Journal of Inclusion Phenomena Guidelines for Authors

1. Aims and Scope

The Journal of Inclusion Phenomena and Molecular Recognition in Chemistry is an inter-disciplinary publication reporting on original research into all aspects of the study of host-guest systems. Examples of specific areas of interest are: The preparation and characterisation of new hosts and new host-guest systems; Crystallographic, spectroscopic, thermodynamic, and theoretical studies; Applications in chromatography and inclusion polymerisation; Enzyme modelling, molecular recognition, and catalysis by inclusion compounds; Intercalates in biological and non-biological systems; Cyclodextrin complexes and their applications in the agricultural, flavouring, food, and pharmaceutical industries; Synthesis, characterisation, and applications of zeolites.

The primary emphasis of the Journal is on the publication of refereed research reports, but preliminary communications are also accepted, particularly if they represent a significant advance in the understanding of inclusion science. Review articles dealing with recent advances in this field are also published periodically.

1.1. RESEARCH ARTICLES

These form the core of the Journal's publications, and should present previously unpublished material which significantly advances our understanding of inclusion science. While there is no prohibition on length, it is felt that manuscripts should not exceed 5000 words accompanied by suitable illustrative material (figures and tables). Articles may be submitted in English, French, or German. For the benefit of the anglophone audience, articles submitted in French or German should be accompanied by an extensive summary in English. Each article will be refereed by two independent reviewers. The Editors' decision to publish or not will be final.

1.2. RESEARCH COMMUNICATIONS

Shorter communications of about 1500 words in length, with three to four illustrative items, if urgent, will be accepted as research communications. They will be subject to the same reviewing standards as full articles.

1.3. LETTERS TO THE EDITOR

Matters arising, brief polemics, announcements of forthcoming events, etc., may be considered for publication as Letters to the Editor. They should be brief and to the point, and should contain no more than one table or figure.

1.4. BOOK REVIEWS

Books on important aspects of inclusion science may be noticed in the Journal. Such reviews will be commissioned by the Editors in Chief. Publishers wishing to have their books noticed in the Journal should submit them to the Journals Office in Dordrecht in the first instance.

1.5. REVIEW ARTICLES

It is not the intention to publish frequent review articles, and so most reviews will be commissioned. Authors intending to review a particular aspect of inclusion science should consult the Reviews Editor, Prof. Fritz Vögtle, Institut für Organische Chemie und Biochemie der Universität Bonn, Gerhard-Domagk-strasse 1, D-5300 Bonn, Germany, Fax: 228–735662, prior to submission of the manuscript.

2. Submitting Your Manuscript

2.1. SUBMISSION

European authors submitting manuscripts to the Journal should send *three copies* to either: The Journals Office, Journal of Inclusion Phenomena, P.O. Box 17, 3300 AA Dordrecht, The Netherlands, or to Dr. Eric Davies, Environmental Science Division, University of Lancaster, Lancaster LA1 4YQ, U.K. Telex: 65111 Lancul G; Fax: 0524–63806.

Authors from Japan should send *three copies* of their article directly to Prof. Yukito Murakami, Department of Organic Synthesis, Faculty of Engineering, Kyushu University, Fukuoka 812, Japan. Fax: 092–641–1825.

Authors from other geographical areas should send *three copies* of their article directly to Prof. J. L. Atwood, Department of Chemistry, University of Alabama, University, AL 35486, U.S.A. Fax: 205–348–8426.

Each manuscript should be accompanied by a covering letter stating the title of the paper, key words describing the main focus of the paper, the authors' names and addresses in full, and any special instructions for the printer (such as: use of non-standard terminology or symbolism, identification of handwritten symbols, etc.).

In cases of multiple authorship of an article, the name and full postal address of the corresponding author must be clearly indicated.

In all correspondence about articles in the Journal, authors are requested to refer to the full title of the paper (or MS Ref. No. when allotted), the title of the Journal, and to indicate clearly the author's own name.

2.2. COPYRIGHT

Authors of papers which are accepted for publication in the Journal will be sent a form requiring them to transfer the copyright of the article to the Publisher. Such a formal notice is necessary in connection with the 1978 U.S. Copyright Law, and authors are requested to sign and return the form without delay, as publication of their paper cannot proceed without its receipt by the Publisher.

2.3. REFEREEING

Each article and communication will be submitted to two referees. Where, in the referees' opinion, revision of the paper is deemed to be necessary, the referees' comments will be passed on to the authors; the identity of the referees will remain anonymous. Papers revised in the light of the referees' comments should be resubmitted, with a covering letter referring to previous correspondence.

2.4. OFFPRINTS

Authors of review articles, research articles, and research communications will receive 25 offprints free of charge. Additional offprints may be purchased if ordered before the relevant issue of the Journal goes to press. An order form for this purpose will be enclosed with the proofs. Orders for offprints received after the Journal as gone to press will only be entertained in exceptional circumstances.

2.5. PAGE CHARGES

There will be no page charges levied against authors or their institutions. Under exceptional circumstances (e.g., reproduction in colour, reproduction of items as fold-outs, etc.) an author may be requested to contribute to the cost of printing.

3. Manuscript Preparation

3.1. MANUSCRIPT

All manuscripts must be typed double-spaced on clean white bond paper of good quality, leaving wide margins for editorial instructions on all sides of the typing area. Type on one side of the paper only. The top copy of the manuscript should be accompanied by two carbon copies, or preferably photocopies, of acceptable quality, including copies of all illustrative material. Each page of the manuscript should be numbered consecutively.

3.2. TITLE

Begin the first word of the title with a capital letter, and thereafter capitalize only proper nouns and standard nomenclature requiring capital letters. Small caps (as in D-glucose) should be indicated with two short horizontal lines under the letter.

Avoid the use of non-standard compound names and laboratory shorthand abbreviations in titles. Check any systematic nomenclature very carefully, by reference to IUPAC rules and/or *Chemical Abstracts*. Be particularly careful in the use of square and round brackets and punctuation in systematic compound names.

3.3. NAME AND AFFILIATION

Always cite your own and your co-authors' names in the same way. Do not vary, for instance, between John H. Smith, J. H. Smith, and J. Henry Smith. A computer-generated bibliography will regard all these variants as different names. It will be assumed that the given name is followed by the family name, even in the care of oriental names. Omit

titles and honorifics such as Lord, Sir, Professor, Doctor, Reverend, Father, etc. The author for correspondence should be indicated in a footnote on the first page.

Use no abbreviations in the affiliation, and give an adequate postal address, including such details as post-code and country.

3.4. DATE OF RECEIPT

Type (Received:

on the line following the affiliation. The Editor may add subsequent data amplifying this notice, such as 'Accepted', 'In final form', etc.

3.5. ABSTRACT

Head the abstract clearly, and separate it from the main text of the article by two or three lines' space.

Type the abstract double-spaced, as for the rest of the article. Avoid the use of displayed chemical or mathematical formulas or equations in the abstract. References to the literature should not be cited in the abstract.

The abstract should preferably be composed as a single paragraph and should state, briefly, the main objectives of the investigation, describe the methodology employed, give a brief summary of the results obtained, and give the principal conclusions. The abstract should not contain any material which does not appear in the paper.

3.6. KEY WORDS

Key words supplied by the authors will be used in a short index at the end of each volume of the Journal. The key words selected should be comprehensive and subject specific. It is not necessary to list the subject area of the Journal's coverage as a key word.

Four key words should be sufficient to cover the major subjects of a given paper, although more can always be supplied if the author deems it necessary. General terms should not appear as the first key words, as they have little use as information retrieval tools (for example: 'beta-cyclodextrin complex preparation properties' is preferable to 'preparation properties complex beta-cyclodextrin').

Please, choose key words to be as specific as possible, and list the most specific first, proceeding to the most general last.

3.7. SUPPLEMENTARY DATA

Authors wishing to supply supplementary data for depositing with the British Library should include the following statement immediately below the key words:

Supplementary Data relating to this article are deposited with the British Library as Supplementary Publication No. SUP (pages).

All such data should be submitted with the manuscript, for forwarding to the British Library.

Notes for Users and Notes for Depositors appear on pp. 187–189 of this issue.

3.8. SECTION HEADINGS

Authors should attempt to employ as few orders of heading as possible. It is in any case

difficult to differentiate typographically between more than three orders of heading, and it is doubtful whether any text can support such fragmentation.

The typist can help to distinguish headings by typing:

- 1. Major Section Headings at the Left of the Page
- 1.1. FIRST SUBHEADINGS AT THE LEFT OF THE PAGE IN CAPITALS
- 1.1.1. Second Subheadings Underlined at the Left of the Page

The recommended order for Major Section Headings is: Introduction, Experimental, Results, and Discussion.

3.9. NOTES AND REFERENCES

Notes which appear at the foot of the page are strongly discouraged. In exceptional circumstances they may be permitted (change of author's location, editorial comment) and should then be indicated by *, **, \dagger , \dagger , \dagger , \dagger , etc.

Notes which are to appear at the end of the article are to be referenced by a superior number, following any punctiation. (As here.) The reference numbers to notes should be continuous throughout the text.

References to the literature should be given between square brackets [292] in the text. The standard form of typing references for Kluwer chemistry publications is:

- 46. A. Smith, B. Jones, and C. Brown: Tetrahedron 44, 197 (1976).
- 47. P. M. Henry: <u>Palladium Catalyzed Oxidation of Hydrocarbons</u> (Catalysis by Metal Complexes v. 2, Ed. B. R. James), pp. 44–77. Reidel (1980).
- 48. J. S. Yoo and R. L. Milam (Atlantic Richfield): U.S. Patent 3,920,763 (1975); <u>C.A.</u> 84, 5859lu (1976).

Always try to include a *Chemical Abstracts* number for items likely to be obscure or unintelligible.

Abbreviate journal titles in the reference section according to the *Chemical Abstracts Service Source Index* (CASSI).

3.10. CHEMICAL FORMULAS

Simple formulas (alkyl derivatives, monocyclics) can be set in type; more complex formulas (multidentate ligands, polycyclics, projection diagrams) can be carefully drawn before photographic reproduction.

Highly complex formulas such as enzymes, macrocycles, etc., should be supplied by the author as camera-ready artwork, drawn approximately twice the finished size, with lettering also to the same scale. *See* directions for artwork in Section 3.13.

Try to prepare all formulas so that they will read horizontally across the page, but be careful to preserve correct stereochemistry when taking structural diagrams direct from other sources.

It is not always possible to insert a chemical equation, formula, or reaction scheme in exact relation to the text. It is preferable to give compounds numbers, therefore, and to refer to them as, for instance, "K(dibenzo-30-crown-10)X(I, X = F, Cl, Br)". Reaction schemes should be treated similarly, and given the caption "Scheme 1" etc.

Substituent alkyl groups or ligands should be referred to as R, R_1 , R_2 ... L, L_1 , L_2 , or R, R', R'' ... L, L', L'', but not as a mixture of the two systems.

Oxidation states should be written Pt(II).

Labelled atoms may be indicated by an asterisk: MeC*O₂H; but isotopes should be written with the mass number to the left, when using the element symbol (¹⁴C), or separated by a hyphen when using the element name (fluorine-19).

Avoid extensive quotation of reaction conditions above arrows in reaction schemes. It is better to write them as notes to the scheme or, in complex cases, to write them as part of the text.

3.11. NOMENCLATURE

Common trivial names are perfectly acceptable (aniline not benzenamine, acetic not ethanoic acid) but laboratory shorthand and non-standard ligand names should be avoided unless defined at first mention. Extensive use of non-standard abbreviations may call for a glossary, which can be included as a final section of the article (before the Acknowledgements) or as an Appendix.

Systematic nomenclature should be produced, so far as possible, in accordance with IUPAC rules. In cases where IUPAC has not yet issued guidelines, the latest issue of the *Chemical Abstracts Index Guide* should be consulted for guidance. It is wise to have systematic nomenclature checked by a colleague in all cases of unusual complexity or difficulty.

3.12. TABLES

All tables should be numbered in sequence using Roman numerals, and each table must be referred to in the text. Head each table 'Table I' etc., and provide a suitable

Table I. Stereoselective reduction of alkylcyclohexanones to thermodynamically more stable cyclohexanols with stoichiometric reagents (A, B) and catalysts (C, D).

R = 0	More stable isomer	Selectivity (%) with			
	401.5	A	В	С	D ^a
2-Me	trans	99		_	_
3-Me	cis	94		_	90
4-Me	trans	99	79 - 81	_	82
4- <i>t</i> -Bu	trans	99	88 – 90	90	96

a non optimized data

 $A = Li(NH_3)$ [55]; $B = LiAlH_4$ [56]; $C = IrH_3(PPh_3)_2$, [S]/[cat] = 38 [52];

 $D = [Ir(3,4,7,8-Me_4-phen)COD]Cl, [S]/[cat] = 1600 [54].$

title on the same line. Do not type tables as part of the manuscript, rather collect them on

separate sheets at the end. Do not use vertical rules in tables. Horizontal rules are used to open and close tables, and to separate headings from the data field. Additionally, short rules may be used to group related classes of headings. Range the data field and the headings left on the columns: do not attempt to centre the headings. Use abbreviations freely in order to save lengthy column headings, but take care to explain non-standard abbreviations in footnotes to the table.

3.13. ILLUSTRATIONS

Both line-drawings and photographs should be used sparingly. All illustrations must be supplied in camera-ready form, be numbered in sequence using Arabic numbers, and each illustration must be referred to in the text. Each illustration must be provided with a caption which is complete enough for the figure to be appreciated without referring to the text.

Line drawings must be submitted as the original, drawn in black ink on good quality tracing paper or draughtsman's film, or as a glossy photographic print. Photocopies, multiliths, Verifax or Xerox copies are not acceptable substitutes.

Drawings should be finished at about twice the desired printed size, and it should be borne in mind that the lettering should also be about $2 \times$ magnified over the printed size. Lettering should be done with a lettering stencil, or with press-on lettering: freehand or typewritten lettering is not acceptable.

Photographs must be supplied as glossy prints. Do not use lettering on the photograph itself, but on an overlay sheet, fixed to the photograph. Register lines on the photograph and on the overlay will ensure an accurate mating of text and image. Micrographs and similar material in which linear dimensions are important should have a scale of length on the overlay sheet.

Collect the captions to all the illustrations on a separate sheet, and make sure that each illustration is clearly identified so that it can be mated with the relevant caption. Write on the backs of photographs in soft pencil, and on line illustrations in light blue pencil: provide the authors' names, the title (or short title) of the paper, the Journal name and the figure number on *each* illustration and, where necessary, indicate which side is the top of the illustration

3.14. SPECTRA

Spectral data should be reported, wherever possible, in numerical form (ν C = O (stretch) 1710 cm⁻¹; m/z: 350(M⁺), 320...). Where spectra must be reproduced, it is preferable to provide a tracing of the most significant portion of the spectrum, with suitably labelled axes, rather than to supply the whole spectrum.

Bear in mind that spectra will be reduced to fit the page dimensions, and much fine structure will thereby be lost.

3.15. CRYSTAL STRUCTURE REPORTS

A research article which is based on a single crystal X-ray diffraction study should contain (1) the lattice constants, crystal system, and space group, (2) the final R value based on F and the number of reflections used in the refinement, (3) a brief description of the experimental methods, (4) the final values of the atomic coordinates, (5) the relevant

bond distances and angles, (6) an analysis of any problems associated with the location of the guest molecules in a host/guest situation, (7) one or more molecular illustrations which display the thermal ellipsoids, if appropriate, and (8) a stereographic view of the unit cell packing if guest molecules are present.

Tables of fractional coordinates should be submitted in the form of camera-ready copy when possible. The tables will be reduced *ca.* 50% before publication. Tables of bond lengths and angles will appear in the manuscript only where pertinent to specific points of discussion. Otherwise, they should be submitted as supplementary material. Wherever possible, stereo diagrams should be submitted to better illustrate the modes of inclusion.

The thermal parameters and observed and calculated structure factors should be deposited as supplementary data (see Section 3.7, above).

A research communication should contain (1), (2), and (7) from above, with (4) and (5) available as supplementary material (along with the thermal parameters and structure factors).

Standard deviations should be given for lattice constants and interatomic parameters.

X-ray powder diffraction data should contain details of the experimental technique and a listing of the *d*-spacings (indexed or unindexed). If the data permit, the crystal system and the possible space groups should be mentioned.

3.16. UNITS

The SI system is strongly recommended. Papers presented in British Imperial or U.S. standard units will not be accepted. It is stressed that whatever system of (metric) units the paper is written in, the usage must be consistent.

3.17. SAFETY

All hazardous procedures must be indicated as such by including a warning of the likely dangers of a given experiment and advice on how to circumvent these dangers.

3.18. PROOFS

Each principal author will receive two proofs of the article, together with an annotated copy of the manuscript. It is requested that authors read their proofs and return them to the Publisher within one week of receipt. It is stressed that the author alone is responsible for the correction of the proofs, and so a very careful reading is necessary. It is a wise precaution to ask a colleague to read the proof, in addition to yourself.

Authors should be aware that the copy-edited manuscript is regarded as definitive: it should be returned to the Publisher together with one corrected set of proofs, and any changes which constitute a departure from the original manuscript may be charged to the author.