CARBOHYDRATE RESEARCH

An International Journal of Molecular Glycoscience

AUTHOR INFORMATION PACK

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DESCRIPTION

The Journal of Analytical and Applied Pyrolysis (JAAP) is devoted to the publication of papers dealing with innovative applications of pyrolysis processes, the characterization of products related to pyrolysis reactions, and investigations of reaction mechanism. To be considered by JAAP, a manuscript should present significant progress in these topics. The novelty must be satisfactorily argued in the cover letter. A manuscript with a cover letter to the editor not addressing the novelty is likely to be rejected without review.

More specifically, the Scope of the Journal includes:

Fundamental pyrolysis research on chemical substances and materials comprising:
- experimental studies of pyrolysis reactions such as chemical mechanism and kinetic investigations; this includes preparative pyrolysis methods for the synthesis of novel compounds and mechanisms of high temperature reactions;
- computational and theoretical studies of reaction mechanism, kinetics, and thermodynamics are acceptable, provided they are directly related to experimental data, either new or previously published, but they must be described adequately in the paper;
- computational processing of pyrolysis data, such as advanced pattern recognition and principal component analysis and other multivariate analyses.

Analytical pyrolysis, i.e. the characterization of a material in inert atmosphere by thermally induced degradation reactions;
- exploring chemical composition and structure of materials by revealing thermal and chemical decomposition reactions leading to products fully identified by chemical and spectroscopic methods;
- applications of analytical pyrolysis in environmental, biological, medical, forensic, cultural heritage, food, geochemical, polymer, and materials science;
- new instrumentation and new analytical methods using pyrolysis reactions or to unravel the chemical composition of pyrolysis products.

Applied pyrolysis dealing with the development of pyrolysis processes for producing valuable chemicals and/or energy carriers (gas, liquid, solid or electricity) and/or materials from fossil or renewable feedstock or waste, the recycling of materials, and the disposal of toxic substances. The manuscript must discuss the relationships between pyrolysis conditions and product characteristics. This topic includes:

- various feedstock (fossil fuels, biomass, wastes, polymers, etc.) and the co-processing of different feedstock;
- various thermal processes (slow and fast pyrolysis, torrefaction, carbonization, high pressure pyrolysis, catalytic pyrolysis, deoxygenation, hydropyrolysis, solvent liquefaction).

The combination of a pyrolysis process with other types of treatment (mechanical, biological, or chemical) or materials characterization is within the scope of the journal only if the main focus of the manuscript is the pyrolysis process. Integrated processes combining pyrolysis reactors and products purification are welcome, if different pyrolysis conditions are studied. The computational modeling of pyrolysis reactors or processes should be related to experimental data, either new or previously published, but they must be described adequately in the paper.

The pyrolysis conditions should be described thoroughly (residence times of solid and vapors, temperature distributions, etc.). The pyrolysis products must be chemically characterized. Catalysts should be physically and chemically characterized before reaction, and, when feasible analysis of catalysts after reaction is also desirable. While this may not always be possible, at least qualitative assessments should be made.

The investigation of pyrolysis of a new feedstock or material with conventional methods, but without new development of the pyrolysis process is not sufficiently novel to be considered by JAAP.

Review articles are invited by the Editors but may also be proposed in writing to the Review Editor. The subject of review articles should be broad enough to appeal to a wide range of readers. Discussion should be concise, but adequate. More detailed discussion may be appropriate in some cases. It is expected that reviews should be critical rather than just catalogs of published data. They should include the most important, recent advances in the topic, whereas papers of low scientific significance should be given very limited coverage.

Out of the scope of JAAP

The Journal does not consider studies based on:
- the activation of carbons and characterization of activated carbons;
- thermal analysis, mass yields without characterization of the pyrolysis products by chemical and spectroscopic methods;
- characterization and application of pyrolysis products, unless clearly related to/aimed at understanding the influence/details of pyrolysis processes and conditions;
- theoretical studies, kinetic modelling etc. which are not complemented with or validated by experimental data
- combustion, gasification or incineration unless specifically related to the interplay between pyrolysis and oxidation reactions.

AUDIENCE

Chemists, Biologists, Biochemists and Medical Researchers/Scientists involved in studies of molecular aspects of glycoscience.

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INTRODUCTION

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Nomenclature and units

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 http://www.chem.qmul.ac.uk/iupac/2carb/.

For visual representation of glycan structures, authors are strongly recommended uisng the Symbol Nomenclature for Glycans (SNFG) that can be found at https://www.ncbi.nlm.nih.gov/books/NBK310273/. All figures depicting glycans with symbols for monosaccharides are required to follow the shapes and colors presented in the current version of the SNFG. Please cite Glycobiology 25: 13231324, 2015. doi: 10.1093/glycob/cwv091 https://www.ncbi.nlm.nih.gov/pubmed/26543186.

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Title Compounds

3.1.1. Methyl 6-*O*-*tert*-butyldimethylsilyl-β-D-allopyranoside (4).

Note that the (numbered) compound is an example of a *title compound*, which should satisfy certain criteria if it is to be listed this way. Convincing evidence for identity and purity must be presented for all new carbohydrate derivatives listed as *title compounds*. Ordinarily, identity 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 criteria used to assess purity should be specified; these should include NMR observations (absence of extraneous lines in a spectrum run at high sensitivity) and chromatographic data (GLC, HPLC, or TLC at high sensitivity). Also desirable are *m/z* values from mass spectra.

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Nomenclature

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If there are published physical constants (mp, [α]D, λmax, etc.) for the compound these should be cited, using the following format:

...allyl 2-acetamido-2-deoxy-[α]-L-glucopyranoside (1α): mp 175176 C, lit.6 172174 C; [α]D25

+155 (*c* 1.43, water), lit.6 +149; 1H 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:

1H NMR (CDCl3): δ 7.35 (d, 1H, J3,4 2.0 Hz, H-3), 5.10 (dd, 1H, J4,5 4.0 Hz, H-4), 4.40 (ddd, 1H,J5,6a 6.5, J5,6b 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-3I, H-3II, H-3 III.

1H (signals and coupling constants assigned) and 13C NMR data are required for all synthetic compounds and must be included as electronic supporting information. A minimum of three pieces of analytical data are required for all known compounds, while five pieces of data are required for all new compounds. The latter must include either C and H analysis or high resolution mass spectrometry data.

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Elemental analysis data

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:

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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, CremerPople puckering parameters (Cremer, D.; Pople, J. A. J. Am. Chem. Soc. 1975, 97, 13541358) 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.

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[4] Cancer Research UK, Cancer statistics reports for the UK. http://www.cancerresearchuk.org/aboutcancer/statistics/cancerstatsreport/, 2003 (accessed 13 March 2003).
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