal points (not decimal commas); use a space for thousands (10 000 and above). For further assistance in matters of editorial style, authors are referred to *The ACS Style Guide*, 3rd ed.; Dodd, J., Ed.; American Chemical Society: Washington, DC, 2005. *Carbohydrate Research* follows *The ACS Style Guide* as a standard for scientific format, including abbreviations, reference style, and points of importance in English style and grammar.

Carelessly prepared manuscripts, i.e., those that do not follow journal format and/or are written in poor English, may be returned to the authors for correction before being submitted for review. For authors whose native language is not English, it is strongly recommended that a person fluent in English review and correct the paper. Commercial technical editing services are also recommended. Elsevier has agreements with a number of firms that specialize in technical science editing.

Use of Word Processing Software
Manuscripts (**all parts**: text, footnotes, tables, figure legends, references) should be prepared with a full double line-space setting of 1 cm (~30 points) in 12-point font, and the pages should be numbered. Left-justified format is encouraged, and double-column formats are unacceptable. Papers for initial review are acceptable in Adobe pdf format with embedded figures and drawings; however, original word processor files are required for final submission to the publisher (these directives are included in the online submission system), as well as drawings and figures provided in separate files in original file formats (e.g., ChemDraw, ISISDraw, ChemWindows and the usual TIFF and JPEG formats). Word breaks with hyphens should be avoided, and hard breaks (return key strokes) should be used only at the ends of paragraphs. Attention to details of typesetting, including choice of roman, italics or boldface type, should be made. Common errors include (1) lack of two spaces after a period at the end of a sentence (full stop); (2) lack of spaces before and after major operators (+, –, ±, = , etc. all have spaces before and after when used in mathematical equations, while +, –, and ± when used to indicate a positive or negative number have no space before the number); (3) spacing for parenthetical constructions [no spaces, e.g., “(A) “ with parentheses, brackets and braces], and (4) a space between a number and the quantity (e.g., 3.0 g, 5 mL, and 12 °C). Consult *The ACS Style Guide* when in doubt.

Article Structure
Articles consist of a title, a listing of the authors with the names and addresses of their institutions, an abstract, a listing of keywords, a body of text including tables, charts and figures, and a reference list. The conventions relating to each of these items can be ascertained by examining a current issue of the journal, and by consulting the following sections of these instructions.

Title
The title should be grammatically correct and specific enough to alert the readers to whom the article is directed when seen in a table of contents or retrieved in a database. If a series title is desired it should be given as a footnote (example below), indicated by a superscript symbol at the end of the main title.

Authors' names
Please provide **one fully spelled-out** given name (forename) for each author, to eliminate confusion with others having the same family name (surname) when the names are listed in an index. Do not use the word "and" anywhere in the list of authors' names. Please indicate the corresponding author(s) authors with an asterisk(s).

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Give the name(s) and address(es) of the institution(s) with which the authors were affiliated when the work was done. Any changed contact information for any of the authors can be placed in a footnote (see "Optional," below).

Footnotes to title page
Standard: "*Corresponding author".
Optional: "*Corresponding author. Present address: (if different from that given in 'institutional affiliations'); fax: (number); e-mail: (address)".
Optional (series title, for example): Synthesis of oligosaccharides related to hyaluronic acid,[1] Part 2.
Additional footnotes: To acknowledge financial support (preferably, this may be done in an Acknowledgements section, as mentioned below), list abbreviations used, etc. indicate by superscript symbols *, †, ‡, §, ¶, ‖. Use of these symbols should be kept to a minimum.

Abstract
The abstract should be concise and describe in one paragraph the work accomplished or results obtained at the level of detail found in *Chemical Abstracts*. The abstract should read independently of the body of the paper, including formula charts and the References section. **Compounds should not be listed by formula number, but should be named, descriptively or formally**. Include a formula number only if it is needed as a 'stand-in' for the name when the compound is mentioned a second time. If references must be cited they should be given in full, as in the following example "[Lee, R. T.; Lee, Y. C., *Carbohydr. Res.*, **1995**, *271*, 131–136.] and not placed in the Reference section.

Graphical Abstract
In addition to the textual Abstract, authors must provide a graphic for a Graphical Abstract for the Table of Contents on a separate page and in a separate file. This should convey the essence of the article in a concise pictorial form. Where necessary, appropriate text, not to exceed 50 words, may be added; in cases where a graphic is absolutely not feasible, text alone may be used. The full title of the paper and the full list of authors will be included by the typesetter. Authors should ensure that their graphic, when reduced, will fit into the allocated space (170 mm wide by 50 mm high) and be readable.

Keywords
At the end of the abstract, provide a list of no more than 6 keywords, i.e., expressions that might serve as search terms in an electronic search of a database. The keyword list may include chemical names and multiple-word terms in which the order is inverted. General terms such as 'synthesis', 'NMR', 'structure', etc., are to be avoided, except as parts of inverted expressions. For example: "*Keywords*: Sugar phosphates; Conformational transitions; *Escherichia coli* 06; Polysaccharides, structure; 2,6-Dioxabicyclo[3.1.1]heptanes; 1,3-Anhydro-6-deoxy-β-$_L$-talopyranose, protected; 6-Deoxy-β-$_L$-talopyranose, protected 1,3-anhydro derivative." Note that the first word of each Keyword is capitalized.

The body of the paper
Typically, the body of a Full Paper comprises numbered sections designated **1. Introduction**, **2. Results and discussion**, and **3. Experimental**. In Notes, the headings Introduction and Results and discussion are not used, and the Experimental Section is numbered **1**.

However, these specific outlines are not obligatory; authors may vary the organization of articles as needed for optimal presentation of their subject matter. Subheadings are used as needed in any of the sections and are indented and numbered 2.1, 2.3, etc., followed by the subheading in boldface type with capitalization of the first word, only (except for words normally capitalized). Subheadings appear on a line that is separate from the text. Sub-subheadings follow, if needed, and are numbered 2.1.1, 2.1.2, etc. These are punctuated with a full stop (period) and are integral with the text that follows. For an example, see the Experimental section which follows.

1. Introduction
State the objectives of the work and provide an adequate background, avoiding a detailed literature survey or a summary of the results.
2. Results and discussion (alternatively 2. Results, 3. Discussion)
In addition to text, this section may contain Tables, Figures, structural formulae, and Schemes, which should be supplied on separate sheets. The preparation of such items is discussed further in these Instructions.
3. Experimental
Typically this section will be divided into subsections, the content of which varies according to the subject matter of the article. Some examples follow:

3. Experimental
3.1 General methods
All reactions were carried out in commercially available dry solvents….
3.2 General procedures for the glycosidation of allyl 2-acetamido-4,6-*O*-benzylidene-2-deoxy-α-$_D$–glucopyranoside (9)
3.2.1 Procedure A using glycosyl trichloroacetimidates. Allyl 2-acetamido-4,6-*O*-benzylidene-2-deoxy….
3.2.2 Procedure B using glycosyl bromides. Allyl 2-acetamido-4,6-*O*-benzylidene-2-deoxy….

For specific compounds, subheaders are used as follows:

3.2 Methyl 6-*O*-*tert*-butyldimethylsilyl-α-$_D$-glucopyranoside (4)

A mixture of **3** (200 mg, 1.03 mmol) and *tert*-butylchlorodimethylsilane was stirred….

Note that 3.2 is a title compound. To be listed as such, the compound must be fully characterized as to identity and purity (discussed in Preparative Procedures, below). If the synthesis of a title compound involves one or more intermediate compounds that have not been fully characterized, then these should be listed as sub-subheadings under 3.2.1, 3.2.2, etc. under the title compound. The final sub-subheading under 3.2 will be the synthesis of the title compound (the compound name is repeated in the sub-subheader line).

Use of abbreviations. In the Experimental section, but not in the Introduction or Results and discussion sections, abbreviations should be employed liberally to economize on space. For the names of reagents, solvents, etc., molecular formulae, or designations indicative of molecular formulae, can be used, and these are preferred over acronyms, but acronyms in common usage and listed in the *The ACS Style Guide* are acceptable. Examples include (but are not limited to) the following: $NaHCO_3$, EtOH, MeOH, Et_2O, DMF, Me_2SO (DMSO), Me_2Si (TMS), HOAc (not HAc), NaOAc. TBDMS (for *tert*-butyldimethylsilyl) is preferred over TBS. Other less frequently used abbreviations, for example, DCM (for dichloromethane) are not to be used; the formula should be used instead (CH_2Cl_2). Abbreviations can also be substituted for common terms such as aqueous (aq), saturated (satd), etc. Units of measure [mL, cm, °, °C, s (seconds), min (minutes), h (hour), etc.] are always abbreviated. For a list of allowable abbreviations, consult *The ACS Style Guide.*

Preparative procedures. In articles dealing with synthetic work, subsections of the Experimental are typically headed with the correct IUPAC names of the intermediates and final products of preparative sequences (‘title compounds’). However, status as title compounds is awarded only to

those compounds for which convincing evidence of **identity** and **purity** (see below) has been obtained. For known compounds prepared in the course of the work a reference is cited when the use of the compound is mentioned. The proper format is as follows: "mp 103–104 °C, lit.[3] mp 100–103 °C. ^{1}H and ^{13}C NMR spectral data matched that reported." If the authors have significantly improved the published synthesis, a separate subsection may be used, entitled "**Preparation of ...[3]**". Preparative details for new compounds obtained as intermediates but not fully purified and characterized should be incorporated into the sub-subsection describing the next title compound in the sequence. If new and important physicochemical or spectral data have been generated, then a sub-subsection **Data for …** can be inserted with or without preparative details.
In descriptions of preparative procedures, quantities of reactants and reagents should be stated in both weight (g, mg, kg) and molar (mol, mmol) units. (For General Procedures, these may most conveniently be put into a Table.) Yields should be reported both by weight and as percent of the theoretical, not in molar units. Care should be exercised to ensure that the same number of significant figures is used for weight and molar amounts, e.g., 1.05 g (2.66 mmol) of compound **3** (both reported to three significant figures).

Characterization of compounds. All compounds that are "title compounds" must be characterized as to *identity* and *purity*. Ordinarily, the identity of a compound is established by NMR and mass spectral data. Authors are urged to include an elemental (combustion) analysis (minimally C and H), with values deviating from the theoretical not more than 0.4% absolute for all compounds where feasible (e.g., for stable compounds prepared on multimilligram scale or larger). When a C and H analysis is not feasible (e.g., very small amounts of material available, the compound is unstable or is an intractable syrup, glass or gum) mass spectral data may be substituted for elemental analysis. For small molecules, high-resolution mass spectral data [e.g., electron-impact mass spectra (HREIMS), fast-atom bombardment mass spectra (HRFABMS), electrospray-ionisation mass spectra (HRESIMS) or other methods] that establish elemental composition are required on samples of acceptable purity. Generally a minimum value of ±0.005 amu of the theoretical *m/z* for the compound is sufficient to verify a molecular formula; however, this may vary with elemental composition, molecular weight and method of measurement (see Sack, T. M.; Lapp, R. L.; Gross, M. L. *Int. J. Mass Spectrom. Ion Proc.***1984**, *61*, 191–213). For larger molecules (MW >1000, oligosaccharides and the like) the softer ionisation techniques [electrospray-ionisation (ESIMS) or matrix-assisted laser desorption ionisation (MALDI) techniques] that give clearly defined molecular ions or molecular ions plus reasonable adducts to unit *m/z* values are satisfactory. For all compounds where classical elemental analyses are not reported, the author is required to provide copies of ^{1}H and ^{13}C NMR spectra run at high sensitivity in the Supplementary Data section that is available in the electronic version of the paper (see Supplementary Data, below). Chromatographic data (GLC, HPLC, or TLC, at high sensitivity) should also be reported in support of purity along with the spectral data.

Listing of physical and spectral data. The preferred order is: mp (if applicable); $[\alpha]_D$ (strongly recommended for optically active compounds); R_f values (if pertinent); spectral data (UV, IR, if recorded); ^{1}H NMR data, followed by ^{13}C NMR data (if not presented in a table); MS data. Punctuate as in the following example.

"...gave needles: mp 83–85 ºC; $[\alpha]_D^{25}$ –110 (*c* 1.4, $CHCl_3$); IR (KBr); *v* 1730 and 1260 (ester), 860 and 840 (Me_3Si), and 710 cm^{-1} (Ph); ^{1}H NMR ($CDCl_3$, 600 MHz): δ..."

If there are published physical constants (mp, $[\alpha]_D$, λ_{max}, etc.) for the compound these should be cited, using the following format:
"...allyl 2-acetamido-2-deoxy-α-L-glucopyranoside (**1**α): mp 175–176 ºC, lit.[6] 172–174 ºC; $[\alpha]_D^{25}$ +155 (*c* 1.43, water), lit.[6] +149; ^{1}H NMR..."

NMR data. NMR data may be presented in either tables or in the text. Tables are preferred for complex NMR assignments and for series of compounds with full assignments. Full assignments

are encouraged using 2D NMR techniques, especially for large, complex structures. For listings as running text please adhere strictly to a uniform style. The following is the preferred format: ^{1}H NMR ($CDCl_3$): δ 7.35 (d, 1H, $J_{3,4}$ 2.0 Hz, H-3), 5.10 (dd, 1H, $J_{4,5}$ 4.0 Hz, H-4), 4.40 (ddd, 1H, $J_{5,6a}$ 6.5, $J_{5,6b}$ 5.5 Hz, H-5),...
Additional conventions used in describing higher order data include, for example, the designation of peaks in COSY spectra: Man H-1,2; HOHAHA tracking: GlcNAc H-2,3,4,5,6a,6b etc.; NOE contacts: Glc H-1, Xyl H-4,5e, etc. For designating resonances in oligosaccharides, the sugar units should be numbered with Roman numerals I, II, III, etc. beginning at the reducing ("upstream") end of the molecule. (See IUPAC Nomenclature for Carbohydrates, 2-CARB-37.2 .) The individual resonances are numbered with Roman numeral superscripts as, for example, the following: H-3^{I}, H-3^{II}, H-3^{III}.

Elemental analysis data. Elemental analysis results follow the last spectral data, in the same paragraph. Use the following format: "Anal. Calcd for $C_{13}H_{17}BrO_8S$: C, 37.78; H, 4.15; Br, 19.34; S, 7.76. Found: C, 37.86; H, 4.13; Br, 19.45; S, 7.84". Note the arrangement of element symbols in the molecular formula: C, H, then the remaining symbols (including metals in salts and complexes) in alphabetical order (standard Hill system).

X-ray crystallographic data. Before submission of the paper, the X-ray data must be filed with and accepted by the Cambridge Crystallographic Data Centre in the usual *CIF* (Crystallographic Information File) file format. Under a section, "Supplementary Data," that is placed just after the Experimental section, a statement is made as follows:
"Complete crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC no. 000000. Copies of this information may be obtained free of charge from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK. (fax: +44-1223-336033, e-mail: deposit@ccdc.cam.ac.uk or via: www.ccdc.cam.ac.uk)."

A subheading in the Experimental section is devoted to the description of the X-ray experiment, the equipment, and other information required for repetition of the experiment. Preferably in a table (alternatively in a paragraph of text) crystal data, particulars of the diffraction analysis, and refinement data (specify the function minimized in the least-squares refinement and the weighting factor used), are presented. A table of atomic coordinates and their related anisotropic thermal parameters, tabulations of torsion angles and hydrogen-bond parameters if appropriate, and a structural drawing showing the nonhydrogen atoms as thermal ellipsoids, prepared with ORTEP or an equivalent program should be provided. Only bond angles and bond lengths that are remarkable or necessary for the Discussion section should be provided in a table. A statement giving the ranges of values observed will suffice, with a comment on any unusual values (i.e., outliers). Sufficient torsion angles should be reported to define the molecular conformation. For ring systems, Cremer–Pople puckering parameters (Cremer, D.; Pople, J. A. *J. Am. Chem. Soc.* **1975**, 97, 1354–1358) or their equivalent should be reported. If hydrogen atoms are included in the final refinement, their coordinates should be included in an appropriate table. If there is any discussion of hydrogen bonding, a statement describing precisely how the hydrogen positions were obtained is necessary, and isotropic temperature factors should be included with the H-atom coordinates. Complete tables of bond lengths, valence angles and torsion angles should be provided in the Supplementary Data section of the paper as submitted to the CCDC. Tables of observed and calculated structure factors are not needed as supplementary data.
Care must be taken to have the crystallographer correctly number the atoms in the molecular structure according to IUPAC rules of nomenclature. This numbering should appear for atoms listed in the tables and in the ORTEP or other structural figure(s). It is recommended that the system C-1, C-2, O-1, etc. be used.

For cases where X-ray crystallography is used to support the structural identification of a synthetic or natural product in a paper devoted largely to synthetic or isolation chemistry, the authors may wish to report only the ORTEP or similar depiction of the molecule(s). At a minimum, a description of the experimental methods and a tabulation of crystal data should be provided as

Supplementary Data to appear with the electronic version of the paper (in addition to filing the data with CCDC, above.)

Papers on X-ray crystallography may appear either as Notes or Full Papers, the former most often used to essentially report the structure of a single or limited number of carbohydrate compounds.

Supplementary data
Elsevier accepts electronic supplementary material to support and enhance your scientific research. Supplementary files offer the author additional possibilities to publish supporting applications, movies, animation sequences, high-resolution images, background datasets, sound clips and more. Supplementary files supplied will, subject to peer review, be published online alongside the electronic version of your article in Elsevier web products, including ScienceDirect: www.sciencedirect.com. The presence of these files will be signified by a footnote to the article title, and by a description included in a 'Supplementary Data' section at the end of the paper. To ensure that your submitted material is directly usable, please ensure that data is provided in one of our recommended file formats. Please also clearly indicate whether data files are either (i) for publication online or (ii) only to be used as an aid for the refereeing of the paper. A Supplementary Data section should be arranged as follows: A title page should be constructed, with "Supplementary Data" at the top and the paper's title and authorship as on the title page. Pages should be numbered S1, S2, etc. Figures should be labelled Figure S1, Figure S2, etc. and have legends. Schemes are similarly numbered Scheme S1, etc. These pages can be scanned images and provided either in word processor format or as Adobe pdf files. Supplementary Data that contain traces of NMR spectra are required for new compounds that lack elemental analysis data (see Characterization of compounds, above). The spectra should be labelled with the structure of the compound and its compound number from the paper. X-ray data are also supplied as Supplementary Data that are filed with the Cambridge Crystallographic Data Centre (see X-ray crystallography section).

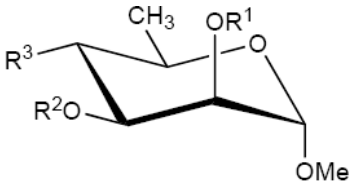
Acknowledgements
This section is not numbered. The inclusion of an Acknowledgements section is optional. Sources of financial support may be recognized here or in a footnote to the title page.

Footnotes
Footnotes should appear at the bottom of the appropriate page and be indicated by the following symbols: *, †, ‡, §, ¶, ‖ .

Figures, schemes, equations and structural formulae:
These should be submitted separately, without legends and must be cited in the text, and numbered in order of appearance with Arabic numerals. Line drawings, structural formulae, and instrument traces (spectra etc.) are preferably done in black on a white background. Colour may be used as appropriate within formulae and line drawings. Drawings produced by computer must be prepared at a resolution of 300 dpi or better and provided in original digital format. Allowing for a 25% reduction in size one column-drawings should be a maximum of 115 mm in width and two column drawings should be a maximum of 230 mm. Please ensure that all illustrations within a paper are consistent in type and quality. Structural formulae should be consistent in size throughout the paper. For Details see: Artwork Guidelines at: http://ees.elsevier.com/car/

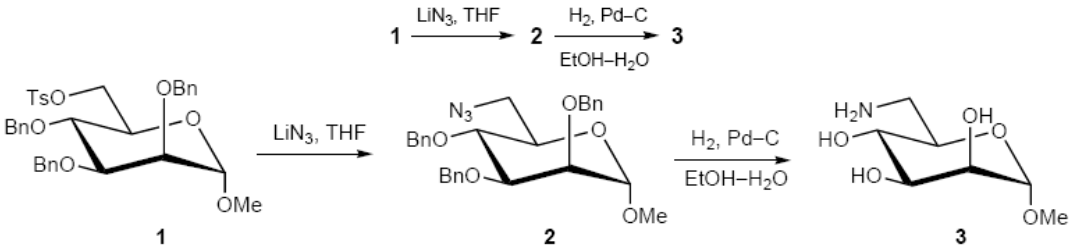
Legends: Labels on the axes of graphs should indicate the parameter being plotted, the units used, and the scale. Use initial capital only, put units of measure in parentheses (for further instructions on this point, see below). A legend is prepared for each figure giving the figure title, if needed an explanation of the symbols used, and any necessary information about experimental conditions. Figure legends should be submitted separately (collected on a separate page and in a separate file) for inclusion in the manuscript.

Structural formulae and schemes: Particular attention should be paid to current conventions for drawing sugar ring structures (tapered thickening of forward edges, etc.). Structural formulae should be grouped for insertion in the text at appropriate points. Such groups need not have a caption, but those showing reaction sequences (i.e., containing arrows) should be designated Scheme 1, Scheme 2, etc. In schemes the general progression of the formula numbers must be **in sequence from left to right** across the page, **regardless of the order of appearance** of the formulae in the text. **That is, compound numbering is determined by appearance in collections of structural formulae or in the scheme(s), which may or may not be the order of appearance in the text.** Where a single structure with R groups represents two or more compounds, the numerical sequence follows the listing below the structure, then resumes its rightward progression. Multiple listings under a single formula should be presented as in the following structure:

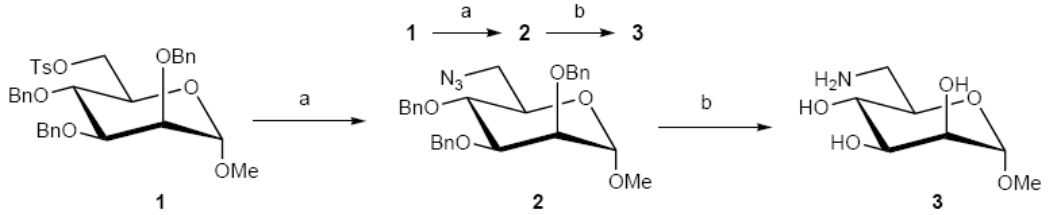


12a: R^1, R^2 = –CMe_2–, R^3 = N_3
12b: R^1, R^2 = –CMe_2–, R^3 = NH_2
12c: R^1 = R^2 = H, R^3 = NH_2
12d: R^1 = R^2 = H, R^3 = NHAc

If reagents and solvents used, and other information on procedures, are to be indicated on a formula scheme, this may be done with abbreviations, molecular formulae, etc. placed along the arrows, taking care to avoid excessive detail:



Alternatively, the information may be given in a legend to the scheme, and keys to the legend placed above the arrows, as in the following example:



In the legend: (a) LiN_3, THF; (b) H_2, Pd–C, EtOH–H_2O

Line width: Lines in drawings, spectral traces, etc. must be sufficiently heavy to remain sharp and distinct after reduction. In case of doubt authors should test drawings by making reduced copies and examining them.

Lettering size and fonts: Similarly, lettering on formulae, figure axes, etc. must be large enough to be **legible after reduction**. This means a height, for capital letters in the reduced copy, of **not less than** 1.5 mm in formula charts, 2.0 mm on the axes of graphs. The preferred font is Helvetica (Arial).

Units of measurement
When quantities given in a table, or presented as scales along the axes of a graph, are derived by multiplication of the true values by ten to a power (10^{n}), the column head or label must indicate **that it is the value, not the unit**, that is multiplied. Thus: 10^{3} × concentration (M), not Concentration ($M \times 10^{-3}$) Cell density (millions of cells/mL), not cell density (10^{6} cells/mL); the latter could be interpreted as (10^{6} × cells/mL).

Tables
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