CrystEngComm

Instructions for Authors (2004)

Also see: www.rsc.org/illustrations and www.rsc.org/electronicfiles

CONTENTS

1.0 General Policy

CrystEngComm is an international journal for the publication of original research concerned with all areas of crystal engineering. The use of electronic media for all stages in the publication process leads to rapid publication times, and the enhanced presentation of the research presented.

All contributions are judged on the originality and quality of scientific content. Thus, articles reporting results which would be routinely predicted or result from application of standard procedures or techniques are unlikely to prove acceptable in the absence of other attributes which themselves make publication desirable.

There are no author charges for publishing in *CrystEngComm*, and authors will receive a FREE pdf of their article, which can be used for reprint purposes.

1.1 Scope of the Journal

Topics covered include:

Properties: Thermodynamics, phase transitional behaviours, solid state reactivity, optoelectronics, NLO, molecular and bulk magnetism, conductivity and super conductivity, absorption and desorption, mechanical.

Target Crystals/Materials: Ionic, molecular, covalent and coordination solids, biominerals and biomimetic materials, synthetic zeolites, liquid crystals, nano and mesoporous crystals, channelled structures.

Techniques: Single crystal X-ray and neutron diffraction, powder diffraction, solid state spectroscopy (IR, Raman, NMR *etc*.), calorimetry and thermogravimetry.

Methods: Modelling and data mining, as well as empirical, semi-empirical and *ab-initio* theoretical evaluation of solids and of intermolecular interactions.

1.2 Full Papers

Full Papers contain original scientific work that has not been published previously. However, work that has been published previously in a short form such as a *CrystEngComm* Communication is normally acceptable, provided that it represents a substantial amplification and extension of the original material. There are no restrictions on the length of a paper.

1.3 *CrystEngComm* Highlights

CrystEngComm Highlights are normally published by invitation of the Editorial Board. However, suggestions from authors are welcome and enquiries regarding the submission of *CrystEngComm* Highlights should be directed to the Managing Editor, Dr J. S. Humphrey (crystengcomm@rsc.org).

Highlights should be long enough to allow the authors to make their principal points – but no longer. The more effectively these are made, and the more accessible the article, the better. The old adage that 'one picture is worth a thousand words' is particularly appropriate in an electronic medium.

1.4 Communications

Preliminary accounts of original and significant work of such importance or novelty that rapid publication is justified may be published in Communication form. Authors should provide in a covering letter a justification as to why they feel that publication of their work as a Communication is warranted. The recommended length is four pdf journal pages, however some flexibility is allowed. *CrystEngComm* Communications should not contain section headings.

Full Papers based upon Communications are welcome, provided that they represent a substantial amplification and extension of the original material.

1.5 Letters

A *CrystEngComm* Letter is a medium for the expression of scientific opinions and views normally concerning material published in *CrystEngComm* or other RSC journals. It is intended that contributions in this format should be published rapidly. *CrystEngComm* Letters are for scientific discussion, and are not intended to compete with media for the publication of more general matters such as *Chemistry in Britain*, or for revision/updating authors' own work. Letters should rarely exceed one pdf journal page in length (about 3 pages of typescript) and should contain no more than 5 references. Where a Letter is polemical in nature, and if it is accepted, a Reply will be solicited from other parties implicated, for consideration for publication alongside the original Letter.

1.6 Submission of Articles

Articles for publication should be submitted using the RSC electronic submission service (www.rsc.org/submissions). On submitting their manuscripts, authors are encouraged to supply the names and addresses of 2–3 potential referees. For a Communication authors should briefly indicate in a covering note or letter the reasons why they feel that rapid publication of their work is justified.

All authors submitting work for publication are required to sign an exclusive Licence to Publish (see www.rsc.org/is/journals/current/coplic.htm).

Rapid publication is aided by careful preparation of text and illustrations. Particular attention is drawn to the use of (i) SI units and associated conventions, (ii) IUPAC nomenclature for compounds and (iii) standard methods of literature citation.

1.6.1 Online Submission of Articles [E-Submissions]. The RSC electronic submission service allows any number of files to be uploaded to the *CrystEngComm* Editorial Office. The following files and information should be provided:

(a) A pdf version, if possible, of the manuscript as a single file (containing text and figures). If a pdf version is not possible, then the file in MS Word format will be acceptable.
(b) Data for deposition with the Electronic Supplementary Information (ESI) service (if appropriate, see Section 3.4).
(c) Details of any relevant preliminary Communications (please give reference or include pdf file).
(d) Names of potential referees.
(e) A justification of why the work merits urgent publication if the submission is a Communication.
(f) Any multimedia files.
(g) A completed Licence to Publish (see www.rsc.org/is/journals/current/coplic.htm)

After electronic submission your file will be acknowledged by the Editorial Office as soon as possible. Authors should contact the Editorial Office if they have not received an acknowledgement within 4 working days.

1.6.2 Requirements for Revised Articles and Material for Proof Preparation. Revised manuscripts may be sent to the Editorial Office by electronic file upload (www.rsc.org/submissions) or crystengcomm@rsc.org.

The revised files should be sent in the formats given in the separate guidelines on submitting files for proof preparation given in Section 3.5.

2.0 Administration

Receipt of a paper will be acknowledged, and the paper will be given a reference number which authors are asked to quote on all their subsequent correspondence. If no such acknowledgement has been received after a reasonable period of time, authors should check with the Editorial Office as to whether the paper or the acknowledgement has gone astray.

Editorial Policy. Every paper will be considered by the Editor, who will then consult with at least two referees. Submission of a manuscript will be regarded as an undertaking that the same material is not being considered for publication by another journal.

Copyright. The whole of the literary matter (including tables, figures, diagrams and photographs) in *CrystEngComm* is subject to copyright and may not be reproduced without permission from the Royal Society of Chemistry and such other Owner of the copyright as may be indicated. However, the Owner may reproduce/republish portions of the Work without seeking permission, provided that any reproduction is accompanied by an acknowledgement in the form:

(original citation) – Reproduced by permission of the Royal Society of Chemistry

To republish/reproduce the whole Work, the copyright Owner must submit a written request to the RSC. The RSC will agree to any reasonable request, provided that the owner ensures that any such republication is accompanied by an acknowledgement (in the above form) of first publication of the Work by the RSC.

Reprints. Electronic reprints (pdf) of each paper are made available free of charge.

3.0 Notes on the Preparation of Articles

3.1 Organisation of Material

(a) Various templates for manuscript preparation are available at www.rsc.org/is/journals/templates/templates.htm
(b) The first page should be set out as follows:

(i) Name and address of the author to whom the proofs and correspondence should be sent.
(ii) Title of the paper.
(iii) Authors' names, including at least one forename or initial for each author; an asterisk should follow the name of the author who is to receive correspondence. An e-mail address may be included at the end of the address of the author who is to receive correspondence.
(iv) The address where the work was carried out; if this is different from the current address of any author wishing to deal with correspondence a footnote indicating the present address of this author should be included. For multiple authors at different locations italic superior letters (*a,b,c*. . . following the asterisk if present) should be used to identify addresses.
(v) Abstract, followed by a horizontal line, in double-line spacing.

(c) Suitable headings and sub-headings should be used in the main text as appropriate (except for Communications in which no headings are used).
(d) Equations and reactions should be numbered sequentially through the text. For example, eqn. (1), reaction (2) *etc*.
(e) Bibliographic references, or Notes and references, should be numbered serially in the text by means of superscript Arabic numerals. Authors are encouraged to check the RSC Reviews web site to ensure that they have cited relevant recent reviews: www.rsc.org/reviews
(f) Notes and references should follow the main text and should have the following format for journal articles: author names, journal title, year of publication, volume, issue, page range, *e.g.*:

1 Heike I. Süss, Martin Lutz and Jürg Hulliger, *CrystEngComm*, 2002, **4**, 610–612.
2 Nicholas J. Turro, *Chem. Commun*., 2002, 2279–2292.

and for books: author names, title, editor, publisher and place of publication, year, page number, *e.g.*:

1 G. R. Desiraju, *Crystal Engineering: The Design of Organic Solids*, Elsevier, Amsterdam, 1989.

(g) Journal titles should be abbreviated according to the Chemical Abstracts Service Source Index (CASSI).
(h) Tables should be prepared on separate pages at the end of the manuscript.
(i) Diagrams should be provided on separate pages at the end of the manuscript and accompanied by a separately typed set of captions. Text and diagrams should not be combined.
(j) Revised manuscripts should also be submitted in electronic form. The guidelines for submission of files for proof preparation are given in Section 3.5.
(k) Communications should include brief details of key experiments (with amounts of reagents used) but more extensive supporting data are not required; these can be provided as supplementary information to assist referees in their assessment of the work.
(l) A graphical contents entry is also required. The format incorporates, where possible, a small graphic (maximum size 4.5 cm in width × 4 cm in depth). Each entry should be presented in such a way as to encourage further perusal of the article, by highlighting the novelty and main feature(s) of interest; excessive lists of results and, in particular, cumbersome formulae should therefore be avoided.

To facilitate rapid processing of your work and to avoid omissions please ensure that submitted manuscripts clearly indicate the desired location of unnumbered graphics in the text, *e.g.* **<structures 1–3 here>**.

3.2 Artwork Guidelines

Please supply graphics in TIFF or EPS format, at a resolution of 600 dpi.

All formulae and figures should be clear and in the case of figures, provided with captions, listed on a separate page. Illustrations should be prepared for a single (83 mm) or double column (171 mm) width. Single column is preferred and the maximum page depth is 233 mm. Artwork sent by post should be supplied at its *final* size so that reduction is not required.

3.2.1 Line Illustrations.

(a) Line illustrations should be drawn in black, using lines of an even and adequate thickness (*e.g.* 1 pt). Curves should be smooth. Broken, dotted and dot-dash lines may also be used. Particular care should be taken to ensure that lines in spectra are of an adequate thickness (*i.e.* not less than 1 pt) for reproduction.
(b) Experimental data points must be of a reasonable size and wherever possible confined to open and closed circles, crosses, squares and triangles. Partly black circles and similar signs frequently become indistinguishable in print.
(c) Avoid the use of shading (tints) that simulate grey and use line shading if appropriate. Diagrams containing several grey shades are unlikely to reproduce successfully.
(d) If possible, lettering should be in an 8 pt Helvetica or Arial font.
(e) For graphs, axis labels should use SI units, separated from quantities with a solidus (*/*) **not** brackets, *e.g.* λ/nm, $10^3(T/\mathrm{K})^{-1}$, 2θ/degrees. Symbols representing physical quantities should be given in italics, *e.g.* *t*/s, and units should be expressed in the form, *e.g.* g ml^{-1} rather than g/ml. Please note that % and ppm are ratios rather than units and should therefore be given in brackets.
(f) Extensive identifying lettering should be placed in the captions, rather than on the figures. Curves may be referred to by (a), (b), (c) *etc*. on the figure.

3.2.2 Structural Formulae.

(a) Structural formulae should be numbered with bold Arabic numerals, *e.g.* **1**, **2**.
(b) Please use the following organic ligand abbreviations: Et, Pr^n, Pr^i, Bu^n, Bu^i, Bu^s, Bu^t, Ph, CO_2H, CO_2R, R, R^1, R^2,. . .
(c) Structures and schemes can be submitted electronically. The settings for ChemDraw 3.5 are:

Drawing settings: chain angle 120°; bond spacing 20% of length; fixed length 0.43 cm; bold width 0.056 cm; line width 0.016 cm, margin width 0.044 cm, hash spacing 0.062 cm.

Text settings: font labels and atom labels should be in 7 pt Helvetica; fractional character widths should be enabled.

To facilitate the submission of structural formulae on disk, the preference files for ChemDraw 3.5 are available from the Society on a 3.5" Macintosh disk. To obtain a copy, please contact the Editorial Office at the Cambridge address. Structural formulae produced on ChemWindow and ISIS/Draw may also be submitted electronically. ChemWindow files should be saved as ChemDraw (<*filename*>.CHM) and ISIS/Draw exported as <*filename*>.TGF

3.2.3 Colour. Colour figures or computer-prepared artwork are encouraged.

(a) Avoid tints or shading and if possible use only the following colours (other colours may not reproduce well):
100% magenta
100% cyan
100% magenta + 100% process yellow (to give red)
100% cyan + 100% process yellow (to give green)
(b) Reproduction of colour figures is best from computer generated artwork which should be saved as TIFF or EPS files at = 600 dpi resolution.

3.3 Nomenclature

Current IUPAC nomenclature and symbolism should be used. Attention is drawn to the following publications in which the rules themselves and guidance on their use are given:

Nomenclature of Inorganic Chemistry, Blackwell Scientific Publications, Oxford, 1990.

Nomenclature of Organic Chemistry, Pergamon, Oxford, 1979.

A Guide to IUPAC Nomenclature of Organic Compounds, Blackwell Scientific Publications, Oxford, 1993.

3.3.1 Units and Symbols. The recommendations of IUPAC should be followed. Their basis is the Système Internationale d'Unités (SI). A detailed treatment is given in the so-called Green Book: *Quantities, Units and Symbols in Physical Chemistry*, Blackwell Scientific Publications, Oxford, 1993.

3.4 Deposition of Supplementary Data

Information (such as spectra, primary kinetic data, computer programs, and output, evidence for amino acid sequences, *etc*.), which accompanies papers may be deposited, free of charge, with the Society's Electronic Supplementary Information service (ESI), either at the request of the author and with the approval of the referees or on the recommendation of referees and with the approval of the author. The final decision, however, lies with the Editor.

Under this scheme, authors should submit articles and the supplementary material to the Journal simultaneously in the normal way, and both will be refereed. If the paper is accepted for publication, electronic supplementary material will be mounted on the RSC web server in an appropriate file format. The supplementary material will be available from the RSC web site at the internet address that will appear in the article.

3.4.1 Preparation and Submission of Material. Authors will be responsible for the preparation of the supplementary material. Electronic material should be supplied where possible in the following file types:

(a) Microsoft Word
(b) WordPerfect
(c) Crystallographic Information File (CIF)
(d) XYZ, MDL MOLFile (MOL) or Brookhaven Protein Databank (PDB) files
(e) JPEG/GIF (maximum size 640 480 pixels)

Authors must identify which manuscript the electronic file is associated with when they send the file to the Editorial Office by entering the name of the manuscript at the top of the electronic file. CIF files should be sent by e-mail or supplied as part of the file upload.

3.5 Guidelines on Submitting Files for Proof Preparation

Successful use of your electronic files should speed up the production process and avoid errors being introduced.

3.5.1 Uploaded Files.
(a) The electronic files for proof preparation (for formats see below) should be for the revised version of the manuscript. At this stage do **not** provide pdf files.
(b) Please supply the manuscript text (incorporating any revisions) and the graphics (for formats see below) as separate files, since these have to go through different production stages.

3.5.2 File Types.
(a) We prefer to receive Microsoft Word files, although we will endeavour to use other electronic versions wherever possible. For other word processors, also save the file as Rich Text Format (.RTF) if possible.
(b) *Graphics*. ChemDraw files (saved as *filename*.CDX) are preferred, but we can also accept ChemWindows (saved as filename.CHM) and ISIS/Draw (exported as *filename*.TGF).
(c) Please do not integrate your graphics files into the word processor document.

3.5.3 Text Details. Please supply the text file as unjustified, ranged left, and without end-of-line hyphenation. Auto-referencing features that bury references within the text should not be used.

3.5.4 Tables. Please include any tables at the end of the text file, and use either the word processor's table editor or tabs for formatting (but not a mixture of the two).

3.5.5 Graphics.
(a) Chemical structures as ChemDraw, ChemWindows and ISIS/Draw files submitted separately to the manuscript.
(b) Artwork (other than structures) as TIFF, EPS or pdf at 600 dpi or greater resolution.
(c) Please supply these separately to the word-processed file.

3.5.6 Consistency. Check the manuscript carefully for consistency, particularly in the representation of chemical formulae, compound names and words with alternative spellings.

We will try to use the supplied data in our production process, but mathematical equations and tables, in particular, may be re-keyed by the typesetter. Page proofs should still be checked closely.

4.0 Single Crystal X-Ray Crystallographic Data

The description of a crystallographic structure determination should be as brief as possible, consistent with the following guidelines, and should be included either at the end of the paper or at the end of the Experimental section. An expanded version of instructions for publication of crystallographic work can be found on the RSC web site (www.rsc.org/is/journals/authrefs/cryst.htm).

4.1 Title and Summary

For a paper reporting a crystallographic structure determination it is not essential to indicate this information in the title, *e.g*. by the words "crystal structure of". Lengthy titles quoting the formula of all the structures determined are strongly discouraged. Whether or not the crystal structure determination is indicated in the title, reference should be made to it in the summary. The summary should not normally contain cell dimensions and other crystal data, although these data may be included for extended solids.

4.2 Presentation of Crystal Data in the Manuscript

If the procedures for data collection and structure analysis were routine, their description should be particularly concise. When the analysis has not been of a routine nature, the authors should briefly detail the procedures used.

4.2.1 For Full Papers. The description may be given in textual or tabular form, although the latter is more appropriate if several structure determinations are being reported in one paper.

A table of selected *bond lengths* and *angles*, with estimated standard deviations, should be restricted to significant dimensions only (for example it is rarely necessary to include data for phenyl rings). Average values may be given (with a range of esds) for chemically equivalent groups or for similar bonds. Differences from expected norms should be noted.

4.2.2 For Communications. Details of the data collection and structure analysis should be given as a note in the Notes and references section.

Selected bond lengths and angles, with estimated standard deviations, should be included in the figure captions and be restricted to significant dimensions only.

4.2.3 Data Required for Presentation in the Manuscript. For both Full Papers and for Communications, the following information should be given in the manuscript:

(1) Chemical formula and formula weight (M).
(2) Crystal system.

(3) Unit-cell dimensions (Å or pm, degrees) and volume, with estimated standard deviations, temperature.
(4) Space group symbol (if non-standard setting give related standard setting).
(5) No. of formula units in unit cell (Z).
(6) Linear absorption coefficient (μ).
(7) Number of reflections measured and/or number of independent reflections and R_{int}.
(8) Final R values (and whether quoted for all or observed data).

For full papers, the description may be given in textual or tabular form, although the latter is more appropriate if several structure determinations are being reported in one paper. For Communications, details of the data collection and structure analysis should be given in a footnote or in the References/ Notes section.

Any tables of selected *bond lengths and angles*, with estimated standard deviations should be restricted to significant dimensions only (for example it is rarely necessary to include data for phenyl rings). Average values may be given (with a range of e.s.d.s) for chemically equivalent groups or for similar bonds. Differences from expected norms should be noted.

4.3 Supplementary Data Required for Assessment and/or Deposition

Authors should submit all supplementary crystallographic data as a Crystallographic Information File (CIF) file *via* file upload or crystengcomm@rsc.org. Authors should combine multiple data sets for a given manuscript into a single file. The individual structures in the combined file must be separated from each other by the sequence #=== END at the beginning of a line. Authors must identify which manuscript the electronic file is associated with when they send the file to the Editorial Office by entering the name of the manuscript at the top of the electronic file.

The information required for deposition includes:

(1) A table of final fractional atomic coordinates.
(2) Any calculated coordinates (*e.g.* hydrogen).
(3) A full list of bond lengths and angles with estimated standard deviations.
(4) A full list of displacement parameters in the form B_{ij} or U_{ij} (in Å^2 or pm^2).
(5) FULL details of the refinement.

A full checklist of data items required for deposition, together with full details for CIF submissions, is available by request from the editorial office or *via* the RSC web pages (http://www.rsc.org/is/journals/authrefs/cryst.htm).

The Cambridge Crystallographic Data Centre (CCDC) have a freely available programme which allows users to add RSC required information to cif files via a user-friendly graphical interface. Download EnCIFer for free at http://www.ccdc.cam.ac.uk/prods/encifer

The IUCR also have a free cif checking facility available at http://checkcif.iucr.org. Authors are encouraged to validate their cif files before submission.

Tables of *structure factors* (F_o, F_c) should not be sent, but copies should be retained by the authors so that they may be made available *via* the Editorial Office if requested.

4.3.1 Deposition of Material at the Cambridge Crystallographic Data Centre.. Supplementary crystallographic data will be deposited by the Society with the Cambridge Crystallographic Data Centre (CCDC) as part of the assessment process. Each structure will be assigned a separate CCDC number that will be quoted in the subsequent crystallographic report. Data will be held in the CCDC's confidential archive until publication of the article, when data for organic and metallo-organic compounds will be entered into the Cambridge Structural Database, and data for inorganic compounds will be forwarded to Fachinformationszentrum Karlsruhe for inclusion in the Inorganic Crystal Structure Database. Post-publication requests for individual data sets (organic or inorganic) should be directed to CCDC, 12 Union Road, Cambridge, UK CB2 1EZ (deposit@ccdc.cam.ac.uk; Fax: +44 (0)1223 336033).

If the article is not published by the RSC, supplementary crystallographic data will remain in the CCDC"s confidential archive. If the crystal structure(s) are subsequently published elsewhere, the CCDC Deposition Number(s) provided in the RSC crystallographic report should be quoted in that publication, and the CCDC advised of the new journal and the appropriate reference. Data will then enter the appropriate database as described above.

4.4 Reference to Crystallographic Work Published in a Preliminary Communication

It is permissible to regard a fully refined crystal structure determination published in a Communication as archival material. If an author does not wish to discuss the structure again at any length in the corresponding full paper, his purpose will be served by a simple reference back to the original communication, and need not re-present the associated data for publication or for the referees. However if these conditions are not fulfilled, the data should be re-presented *in full* and will be re-published if considered necessary.

4.5 Reference to Unpublished Crystallographic Work

There may be cases (other than that just described) when an author wishes to publish a paper in which the result of a crystal structure determination is discussed, but does not wish to include details or extensive discussion. The author may not even wish to include the crystallographer as co-author (for example when the determination is carried out by a commercial company). If the author is able to show the referees that this procedure is appropriate, it will be allowed provided that it does not lead to unnecessary fragmentation. However the author must provide, as supplementary information, sufficient data relating to the crystal structure determination to allow a referee to make sure that the point made is correct, and coordinates *etc*. will be deposited at the Cambridge Crystallographic Data Centre (or the Fachinformationszentrum Karlsruhe). The brief published description of the determination should be supplemented by appropriate reference to 'unpublished work'.

5.0 Multimedia

While not a requirement for publication, authors are encouraged to make the most of the latest technology to enhance the presentation of their work. These notes outline how this can be achieved, and also the formats preferred. Use of these formats will ensure that articles are published in the quickest time possible. All article information must be submitted electronically.

Some example figures, and a tutorial on how readers can get the most out of enhanced figures, are available at www.rsc.org/is/journals/current/e-only/tutorial3.htm

5.1 Spectra *etc.*

Certain software packages allow spectra, HPLC traces *etc.* from a spectrometer to be saved in the JCAMP-DX format. The file specifications for some of these packages are available free from the IUPAC Working Party on Spectroscopic Data Standards (JCAMP-DX) website (http://www.isas-dortmund.de/projects/jcamp/jcamp.htm).
Plots in JCAMP-DX format can then be displayed using the Chime™ plug-in and expanded and manipulated on screen. Providing JCAMP-DX files allows readers to save spectra for direct comparison with their spectra.

5.2 Movies

Authors are encouraged to include movies in their articles in those instances where a static image will not satisfactorily convey the information presented. Authors are requested to prepare their movies in a commonly used format, such as mpeg, or quicktime. Since movies tend to use a lot of memory, authors are requested to keep such presentations as small as possible, in order to reduce download times for readers. The appropriate file extension should be attached to each video file, for example *.qt* or *.mov* for quicktime, *.mpeg*, *etc*.

Acceptable file types include:

MPEG
Quicktime

5.3 Molecular Information

Authors presenting molecular coordinates from crystallographic or modelling studies in their submitted articles can benefit from presenting such results in Brookhaven protein databank (PDB), MDLI Molfile or xyz format. While coordinates provided by most crystallographers normally come in SHELX format, conversion of SHELX to PDB can be easily accomplished using SHELX93, Chem3D or Babel. The crystallographer, however, must ensure that all the molecular coordinates are written out (not just the unique asymmetric atoms), when the file is created.

Advice on the preparation of suitable files is available from the Editorial Office, and in some cases, the Editorial Office will be able to convert CIF files to 3D xyz files on behalf of the authors. Authors requesting this service should clearly state this in their submission letter (crystengcomm@rsc.org).

Acceptable file types include:

Brookhaven PDB
MDL MOL
XMOL XYZ
MDLSketch
RASMolScript
CSML

5.4 Three-Dimensional Images

3D images of, for example, results from molecular modelling or molecular orbital calculations can be displayed as 3D images, which allow readers to rotate, zoom in *etc*. to inspect the figures more closely. These figures can be viewed using the free Chime™ Plug-in, or Cosmoplayer, which are available from www.rsc.org/suppdata/plugin.htm

Acceptable file types include:
MOPACInput
GaussianInput
VRML