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RESEARCH

INSTRUCTIONS TO AUTHORS 2004

General Information

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, 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 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 or data from the literature. Specific directions for the presentation of X-ray data are given below under "Results and discussion".

Contributions to *Carbohydrate Research* may be in the form of:
Perspectives—these are critical reports reviewing important research but also giving a personal outlook on 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.
Rapid Communications—these are published for the early communication of important and original advances. While an Experimental section is generally not necessary, in synthetic papers all new compounds must be adequately characterised (see **Preparative procedures** which follows). Rapid Communications may be of a preliminary nature. It is expected that a detailed, expanded version will be published as soon as possible after publication of the communication. Their handling will be expedited at all stages of publication, and online submission to an Editor is encouraged.

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.

For all contributions authors are encouraged to write in English, but articles are also published in French or German. In English language manuscripts either British or American (U.S.) spelling may be adopted; however, the spelling chosen should be used consistently.

Manuscripts may be sent to any of the Editors, either by post or by using the online submission system. Detailed instructions will be found below.

Preparation of Manuscripts

Overview

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. For further assistance in matters of editorial style authors are referred to *The ACS Style Guide*, 2nd ed.; Dodd, J., Ed.; American Chemical Society: Washington, DC, 1997. *Carbohydrate Research* follows the *Style Guide* as a standard. Authors are requested to give attention to the instructions given here and to examine a recent issue of the journal when preparing their manuscripts. Carelessly prepared manuscripts may be returned to the authors for correction before being processed.
Manuscripts (**all parts**: text, footnotes, tables, figure legends, references) should be printed with a line-space setting of 1 cm (~30 points) and should be paginated. Avoid making word breaks with hyphens, and use hard breaks (return key) only at the ends of paragraphs.

Chemical and biochemical nomenclature
The nomenclature of all carbohydrates and glycoconjugates should follow the recommendations of the IUPAC–IUBMB Joint Commission on Biochemical Nomenclature: ''Nomenclature of Carbohydrates (Recommendations 1996)'' published in *Pure Appl. Chem.* **1996**, *68*, 1919–2008 as well as *Carbohydr. Res.* **1997**, *297*, 1–92 and elsewhere, including the World-Wide Web at www.chem.qmul.ac.uk/iupac/2carb
For any enzyme having a substantial role in an article, the EC number should be cited when the enzyme is first mentioned. A complete and definitive list of EC numbers, which updates the printed version (*Enzyme Nomenclature*, Academic Press, 1992), can be found on the World-Wide Web at www.chem.qmul.ac.uk/iubmb/enzyme

Title
The title should be specific enough to alert the readers to whom the article is directed when seen in a table of contents, database, etc. 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 with an asterisk.

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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.

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Optional (series title, for example): Synthesis of oligosaccharides related to hyaluronic acid☆, Part 2.
Additional footnotes: to acknowledge financial support (preferentially, this may be done in an Acknowledgements section, as mentioned below), list abbreviations used, etc.—indicate by superscript symbols *, †, ‡, §, ¶, ‖, keep to a minimum.

Abstract (Required of all Papers)
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 be independent 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.]''
For papers written in French or German, authors are asked to provide an English version of the Abstract, in addition to the version in the language of the paper.

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In addition to the textual Abstract, authors are requested to provide a Graphical Abstract on a separate page. This should aim at presenting the essence of the article in a concise pictorial form. Authors should provide a suitable graphic and appropriate text, not exceeding 50 words. The full title of the paper and the full list of authors will be included by the typesetter. Authors should ensure that their graphic and text will fit into the allocated space (170 mm wide by 50 mm high) along with the title of their paper and the list of authors.

Keywords
At the end of the abstract, provide a list (typically 3–6) of 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.''

The body of the paper

Typically the body of a Full Paper comprises sections designated Introduction, Results and discussion, and Experimental. In Notes, the headings Introduction and Results and discussion are normally not used, and Rapid Communications typically lack an Experimental section. However, these specific outlines are not obligatory; authors may vary the organization of articles as needed for optimal presentation of their subject matter.

1. Introduction

The Introduction should briefly state the rationale for the work reported, with citations to the immediately relevant literature, and indicate the scope of the work. Please avoid lengthy surveys of the literature, except of course when perspective (review) articles are involved.

List references by number, **in the order in which they are cited in the text**. The numbers should be indicated by superscript Arabic numerals and appear after any punctuation thus: [1,2]

2. Results and discussion (alternatively 2. Results, 3. Discussion)

In addition to text this section may contain Tables, Figures, formula charts, and Schemes, which should be supplied on separate sheets. The preparation of such items is discussed further on in these Instructions.

If subheadings are used, these are integral with the immediately following text, as illustrated under **Experimental**.

Presentation of X-ray crystallographic data. In addition to the usual table or paragraph of text giving crystal data, particulars of the diffraction analysis, and refinement data (specify the function minimized in the least-squares refinement and the weighting factor used), authors should include 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.

Where bond lengths and valence angles are normal, listings of the individual values ordinarily make no significant contribution to the published paper. 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 pyranose and furanose rings, Cremer–Pople puckering parameters 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 as a supplement for use by referees. Tables of observed and calculated structure factors are not needed as supplementary data.

X-Ray crystallographic data are being increasingly used in structural correlations, as described for example in *Structure Correlation*, Burgi, H.-B., Dunitz, J.D., Eds.; VCH: Weinheim, 1994; Vols. 1 and 2. Thus, authors are encouraged to contribute a complete list of data in CIF (Crystallographic Information File) format to the Cambridge Crystallographic Database (see www.ccdc.cam.ac.uk for further information) before the paper is submitted. A footnote indicating this fact should be included in the manuscript "CCDC . . . contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk)." Please submit a copy of the CIF data when you submit your manuscript.

3. Experimental

Typically this section will be divided into subsections, the content of which varies according to the subject matter of the article.

Subsection examples:

3.1. General methods

Optical rotations were determined with a Jasco Model DIP polarimeter for solutions in $CHCl_3$ . . .

3.1.1. Methyl 6-*O*-*tert*-butyldimethylsilyl-β-D-allopyranoside. A mixture of **3** (200 mg, 1.03 mmol) and *tert*-butylchlorodimethylsilane. . .

3.1.1.1. Biological activity. The compound methyl 6-*O*-*tert*-butyldimethylsilyl-β-D-allopyranoside was found to have biological activity when...

Note that 3.1.1 is an example of a **title compound**, which should satisfy certain criteria if it is to be listed this way (see later).

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 (except at the beginning of a sentence), and these are preferred over acronyms, e.g., $NaHCO_3$, Et_2O, Me_2SO (not DMSO), Me_4Si (not TMS), HOAc (not HAc), NaOAc. Abbreviations can also be substituted for common terms such as aqueous (aq), saturated (satd), etc. Units of measure [mL, cm, °, 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 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** 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 or, 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 should be incorporated into the subsection describing the next title compound in the sequence.
In descriptions of preparative procedures quantities of reactants and reagents should be stated in both weight (g, mg, kg) and molar (mol, mmol) units. Yields should be reported both by weight and as percent of the theoretical.
Ordinarily, the identity of a compound is established by NMR and mass spectral data. As evidence of purity, authors are required to include an elemental (combustion) analysis (minimally C and H), with values deviating from the theoretical not more than ±0.4% absolute. When a C and H analysis is not feasible (e.g., very small amounts of material available) the author should enclose copies of pertinent NMR spectra run at high sensitivity. Also desirable are *m/z* values from mass spectra (high-resolution EIMS or low-resolution FAB- or ESIMS) and chromatographic data indicative of purity (GLC, HPLC, or TLC, at high sensitivity).

Listing of physical data. The preferred order is: mp (if applicable); $[\alpha]_D$ (normally required for chiral compounds); R_f values (if pertinent); electronic-spectral data (UV, IR, if recorded); NMR data (if not presented in a table); MS. Punctuate as in the following example.
"...gave needles: mp 83–85 °C; $[\alpha]_D^{25}$ – 110° (*c* 1.4, $CHCl_3$); IR (KBr); *v* 1730 and 1260 (ester), 860 and 840 (Me_3Si), and 710 cm^{-1} (Ph); ^1H NMR..."

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 °C, lit.[6] 172–174 °C; $[\alpha]_D^{25}$ +155° (*c* 1.43, water), lit.[6] +149°; ^1H NMR..."

NMR data. Authors are encouraged to use tables for the presentation of NMR data. For listings as running text please adhere strictly to a uniform style. The following is the preferred format:

^1H NMR ($CDCl_3$): δ 7.35 (d, 1-H, $J_{3,4}$ 2.0 Hz, H-3), 5.10 (dd, 1-H, $J_{4,5}$ 4.0 Hz, H-4), 4.40 (ddd, 1-H, $J_{5,6a}$ 6.5, $J_{5.6b}$ 5.5 Hz, H-5),...

Note that additional couplings contributing to the multiplicity of δ 5.10 ($J_{4,3}$) and δ 4.40 ($J_{5,4}$) are not listed because the values have already been recorded as $J_{3,4}$ and $J_{4,5}$, respectively. 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.
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 arrrangement of element symbols in the molecular formula: C, H, then the remaining symbols in **alphabetical order** (standard Hill system).

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.

Supplementary data

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References

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Journal articles: List **all** authors, taking great care with the spelling of authors' names; include diacritical marks (umlaut, acute accent, etc.) when these appear in the original. Journal abbreviations should follow the *Chemical Abstracts Service Source Index* (*CASSI*) style (an electronic version of CASSI which lists most of the abbreviations is available on-line at www.cas.org/sent.html).

1. Borén, H. B.; Garegg, P. J.; Wallin, N. H. *Acta Chem. Scand.*, **1972**, *26*, 1082–1086. **(Inclusive pages are required)**.

Patents:

2. Ledrut, H. U.S. Patent 2,551,982, 1951; *Chem. Abstr.*, **1952**, *51*, 7128i. [If possible include a reference to *Chemical Abstracts,* or to the *World Patent Index* (Derwent Publishers).]

Abstracts of papers given at meetings:

3. Edye, L. A.; Clarke, M. A. *Abstracts of Papers*, 208th National Meeting, American Chemical Society, Washington, DC, August 1994; CARB 7.

Monographs:

4. Armstrong, E. F.; Armstrong, K. F. *The Carbohydrates*, 5th ed., Longmans, London, 1934, pp 106–115.

Multiauthor volumes:

5. Wolfrom, M. L.; Szarek, W. A. Halogen Derivatives. In *The Carbohydrates*, *Chemistry and Biochemistry*, 2nd ed., Pigman, W.; Horton, D., Eds.; Academic Press, New York, 1972; Vol. 1A, pp 239–251.

Thesis:

6. Cato, S. J. Ph.D. Thesis, University of Florida, 1987.

Footnotes

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

Tables

Many types of data can be most effectively presented in tabular form. Authors should consult a current issue (or the free online sample copy at www.elsevier.com/locate/carres in the Author Gateway section) for examples of the style employed by *Carbohydrate Research*. Tables are numbered in sequence as they are to appear in the text, using **Arabic** numerals. *Vertical lines should not be used.*

Title: The title should accurately and concisely describe the content of the table. It should be understandable, at least in a general way, without reference to the text. Units of measure should not be given in the title.

Column headings: these should be short—use abbreviations where possible. Most important, column headings should **name the parameter** listed in the column or group of columns below. Units of measure should be specified here; for further instructions on this point, see ''Units of Measurement'' below.

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These should be submitted separately, without legends and must be cited in the text, numbered in order of appearance with Arabic numerals. Line drawings, structural formulae, and instrument traces (spectra etc.) must be done in black on a white background. Charts and drawings produced by computer must be prepared at a resolution of 300 dpi or better. All graphics (including chemical structures) must be supplied camera-ready. 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.

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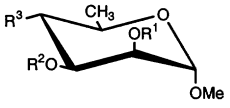
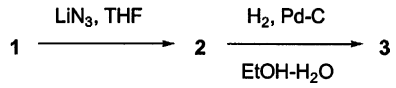
Formula charts and schemes: Particular attention should be paid to current conventions for drawing sugar ring structures (tapered thickening of forward edges, etc.). Structural formulae should be grouped for insertion in the text at appropriate points. Such groups need not have a caption, but those showing reaction sequences (i.e., containing arrows) may be designated Scheme 1, Scheme 2, etc. In charts and 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. Where a single structure with R groups represents two or more compounds, the sequence follows the listing below the structure, then resumes its rightward progression. Multiple listings under a single formula should be in 'tabular' format, as in the following example.



	R^1	R^2	R^3
12	H	H	NH_2
13	H	H	NHAc
14	-CMe_2-		N_3
15	-CMe_2-		NH_2
16	-CMe_2-		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:



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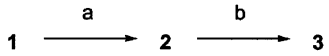

In legend: (a) LiN_3, THF; (b) H_2, Pd–C, EtOH–H_2O

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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: $10^3 \times$ concentration (M), not Concentration ($M \times 10^{-3}$).
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