# Sample Paper Using the IUCr LaTeX Macro Package[1]

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This document describes how to obtain and use the *iucr* LaTeX macro package for submitting articles in LaTeX2$\varepsilon$ format to IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*).



## 1. Purpose

The International Union of Crystallography (IUCr) publishes a number of specialist scientific journals, many containing complex mathematics. The journal articles are held as electronic files for typesetting and electronic publication. The common format for the article files is SGML, an ISO standard that allows a specific structure to be defined for a class of documents through a machine-readable *document type definition* (DTD). Detailed markup of the article with SGML codes allows portions of the article to be indexed, hyperlinked or stored in databases. Mathematical formulae within the document are encoded in TeX (Knuth, 1984), a portable technical typesetting language.

Authors may submit papers to the IUCr in a variety of electronic formats, some more suitable than others for automated translation to SGML. A particularly suitable format is already widespread in many scientific disciplines, namely a structured dialect of TeX known as LaTeX (Lamport, 1986).

The IUCr has produced a macro package (*iucr*) that may be used by authors familiar with LaTeX version 2$\varepsilon$ to create articles that can easily be translated to SGML. This document describes how to use the package. It has been prepared using the package itself, and refers to some of its own contents to illustrate relevant points.

Full details of how to obtain the IUCr LaTeX macro package are given in Appendix A.

## 2. Structure of the paper

The following skeleton outline indicates the structure of a typical paper in LaTeX format; portions in parentheses are optional. A file **template.ltx** is available by ftp from the IUCr, and includes this structure with some additional material that is described below. Frequent reference will be made to this file (it will usually just be called 'the template'). Authors should acquire a copy of the template as the basis of their journal submission; it is possible, however, to construct a satisfactory paper from scratch by following the instructions in this document.

A copy of the template is included as Appendix D.

```
% ------ The front matter (heading section) ---
\documentclass{iucr}
\begin{document}

\title{...}
(\shorttitle{...})

  (\author...)
  \cauthor...
  \aff...

(\shortauthor{...})
(\vita{...})

\maketitle

\begin{synopsis}
...
\end{synopsis}

\begin{abstract}
...
\end{abstract}

% ------ The main body of the text ------------
\section{...}

   Text text text ...

   \subsection{...}

   Text text text ...

      \subsubsection{...}

   Text text text ...

\section{...}

   Text text text ...

% ------ The back matter ----------------------
(\appendix
```

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[1] Version 2

*Joe Soape is an archetypal generic author, whose association with the much-travelled Kilroy has extended over many years. He travels to work each day on a Clapham omnibus.*

*John Doe is also a generic individual with extensive experience of legal and forensic matters.*

```
   \section{...}

   Text text text ...
)

(\ack{...})

\begin{references}
   \reference{...}
\end{references}

\end{document}
```

## 3. Style of the paper

The same template is used for submitting papers of all types to all the IUCr journals. Different printing styles are used for different types of papers and across different journals, and the author should indicate the required style for the finished paper.

The article *must* begin with a line invoking the IUCr document class; the minimum required is

```
\documentclass{iucr}
```

to indicate that LaTeX should load and implement the macros for IUCr journal articles.

**The initial submission to a journal Coeditor should use the 'preprint' option** to produce a single-column double-spaced version suitable for examination and annotation by referees. This may be achieved by modifying the first statement in the file to

```
\documentclass[preprint]{iucr}
```

**The final version of the paper should then be prepared in the appropriate style**, and adjustments made to the layout of mathematical equations, tables, figure widths *etc.* to ensure that such components fit the journals' multi-column layout.

*Note, however, that the actual page layout of the journals is* ***not*** *performed using LaTeX; it is therefore not worth spending time trying to fit the figures and tables into a proper balanced page layout. Except when used in the preparation of camera-ready conference proceedings, the different page styles are used* ***only*** *to allow authors to break equations and establish suitable scaling factors for figures.*

If the paper is intended for publication in *Acta Crystallographica Section A* (*Acta A*) or *Journal of Applied Crystallography* (*JAC*), the `\documentclass` statement *may* include the option `a` (in square brackets). If the paper is a *Short Communication*, the additional option `short` is *required*.

If the paper is intended for publication in *Acta Crystallographica Section B* or *Acta Crystallographica Section D* (*Acta B*, *Acta D*), the `\documentclass` statement *must* include the option `d` (in square brackets). If the paper is a short contribution, such as a *Short Communication* or *Crystallization Paper*, the additional option `short` is required.

If the paper is intended for publication in *Journal of Synchrotron Radiation* (*JSR*), the `\documentclass` statement *must* include the option `s` (in square brackets). If the paper is a *Short Communication*, the additional option `short` is required.

| | |
|---|---|
| *Acta A, JAC* full article | `\documentclass{iucr}` |
| *Acta B, D* full article | `\documentclass[d]{iucr}` |
| *JSR* full article | `\documentclass[s]{iucr}` |
| *Acta A, JAC* short article | `\documentclass[short]{iucr}` |
| *Acta B, D* short article | `\documentclass[d,short]{iucr}` |
| *JSR* short article | `\documentclass[s,short]{iucr}` |

If a paper has been submitted as a camera-ready document for a conference proceedings issue of the journal, the option `conference` should be supplied, *e.g.*

| | |
|---|---|
| *JAC* conference paper | `\documentclass[conference]{iucr}` |
| *JSR* conference paper | `\documentclass[s,conference]{iucr}` |

For such papers, the submission instructions might also request that authors use the `nohead` option to remove the running headlines and footers (these will be added by the editorial office during the subsequent preparation for printing).

A full list of available package options is supplied as Appendix B.

## 4. The header of the paper

Information about the paper's title, its authors and their affiliations, and such descriptive portions of the paper as the *Abstract*, *Synopsis* (which appears as a brief description of the paper in the Table of Contents of an issue) or *keywords* is included in the *header* or *front matter* of the paper.

### 4.1. The document preamble

The template contains identifiers that encode bibliographic and production information about the document. The author may not know all the details that are required, but should fill in any information that is known, and leave the remaining default values for IUCr editorial staff to update.

The template includes a complete list of allowed article type codes.

```
\paperprodcode{a000000} % Production code
\paperref{xx9999}       % Editorial reference
\papertype{FA}          % Type of article
                        %   FA - Full article
                        %   SC - Short Comm.
\paperlang{english}     % Language
\journalcode{A}         % Which journal?
                        %   A - Acta Cryst. A
                        %   B - Acta Cryst. B
                        %   C - Acta Cryst. C
                        %   D - Acta Cryst. D
                        %   D - Acta Cryst. E
                        %   J - J. Appl. Cryst.
                        %   S - J. Synchr. Rad.
\journalyr{2000}
\journaliss{1}
\journalvol{56}
\journalfirstpage{000}
\journallastpage{000}
\journalreceived{0 XXXXXXX 0000}
\journalaccepted{0 XXXXXXX 0000}
\journalonline{0 XXXXXXX 0000}
```

The printout of the article's dates of receipt and acceptance and its online publication date can be suppressed by supplying the argument `\relax` to the last three commands.

### 4.2. The document proper

The body of the document is introduced with the line

```
\begin{document}
```

This must appear *after* the preamble, and *before* the title or any other content.

### 4.3. Title

Give the title of the paper as an argument to the macro `\title`. The title will usually be incorporated in a footer to the pages of the journal. Often the full title is too long to fit within the footer. If it is necessary to indicate a shorter form of the title for use in the footer, use the macro `\shorttitle`

```
\title{Sample Paper Using the IUCr \LaTeX{}
       Macro Package}
\shorttitle{IUCr \LaTeX{} sample}
```

If a title footnote is required, the `\footnote` macro should be invoked *inside* the argument to the `\title` macro, *e.g.*

```
\title{Sample Paper Using the IUCr \LaTeX{}
       Macro Package\footnote{Version 2}}
```

### 4.4. Author group

The list of the authors' names and addresses forms the *author group* of the paper. The macros `\cauthor`, `\author` (for names of correspondence and other authors respectively) and `\aff` (for *affiliations*) should be used. If the paper has a single author, the form of the entry will look like this:

```
\cauthor{J.}{Soape}{soap@bath.tub}{}
\aff{Baskerville Lodge, \city{Dartmoor}, Devon,
     \country{England}}
```

The author's given name(s) or initial(s) appear within the first set of curly braces, the surname (*i.e.* family name) in the second set. The third braces give the author's e-mail address, and the fourth the correspondence address (where this differs from the affiliation printed in the paper). **The third and fourth sets of braces must be present, even if they are empty.**

The associated address is given as the argument to the `\aff` macro. The country should be indicated by the `\country` macro; the city of residence *may* (but need not) be indicated by the `\city` macro. These are both included within the outer set of braces that delimit the argument of the `\aff` macro.

If there are multiple authors, the simpler `\author` macro is used for all but the correspondence author. A paper may have only *one* correspondence author. For example,

```
\author{J.}{Soape}
\author{A. N.}{Author}
\cauthor{John}{Doe}{doe@any.where}{}

\aff{Baskerville Lodge, \city{Dartmoor}, Devon,
     \country{England}}
```

Where there are multiple addresses, each author should be linked to a corresponding address by a small letter enclosed in square brackets immediately following the name of the relevant macro,

```
\author[a,b]{J.}{Soape}
\author[b]{A. N.}{Author}
\cauthor[a]{John}{Doe}{doe@any.where}{}

\aff[a]{Baskerville Lodge, \city{Dartmoor},
        Devon, \country{England}}
\aff[b]{3 Watery Way, \city{Full Fathom} 5,
        \country{Atlantis}}
```

Two other macros exist to modify an author's name; these should both appear *inside* the braces delimiting the surname. They are `\nee` to describe a married woman's original surname (*e.g.* `\author{J.}{Jackson \nee{Jones}}`, producing the text 'J. Jackson (*née* Jones)'), and `\jr` to indicate a dynastic relationship. The macro `\jr` by itself produces the text 'Jr'; with an argument *in square brackets* it produces the text provided, *e.g.* `\author{H. H.}{Hackenbusch\jr[III]}` produces the text 'H. H. Hackenbusch III'.

Footnotes associated with the authors' names *must* use the `\aufn` macro, which must follow the last mandatory argument of each occurrence of the `\author` or `\cauthor` macros:

```
\cauthor[a]{John}{Doe}{doe@any.where}{}\aufn{On
     leave from Institute of Advanced Research,
     Albany, Ruritania.}
```

### 4.5. Author biography

Occasionally a biographical note for an author or authors is required (usually for Lead Articles, Topical Reviews, or other invited contributions). The `\vita` macro is used to supply the required information; if there is more than one author, a line containing `\\` should separate the individual entries:

```
\vita{Joe Soape is an archetypal generic
      author, whose association with the
      much-travelled Kilroy has extended
      over many years. He travels to work
      each day on a Clapham omnibus.
\\
     John Doe is also a generic individual with
     extensive experience of legal and
     forensic matters.}
```

### 4.6. Other information

Some journals require other ancillary information to be conveyed in the article header. These may be supplied at this point in the document.

*Journal of Synchrotron Radiation* requires one or more key words or phrases for indexing purposes. These may be supplied with the macro `\keyword`, *e.g.*

```
\keyword{X-ray diffraction}
\keyword{muscle}
```

On rare occasions (especially for conference proceedings) an editor may request that keywords be printed in other journals. In such a case the document class line should be changed to include the `keywords` option, *e.g.*

```
\documentclass[a,keywords]{iucr}
```

Conversely, the `nokeywords` option may be used to suppress the output of the keywords terms in styles where they are printed by default.

*Acta Crystallographica Section D* requires reference codes for structures deposited in the Protein Data Bank. Use the macros `\PDBref` and `\NDBref`, *e.g.*

```
\PDBref[dethiobiotin synthetase]{1byi}
\NDBref[d(G$_4$CGC$_4$)]{ad0002}
```

### 4.7. maketitle

The command `\maketitle` should be included before the synopsis (or, if no synopsis is present, before the abstract). This command instructs LaTeX to output the authors and affiliations in the correct style. If it is not present, the information will in many cases nevertheless be output correctly; but several error messages may be generated by LaTeX.

### 4.8. Synopsis

All IUCr journals require the author to provide a brief synopsis of the paper, a couple of sentences in length, which is printed on the journal contents pages. There is a *synopsis* environment which should be used for this purpose:

```
\begin{synopsis}
Documentation of the IUCr \LaTeX{} macro
package and a demonstration of its
use in constructing a paper for an
IUCr journal.
\end{synopsis}
```

By default, the synopsis is printed only for the `preprint` option. If it is necessary for some reason to display the synopsis within other styles, the option `synopsis` may be added, *e.g.*

```
\documentclass[d,conference,synopsis,nohead]{iucr}
```

will print the synopsis at the end of an unornamented conference-style paper for *Acta Crystallographica Section D*. When printed, the synopsis appears on the LaTeX printout within parallel horizontal rules at the end of the document.

### 4.9. Abstract

The abstract of the paper should be given in the *abstract* environment,

```
\begin{abstract}
This document describes how to obtain and use
the \emph{iucr} \LaTeX{} macro package for
submitting articles in \LaTeX{}2$\varepsilon$
format to IUCr journals (\emph{Acta
Crystallographica, Journal of Applied
Crystallography, Journal of
Synchrotron Radiation}).
\end{abstract}
```

The abstract must always be a single paragraph. It may *not* contain footnotes.

## 5. The main body of the paper

The main body of the paper has a relatively simple structure; it consists of a sequence of sections, which may contain subsections or subsubsections. It may also include appendices (introduced by the `\appendix` command) which themselves contain sections or sub- and subsubsections. (Details of how to mark up appendices are included as Appendix C.)

The sectional elements of the paper contain the text, broken into paragraphs that are separated in the LaTeX source by blank lines. The text may include mathematics (discussed in a separate section below), figures and tables.

### 5.1. A note on single- and double-column formats

The current template uses the *multicol* package to permit double-column typesetting in the style of the IUCr journals. The main purpose of this is to ensure that the author knows where long mathematical formulae should be broken in order to fit into the journal column widths.

It may occasionally be necessary to switch off double-column setting (or to restrict it to certain portions of an article that relies heavily on long mathematical formulae or wide tables that cannot conveniently be fitted into a single column of the journal).

Within the body of the paper, double-column setting is switched off by the statement

```
\onecolumn
```

and may be re-invoked by the declaration

```
\twocolumn
```

In short contributions to some sections of *Acta Crystallographica* three-column setting is used. The macro `\threecolumn` is also available for switching explicitly to such a mode.

The present version of the *multicol* package does not permit figures, tables or other 'floats' within the multi-column portion of the article; this is partly the reason why figures and tables should be inserted at the end of the article (see later).

### 5.2. Sectioning

The text may contain sections nested to a depth of 3, *i.e.* sections, subsections and subsubsections, introduced respectively by the macros `\section`, `\subsection` and `\subsubsection`. The title of the section should follow as an argument to the sectioning command. **N.B. Please leave a blank line above and below these commands in the source file.**

```
\subsection{Sectioning}

The text may contain sections nested to a depth
of 3, \emph{i.e.} sections, subsections
```

Please employ the usual LaTeX convention of leaving one or more blank lines to indicate paragraph breaks. However, displayed equations and embedded figures should *not* be placed in separate paragraphs. If it is desired to include some visual white space in the LaTeX source file (and it can certainly be helpful to lay out complex mathematics neatly and clearly to permit later editing), lines containing only a % symbol (the LaTeX comment code) may be used for visual punctuation, *e.g.*

```
as seen in the equation
%
\begin{equation}
     x^n + y^n = z^n
\end{equation
%
and discussed elsewhere...
```

### 5.3. Changes of typeface

Within the body of the text, portions of italic or bold-face type may be indicated by the *textit* and **textbf** macros. The material to be typeset in a different face should be passed as the argument to these macros, and *not*, as is sometimes done, included within an open macro declaration inside braces; *i.e.* use

```
\textbf{bold-face type}
```

and **not**

```
{\textbf bold-face type}
```

However, in keeping with the spirit of LaTeX, it is generally better style to use the `\emph` macro to highlight text that is to be emphasised, rather than using specific font commands such as `\textit`.

### 5.4. Footnotes

The use of footnotes in the main body of the paper is discouraged, but where their use is unavoidable they may normally be handled with the standard LaTeX `\footnote` macro. This will produce footnotes across the full width of the page, with automatic numbering.

Exceptionally, however (specifically where camera-ready documents are to be prepared strictly in the style of the journals), manual placement of footnotes is possible[2].

The macro `\fnmark` is used to indicate the location in the text of the current footnote marker. Footnotes are numbered in sequence through an article. If it is necessary to over-ride the automatic number generation, an optional argument (in square brackets) may be supplied. The `\fnmark` macro does not print a space after the footnote marker, so when used in the body of a sentence will often be followed by an empty pair of braces to ensure that a space is printed,

```
The use of a footnote marker\fname{} causes a
superscript numeral to be printed; the numbers
are auto-incremented. Very occasionally\fname[3],
a specific number needs to be given in square
brackets.
```

The actual text of the footnotes is given as an argument to the `\fntext` macro. Although the footnote numbers are automatically tracked by the `\fnmark` macro, the number associated with each footnote *must* be given in square brackets as the first argument to the `\fntext` macro. If the number is omitted, the footnote will be printed without a number.

The user must collect together footnotes handled in this way at the relevant location in the text so that they will be printed at the foot of the first or second column, as required. The macro `\footnotes`, immediately preceding the first `\fntext` macro of a group, will print the separator rule (horizontal line).

It is the responsibility of the user to ensure that paragraphs that need to be broken to allow placement of the footnotes are correctly formatted. An example of how to do this with the `\breakpar` and `\noindent` commands is shown in the example.

[2] The default placement of footnotes across the full page width is a shortcoming of the way in which floats are handled by the *multicol* package. Use of the macros described here allows manual placement in either column.

```
... may be necessary to break a paragraph
\breakpar

\footnotes
\fntext[1]{Note the use of empty braces after a call
          to the fnmark macro to ensure that a
          space is printed.}
\fntext[3]{When the normal numbering is overridden
          by the use of an optional argument to
          fnmark, one must remember to change the
          footnote text numbering accordingly.}

\noindent
to allow placement of the footnotes.
```

## 6. Mathematics

The standard LaTeX conventions for typesetting mathematics should be employed. In-line equations are delimited by the `\(` and `\)` constructs, so that an equation embedded within running text such as `\(x^n+y^n=z^n\)` would print as $x^n+y^n=z^n$. Displayed equations without numbering are obtained with the `\[` and `\]` constructs, *e.g.*

```
\[ x = -b \pm \frac{\sqrt{b^2-4ac}}{2a} \]
```

displays as

$$x = -b \pm \frac{\sqrt{b^2-4ac}}{2a}$$

Numbered display equations are obtained with the *equation* environment,

```
\begin{equation}
x = -b \pm \frac{\sqrt{b^2-4ac}}{2a}
\end{equation}
```

yielding

$$x = -b \pm \frac{\sqrt{b^2-4ac}}{2a} \tag{1}$$

## 7. Acknowledgements and references

### 7.1. Acknowledgements

The acknowledgements should appear in a single paragraph as argument to the `\ack` macro:

```
\ack{The assistance and knowledge of \TeX{},
     \LaTeX{} and SGML of many members of the
     IUCr editorial staff are acknowledged.}
```

### 7.2. References

Reference lists may be built up in two ways: manually, or with the assistance of the BibTeX program and associated bibliographic database files.

**7.2.1. Plain citations** If bibliographic references are being handled manually, they should be cited in the text using the Harvard system which employs the surname of the author and year of publication. Parenthetic allusions (Parthé & Gelato, 1984) may be made by including the authors' names and the date of publication within parentheses; direct textual references normally have the date in parentheses, as in this reference to the work of Rauch (1976).

The reference list is then built up by establishing a *references* environment, and placing each cited work within a `\reference` entry:

```
\begin{references}
\reference{Parth\'e, E. \& Gelato, L. (1984).
   \emph{Acta Cryst.} A\textbf{40}, 169--183.}
\reference{Rauch, H. \& Petrascheck, D. (1976).
   \emph{Grundlagen f\"ur ein
   Laue-Neutroneninterferometer Teil 1:
   Dynamische Beugung.} Report AIAU 74405b.
   Atominstitut der \"Osterreichischen
   Universit\"aten, Austria.}
\end{references}
```

**7.2.2. Using BibTEX** The BibTEX program package may be used to handle citations and reference lists, such as to the seminal work of Pauling (1989) and other multi-author articles (Parthé & Gelato, 1984). The IUCr bibliography style file **iucr.bst** should be obtained and loaded in a public directory to obtain correctly-formatted reference lists and citations.

In this case the in-text citation is handled by the normal BibTEX conventions. Note in the following listing the use of the commands `\citeasnoun` and `\cite` to obtain citations that occur as part of the running text or as parenthetic insertions respectively.

```
The Bib\TeX{} program package may be used to
handle citations and reference lists, such
as to the seminal work of \citeasnoun{pauling89}
and other multi-author articles \cite{pargel84}.
```

The references section is invoked by placing the declaration

```
\referencelist[foo,bar]
```

just before the `\end{document}` statement. The `\referencelist` command takes a list of names of bibliographic databases as its argument in square brackets (in this example, the references would be found in either of the files **foo.bib** or **bar.bib** in the author's filesystem). **Any such bibliographic database files must accompany the submission.** If the `\referencelist` command is given without any argument, the bibliographic information is expected to be in a file called **iucr.bib**. Generation and formatting of the reference list itself is handled by BibTEX.

See Lamport (1986) for further information about BibTEX. An example of a sequence of LATEX/BibTEX runs necessary to generate the final version of this document is given in Appendix A.

## 8. Floating objects (tables and figures)

As mentioned previously, floats such as tables and figures are not handled properly within the double-column environment provided by the *multicol* package; they are also not yet automatically handled by the page make-up software in use at the Editorial offices. Therefore, tables and figures are best placed *after* the rest of the document.

An exception is made for papers solicited as camera-ready conference proceedings. In these cases, the author should manually place tables and figures within the text at the top or bottom of columns where possible; or between paragraphs if unavoidable.

### 8.1. Tables

Several LATEX styles exist for tables (because they are complicated objects that exist in a variety of styles). It is likely that the table translator will pose the greatest number of problems. Currently we recommend authors to use the *tabular* style for simple tables. Other table packages, such as *supertabular* or *longtable* may be used for complex tables at the author's discretion.

Authors should, however, be aware that it might be counterproductive for them to expend too much effort in producing LATEX tables that are visually attractive, since at a detailed level they may conflict with the layout requirements of the SGML version of the tables that will ultimately be produced.

**8.1.1. Simple tables using the *tabular* style** Table 1 shows a simple table set using the following code:

```
\begin{table}
\caption{Example table}
\begin{tabular}{llccrc}
     & Triplets &       &        & +ve  quartets
                                          &       \\
$E_3$& no.      & \%    & $E_4$ & no.    & \%    \\
\hline
6.0  &   21     & 100   & 6.0   &    185 & 100   \\
4.0  &  143     & 100   & 4.0   &   1213 & 100   \\
3.0  &  353     & 100   & 3.0   &   3295 & 100   \\
2.5  &  583     &  99.8 & 2.5   &   5813 &  99.8 \\
2.0  &  980     &  99.7 & 2.0   & 10,006 &  99.5 \\
1.5  & 1823     &  99.2 & 1.5   & 13,114 &  98.8 \\
1.0  & 3395     &  96.9 &       &        &       \\
\end{tabular}
\end{table}
```

In this example, the `{llccrc}` argument instructs the `tabular` environment to align material within the six tables of the columns against the left margin (`l`), centred (`c`), or aginst the right margin (`r`) of each table cell.

**Table 1**
Example table

| | Triplets | | | +ve quartets | |
|---|---|---|---|---|---|
| $E_3$ | no. | % | $E_4$ | no. | % |
| 6.0 | 21 | 100 | 6.0 | 185 | 100 |
| 4.0 | 143 | 100 | 4.0 | 1213 | 100 |
| 3.0 | 353 | 100 | 3.0 | 3295 | 100 |
| 2.5 | 583 | 99.8 | 2.5 | 5813 | 99.8 |
| 2.0 | 980 | 99.7 | 2.0 | 10,006 | 99.5 |
| 1.5 | 1823 | 99.2 | 1.5 | 13,114 | 98.8 |
| 1.0 | 3395 | 96.9 | | | |

### 8.2. Figures

Figures may be included using the following segment of code as an example:

```
\begin{figure}
\caption{Example of PostScript figure.}
\includegraphics{fig1}
\end{figure}
```

If no file extension is supplied, then the graphics driver routines available through LaTeX graphics packages (usually *dvips* or *pdflatex*) will search the current directory for files beginning with the name supplied and with extension suitable for the supported graphics file formats (*e.g.* .eps, .ps for *dvips*, .png, .jpg, .pdf for *pdflatex*). If figures in a supported format are not available, each figure caption should nevertheless be supplied in the form above. (That is, set up a *figure* environment around each `\caption` entry.)

If the space that will be occupied by a figure is known, it is possible to reserve that space in the document by creating a dummy PostScript file that indicates the *bounding box* of the figure. Fig.1 indicates the reference points at the lower-left and upper-right corners of a rectangular box that is said to *bound* the figure. The $x$, $y$ coordinates of these reference points (measured in *points* or units of $\frac{1}{72}$ of an inch) are specified in a PostScript `%%BoundingBox` directive. In other words, if the PostScript figure reproduced here as Fig. 1 were unavailable, a file fig1.ps containing the two lines

```
%!
%%BoundingBox: 0 0 120 200
```

could be constructed to reserve the appropriate space for later insertion of the figure (the line containing `%!` is an obligatory header for PostScript files).

If it is necessary to scale a figure to fit into the available space, the command `\scalebox` may be used as in this example (to scale by 80%):

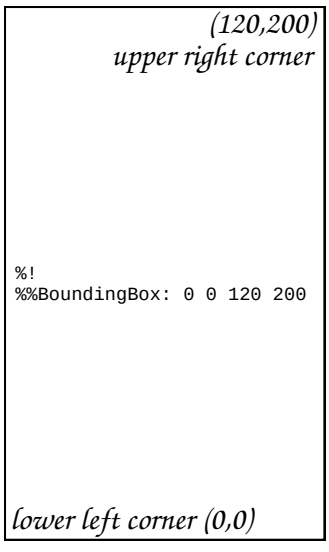


**Figure 1**
Example of PostScript figure.

```
\scalebox{.8}{\includegraphics{fig1}}
```

Note how the `\includegraphics` command is enclosed in braces.

**8.2.1. Advanced handling of graphics** The handling of figures described above depends on the availability of the LaTeX *graphics* package. More sophisticated graphics handling is possible if the *graphicx* package is available. To use *graphicx* in place of *graphics*, the following line should be added to the preamble of the document, just after the `\documentclass{iucr}` line:

```
\RequirePackage{graphicx}
```

Then rotation of a figure through a right angle (for example) could be accomplished with the command

```
\includegraphics[angle=90]{fig1}
```

See local documentation of the *graphicx* package for further information.

## 9. Conference abstracts

From time to time the IUCr publishes abstracts of Conference proceedings as supplements to its journals. A conference abstract may be submitted in a suitable format by using the `abstract` option to the `\documentclass` statement, *i.e.*

```
\documentclass[abstract]{iucr}
```

For a conference abstract, only the following components are required: a title (using the `\title` macro); the author names and affiliations as described in Section 4.4; keywords (Section 4.6 – note that for Conference abstracts the `keyword` option is *not* required in the `\documentclass` line); the body of the abstract within an *abstract* environment; and a reference list constructed as plain citations (Section 7.2.1). For Conference abstracts *only*, references should be indicated by numbers in square brackets, [1], [2], *etc.*, in the text. Numbering is generated automatically within the reference list.

Figures and tables may also be used sparingly in Conference abstracts. They are treated in the same way as other document types, and should be positioned at the appropriate locations within the body of the abstract.

A distinct template for Conference abstracts is available as the file **abstemplate.ltx** (see Appendix A for availability). A sample Conference abstract is included as Appendix E.

## 10. Miscellaneous notes

### 10.1. Changed font encoding

A LaTeX warning similar to the following may appear when modes other than the *preprint* mode are used:

```
LaTeX Font Warning: Encoding `OML' has changed to
(Font)              `OT1' for symbol font `letters'
                    in the math version `bold' on
                    input line 485.
```

This is harmless (indicating some internal font manipulations) and may be ignored.

### 10.2. Fonts unavailable

The journal styles use the LaTeX new font selection scheme and attempt to use PostScript fonts in the Times, Helvetica and Palatino families where available. These are accessible to many LaTeX distributions. If they are not available, however, the *preprint* mode should nonetheless function satisfactorily using only the Computer Modern fonts that come as standard with the great majority of TeX distributions.

Some authors may find that they have Times PostScript fonts available, but not Palatino, which is used in several of the article styles. In this case they may add the `nopalatino` option to their `\documentclass` declaration.

Authors with access to Optima PostScript fonts may use the `optima` option with the `\documentclass` declaration to produce a result identical to that obtained in the editorial/production office. For copyright reasons, these fonts are not freely distributable.

### 10.3. Underfull and overfull boxes

LaTeX will report underfull and overfull boxes (corresponding to text which does not properly fill the contents of a line or page). While these messages can indicate real problems and should be investigated, it must be remembered that the journal pages will not be typeset using LaTeX, and it is therefore a waste of time to try to eliminate all such warnings.

### 10.4. Direct creation of PDF

The option `pdf` in the documentclass invocation will allow the file to be processed by the pdfLaTeX command where available, so producing an output file in Adobe Portable Document Format (PDF). In such a case, the author should include figures in PDF rather than PostScript format. Details of the pdfLaTeX package are available from http://tug.org/applications/pdftex.

### 10.5. Improvements to the class file

Reports of bugs and suggestions for improvements to the class file are welcome, and should be addressed to Brian McMahon at the IUCr (bm@iucr.org).

## Appendix A
## Obtaining the IUCr LaTeX package

The LaTeX package may be obtained by anonymous ftp from the IUCr server **ftp.iucr.org**. Login as user *anonymous* and supply your email address as password. Change to the templates/latex directory. Transfer in text mode the following files (only the first two are essential for the use of the package):

**iucr.cls**, the class file containing all the macros detailed in this document;

**template.ltx**, the skeleton template file used to construct a submission;

**abstemplate.ltx**, the template file used for Conference abstracts *only*;

**documentation.ltx**, this document;

**fig1.ps**, the PostScript figure included in this document as an example;

**iucr.bib**, a BibTeX bibliography file for this document;

**iucr.bst**, the IUCr BibTeX style file.

Test your ability to run LaTeX on this file. A *complete* processing run will involve three passes of the LaTeX program and one of BibTeX; on a typical Unix workstation, the processing run will usually require the commands

```
% latex documentation.ltx
% bibtex documentation
% latex documentation.ltx
% latex documentation.ltx
```

If successful you should be able to preview the documentation on screen (*e.g.* with the Unix *xdvi* program) or print it (*e.g.* with Unix *dvips*).

If the tests are successful, the package file **iucr.cls** should be installed in a public class directory (the location of which will be system dependent) or copied into any directory containing files which are processed with the *iucr* package.

### A.1. Compatibility

The *iucr* package has been designed for LaTeX2$\varepsilon$ and will only work with that format. The development version of LaTeX was `LaTeX2e <1998/12/01> patch level 1` as distributed on the TeX User Group TeXLive4 CD-ROM (see http://www.tug.org/texlive/ for details).

### A.2. Ancillary packages

The *iucr* macros also use a number of public packages that are distributed with LaTeX (*e.g. nfss, multicol, dvips, float, harvard, tabularx*). If these are not available on your system, they may be found in the **utilities** subdirectory of the ftp directory indicated above. If a required package is not available at your site or in the **templates/latex/utilities** subdirectory, please send an email to **bm@iucr.org** for assistance.

## Appendix B
## Complete list of package options

The table below summarises the options available to modify the behaviour of the *iucr* package. All those relevant to the current journal article styles have been discussed in the body of the current article.

In general, one may select a single page style and concatenate other options in a comma-separated list. Where mutually exclusive options are listed, precedence is assigned based on the order of definitions within the class file, and so is not predictable.

The *vanilla* style provides a two-column style with typography similar to that used in *Acta Crystallographica* but without a number of the journal-specific features. The *it* style is for use by authors of chapters of *International Tables for Crystallography*. The *o* and *x* styles recreate an earlier page layout of the journals and are retained purely for historical interest.

**Table 2**
One or more of the options listed below may be added in square brackets to the declaration of the document class.

| | |
|---|---|
| *Journal styles* | |
| (no options) | *Acta A*/*JAC* full article (default) |
| `a` | *Acta A*/*JAC* |
| `c` | *Acta C* |
| `d` | *Acta B*/*Acta D* |
| `e` | *Acta E* |
| `s` | *JSR* |
| *Article styles* | |
| `full` | full article (default) |
| `short` | short communication |
| `conference` | conference paper |
| *Other styles* | |
| `preprint` | preprint (1 col., wide-spaced) |
| `it` | International Tables chapter |
| `abstract` | Conference abstracts |
| `vanilla` | vanilla (general) style |
| `o` | old *Acta A*/*JAC* |
| `x` | old *JSR* |
| *Special directives* | |
| `nohead` | do not print page header/footer |
| `keywords` | print keywords (default for *JSR* and conference abstracts) |
| `nokeywords` | do not print keywords |
| `synopsis` | print synopsis (default in preprint) |
| `nosynopsis` | do not print synopsis |
| `pdf` | allow processing with pdflatex |
| *Font selections* | |
| `optima` | use Optima fonts |
| `nopalatino` | do not use Palatino fonts |

## Appendix C
## Marking up appendices

### C.1. Placement

Appendices are regarded in the IUCr DTD as an integral part of the *body matter* of the paper, unlike in many other DTDs, including the ISO 12083 standard for scientific articles, where they are deemed to be part of the *back matter*. This means that they are inserted *before* the acknowledgements section.

### C.2. Invocation

The appendices form the last portion of the body matter, and are introduced by a single declaration of the form

```
\appendix
```

Thereafter, each appendix should be considered as a new section, and may contain subsections and subsubsections, following the same structure as the main body of the text. Appendix headings are generated automatically, *e.g.*

```
\appendix
\section{Marking up appendices}

\subsection{Placement}

Appendices are regarded in the IUCr DTD...
```

## Appendix D.
## The template.ltx template file

Below is given a complete listing of the template file **template.ltx**. The article that you are now reading was constructed using version 1.2 of the template, and you may find it useful to examine its source code (it is available as the file **documentation.ltx** in the IUCr macro distribution package).

```
%-------------------------------------------------------------------------------
% Template file for the submission of papers to IUCr journals in LaTeX2e
% using the iucr document class
% Copyright 1999-2003 International Union of Crystallography
% Version 1.2 (11 December 2002)
%-------------------------------------------------------------------------------

\documentclass{iucr}              % DO NOT DELETE THIS LINE

     %-------------------------------------------------------------------------
     % Information about the type of paper
     %-------------------------------------------------------------------------
     \paperprodcode{a000000}      % Replace with production code if known
     \paperref{xx9999}            % Replace xx9999 with reference code if known
     \papertype{FA}               % Indicate type of article
                                  %   FA - research papers (full article)
                                  %   SC - short communications
                                  %   FC - fast communications
                                  %   LA - lead article
                                  %   TR - topical review
                                  %   XL - crystallization papers
                                  % (Following categories rarely in LaTeX)
```

```
                                %   AA - abstracts
                                %   AD - addenda and errata
                                %   AI - inorganic compounds
                                %   AM - metal-organic compounds
                                %   AO - organic compounds
                                %   BC - books received
                                %   BR - book reviews
                                %   BI - biography
                                %   CA - cif applications
                                %   CD - crystal data
                                %   CE - current events
                                %   CI - inorganic compounds
                                %   CL - calendar of events
                                %   CM - metal-organic compounds
                                %   CN - cryocrystallography papers
                                %   CO - organic compounds
                                %   CP - computer programs
                                %   CR - crystallographers
                                %   CS - scientific comment
                                %   ED - editorial
                                %   EI - inorganic compounds
                                %   EM - metal-organic compounds
                                %   EO - organic compounds
                                %   FI - inorganic compounds
                                %   FM - metal-organic compounds
                                %   FO - organic compounds
                                %   IP - issue preface
                                %   IU - iucr
                                %   LE - letters to the editor
                                %   LN - laboratory notes
                                %   ME - forthcoming meetings/short courses
                                %   MR - meeting reports
                                %   NN - notes and news
                                %   NP - new commercial products
                                %   OB - obituaries
                                %   PA - computer program abstracts
                                %   RI - reference information
                                %   SG - structural genomics papers
                                %   SI - short format inorganic compounds
                                %   SM - short format metal-organic compounds
                                %   SO - short format organic compounds
                                %   SP - short structural papers
                                %   SR - software reviews
                                %   TE - teaching and education

    \paperlang{english}         % Can be english, french, german or russian
    %-------------------------------------------------------------------------
    % Information about journal to which submitted
    %-------------------------------------------------------------------------
    \journalcode{A}             % Indicate the journal to which submitted
                                %   A - Acta Crystallographica Section A
                                %   B - Acta Crystallographica Section B
                                %   C - Acta Crystallographica Section C
                                %   D - Acta Crystallographica Section D
                                %   E - Acta Crystallographica Section E
                                %   J - Journal of Applied Crystallography
                                %   S - Journal of Synchrotron Radiation
        %-----------------------------------------------------------------------
        % The following entries will be changed as required by editorial staff
        %-----------------------------------------------------------------------
    \journalyr{2003}
    \journaliss{1}
    \journalvol{59}
    \journalfirstpage{000}
    \journallastpage{000}
    \journalreceived{0 XXXXXXX 0000}
    \journalaccepted{0 XXXXXXX 0000}
    \journalonline{0 XXXXXXX 0000}

\begin{document}                % DO NOT DELETE THIS LINE
```

```
     %-------------------------------------------------------------------------
     % The introductory (header) part of the paper
     %-------------------------------------------------------------------------

     % The title of the paper. Use \shorttitle to indicate an abbreviated title
     % for use in running heads (you will need to uncomment it).

\title{Title of Paper}
%\shorttitle{Short Title}

     % Authors' names and addresses. Use \cauthor for the main (contact) author.
     % Use \author for all other authors. Use \aff for authors' affiliations.
     % Use lower-case letters in square brackets to link authors to their
     % affiliations; if there is only one affiliation address, remove the [a].

\cauthor[a]{Forename}{Surname}{email}{address if different from \aff}
\author[b]{Forename}{Surname}

\aff[a]{First affiliation address \country{England}}
\aff[b]{Second affiliation address}

     % Use \shortauthor to indicate an abbreviated author list for use in
     % running heads (you will need to uncomment it).

%\shortauthor{Soape, Author and Doe}

     % Use \vita if required to give biographical details (for authors of
     % invited review papers only). Uncomment it.

%\vita{Author's biography}

     % Keywords (required for Journal of Synchrotron Radiation only)
     % Use the \keyword macro for each word or phrase, e.g.
     % \keyword{X-ray diffraction}\keyword{muscle}

%\keyword{keyword}

     % PDB and NDB reference codes for structures referenced in the article and
     % deposited with the Protein Data Bank and Nucleic Acids Database (Acta
     % Crystallographica Section D). Repeat for each separate structure e.g
     % \PDBref[dethiobiotin synthetase]{1byi} \NDBref[d(G$_4$CGC$_4$)]{ad0002}

%\PDBref[optional name]{refcode}
%\NDBref[optional name]{refcode}

\maketitle                        % DO NOT DELETE THIS LINE

\begin{synopsis}
Supply a synopsis of the paper for inclusion in the Table of Contents.
\end{synopsis}

\begin{abstract}
Abstract goes here.
\end{abstract}


     %-------------------------------------------------------------------------
     % The main body of the paper
     %-------------------------------------------------------------------------
     % Now enter the text of the document in multiple \section's, \subsection's
     % and \subsubsection's as required.

\section{Section title}

Text text text text text text text text text text text text text text
text text text text text text text.

\subsection{Title}

Text text text text text text text text text text text text text text
text text text text text text text.
```

```
\subsubsection{Title}

Text text text text text text text text text text text text text text
text text text text text text text.


     % Appendices appear after the main body of the text. They are prefixed by
     % a single \appendix declaration, and are then structured just like the
     % body text.

\appendix
\section{Appendix title}

Text text text text text text text text text text text text text text
text text text text text text text.

\subsection{Title}

Text text text text text text text text text text text text text text
text text text text text text text.

\subsubsection{Title}

Text text text text text text text text text text text text text text
text text text text text text text.


     %-----------------------------------------------------------------------
     % The back matter of the paper - acknowledgements and references
     %-----------------------------------------------------------------------

     % Acknowledgements come after the appendices

\ack{Acknowledgements}

     % References are at the end of the document, between \begin{references}
     % and \end{references} tags. Each reference is in a \reference entry.

\begin{references}
\reference{Author, A. \& Author, B. (1984). \emph{Journal} \textbf{Vol},
first page--last page.}
\end{references}

     %-----------------------------------------------------------------------
     % TABLES AND FIGURES SHOULD BE INSERTED AFTER THE MAIN BODY OF THE TEXT
     %-----------------------------------------------------------------------

     % Simple tables should use the tabular environment according to this
     % model

\begin{table}
\caption{Caption to table}
\begin{tabular}{llcr}      % Alignment for each cell: l=left, c=center, r=right
 HEADING    & FOR        & EACH       & COLUMN     \\
\hline
 entry      & entry      & entry      & entry      \\
 entry      & entry      & entry      & entry      \\
 entry      & entry      & entry      & entry      \\
\end{tabular}
\end{table}

     % Postscript figures can be included with multiple figure blocks

\begin{figure}
\caption{Caption describing figure.}
\includegraphics{fig1.ps}
\end{figure}

\end{document}                    % DO NOT DELETE THIS LINE
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

## Appendix E.
## Example of a Conference abstract

The example below demonstrates how a short Conference abstract may be presented using the `abstract` option in the `\documentclass` specification. Such abstracts are normally requested for camera-ready preparation of Conference proceedings volumes such as those produced for IUCr Congresses and other large international meetings.

```
%-------------------------------------------------------------------------------
% Template file for the submission of conference abstracts to IUCr journals
% in LaTeX2e using the iucr document class (iucr.cls version 2.0beta 13
% dated 2003/11/24 or later)
% Copyright 2003 International Union of Crystallography
% Version 1.0 (24 December 2003)
%-------------------------------------------------------------------------------

\documentclass[abstract]{iucr}              % DO NOT DELETE THIS LINE

\begin{document}                  % DO NOT DELETE THIS LINE

     %-------------------------------------------------------------------------
     % The introductory (header) part of the abstract
     %-------------------------------------------------------------------------

     % The title of the abstract.

\title{Example conference abstract}

     % Authors' names and addresses. Use \cauthor for the main (contact) author.
     % Use \author for all other authors. Use \aff for authors' affiliations.
     % Use lower-case letters in square brackets to link authors to their
     % affiliations; if there is only one affiliation address, remove the [a].

\cauthor{Brian}{McMahon}{bm@iucr.org}{}

\aff{IUCr, 5 Abbey Square, Chester CH1 2HU, \country{UK}}

     % Keywords. Use the \keyword macro for each word or phrase, e.g.
     % \keyword{X-ray diffraction}\keyword{muscle}

\keyword{\LaTeX}
\keyword{example}
\keyword{conference abstract style}

\maketitle                        % DO NOT DELETE THIS LINE

     %-------------------------------------------------------------------------
     % The main body of the abstract
     %-------------------------------------------------------------------------
\begin{abstract}
This is an example of a conference abstract, such as might be supplied to
an IUCr Congress[1]. It uses a subset of the macros and commands of the
\textit{iucr} macro class, as documented in the class user guide[2]. The
entire text of the abstract should be confined to a single column of
printed text, and preferably should be presented as a single paragraph of
text. References are indicated by bracketed numbers in the text; the
numbering in the reference list is autogenerated, and so the author must
take care to match the numbering correctly. Although discouraged, figures
and tables may be embedded within the abstract text where essential; for
brevity they are omitted from this example, but templates are provided in
the abstemplate.ltx file[3].
\end{abstract}

     %-------------------------------------------------------------------------
     % The back matter of the abstract - references
     %-------------------------------------------------------------------------
     % References are at the end of the document, between \begin{references}
     % and \end{references} tags. Each reference is in a \reference entry.

\begin{references}
```

```
\reference{International Union of Crystallography (2002). Abstracts of the
XIX IUCr Congress, Geneva, Switzerland, 6--15 August 2002. \textit{Acta Cryst.}
A\textbf{58} Suppl.}
\reference{International Union of Crystallography (2003). \textit{Sample
Paper Using the IUCr \LaTeX{} Macro Package}.
http://www.iucr.org/iucr-top/journals/latex/documentation.pdf}
\reference{International Union of Crystallography (2003). Template file for
  Conference abstracts using the iucr.cls \LaTeX{} style.
ftp://ftp.iucr.org/templates/latex/abstemplate.ltx}
\end{references}

\end{document}                    % DO NOT DELETE THIS LINE
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

The assistance and knowledge of TEX, LATEX and SGML of many members of the IUCr editorial staff are acknowledged. Thanks are due to Bruce Ravel, Julie Cross, Matt Newville, Klas Andersson, Phil Bentley, Loic Bertrand, Gunnar Thorkildsen, Chris Cousins, Thomas Proffen, Christian Anders Cumbaa and other users who provided valuable feedback during the development of the macros and associated templates.

## References

*(This block generated from the* references *environment, the other by BibTEX.)*

Parthé, E. & Gelato, L. (1984). *Acta Cryst.* A**40**, 169–183.

Rauch, H. & Petrascheck, D. (1976). *Grundlagen für ein Laue-Neutroneninterferometer Teil 1: Dynamische Beugung.* Report AIAU 74405b. Atominstitut der Österreichischen Universitäten, Austria.

## References

Knuth, D. E. (1984). *The TEXbook*. Addison-Wesley.

Lamport, L. (1986). *LATEX A Document Preparation System*. Addison-Wesley.

Parthé, E. & Gelato, L. (1984). *Acta Cryst.* A**40**, 169–183.

Pauling, L. (1989). *Proc. Natl Acad. Sci USA*, **86**, 8595–8599.

Rauch, H. & Petrascheck, D. (1976). *Grundlagen für ein Laue-Neutroneninterferometer Teil 1: Dynamische Beugung*. Report AIAU 74405b. Atominstitut der Österreichischen Universitäten, Austria.