

1.1. Sample *International Tables* Chapter Using the IUCr L^AT_EX Macro Package¹

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Abstract

This document describes how to obtain and use the *iucr* L^AT_EX macro package for submitting chapters in L^AT_EX2 ϵ format to the IUCr *International Tables for Crystallography* series.

Keywords: L^AT_EX; class file; documentation; *International Tables for Crystallography*.

1.1.1. Purpose

The International Union of Crystallography (IUCr) publishes a respected series of reference volumes, known as the *International Tables for Crystallography*, containing complex mathematics and extensive tables. The chapters are held as electronic files for typesetting, electronic publication, and as source for subsequent revisions. The common format for the 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 material to be indexed, hyperlinked or stored in databases. Mathematical formulae within the document are encoded in T_EX (Knuth, 1984), a portable technical typesetting language.

Contributing authors may submit chapters 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 T_EX known as L^AT_EX (Lamport, 1986).

The IUCr has produced a macro package (*iucr*) that may be used by authors familiar with L^AT_EX version 2 ϵ to create chapters 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 L^AT_EX macro package are given in Appendix A.

1.1.2. Structure of the chapter

The following skeleton outline indicates the structure of a typical chapter in L^AT_EX 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 submission; it is possible, however, to construct a satisfactory chapter from scratch by following the instructions in this document.

A copy of the template is included as Appendix C.

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

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

```
\author...
\author...

(\shortauthor{...})

(\keyword{keyword1}\keyword{keyword2} ...)

\maketitle

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

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

Text text text ...

\subsection{...}

Text text text ...

\subsubsection{...}

Text text text ...

\sectioniv{...}

Text text text ...

\sectionv{...}

Text text text ...

\section{...}

Text text text ...

% ----- The back matter -----
(\appendix
\section{...}

Text text text ...
)

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

\end{document}
```

1.1.3. Style of the chapter

The same class file is used for submitting chapters of *International Tables for Crystallography* as is used for submitting articles to the

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IUCr journals. Different printing styles are used in the *Tables* and journals, and the author *must* indicate the required style by starting the chapter with the line

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

to indicate that L^AT_EX should load and implement the *International Tables*-specific macros for IUCr publications.

Normally an author will provide keywords and an abstract for the chapter. If these are present, but for some reason it is desired not to print them, the file should start instead with the line

```
\documentclass[it,itnoabstract]{iucr}
```

The normal submission format uses a small page size to accommodate marginal annotations on US letter or A4 printouts. If it is desired to print at the full size of an *International Tables* volume (e.g. as directed by the Editorial Office or to test lay out complex multi-line equations in final form), the *fullsize* option may be used:

```
\documentclass[it,fullsize]{iucr}
```

If the part and chapter number of the contribution are known, they should be supplied using the `\part` and `\chapter` macros. If known, the title of the part should also be supplied using the macro `\parttitle`; this is printed as a running head on left-hand pages.

```
\part{1}
\parttitle{Submissions to \emph{International Tables}}
\chapter{1}
```

The beginning of the chapter is then indicated with the line

```
\begin{document}
```

1.1.4. The heading of the chapter

Information about the chapter's title and authors is included in the *header* or *front matter* of the chapter.

1.1.4.1. Title

Give the title of the chapter as an argument to the macro `\title`. The title will usually be printed as a running head on right-hand pages of the journal. Sometimes the full title is too long to fit as a running head (which normally has fewer than 60 characters). If it is necessary to indicate a shorter form of the title for use as a running head, use the macro `\shorttitle`.

```
\title{Sample \emph{International Tables} Chapter
Using the IUCr \LaTeX{} Macro Package}
\shorttitle{IUCr \LaTeX{} sample for \emph{IT}}
```

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

```
\title{Sample \emph{International Tables} Chapter
Using the IUCr \LaTeX{} Macro
Package\footnote{Version 2.1.10}}
```

1.1.4.2. Author group

The list of authors' names forms the *author group* of the chapter. The macro `\author` should be used:

```
\author{J.}{Soape}
\author{A. N.}{Author
```

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.

Two macros exist to modify an author's name: these should

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 argument of the `\author` macro:

```
\author{John}{Doe}\aufn{Deceased.}
```

1.1.4.3. maketitle

The command `\maketitle` should be included before the first section of text. This command instructs L^AT_EX to output the authors in the correct style. If it is not present, the information will in most cases be output correctly; but error messages may be generated by L^AT_EX.

1.1.5. The main body of the chapter

The main body of the chapter 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.

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

1.1.5.1. A note on single- and double-column formats

The current template uses the *multicol* package to permit double-column typesetting.

It may occasionally be necessary to switch off double-column setting (e.g. if there are portions of the chapter that rely heavily on long mathematical formulae or wide tables that cannot conveniently be fitted into a single column).

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

```
\onecolumn
```

and may be re-invoked by the declaration

```
\twocolumn
```

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

1.1.5.2. Sectioning

The text may contain sections nested to a depth of 5, *i.e.* sections, subsections, subsubsections, and 4th- and 5th-level section, introduced respectively by the macros `\section`, `\subsection`, `\subsubsection`, `\sectioniv` and `\sectionv`. 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}
```

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Please employ the usual L^AT_EX 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 L^AT_EX 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 L^AT_EX 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...
```

1.1.5.3. 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 L^AT_EX, 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`.

1.1.5.4. Computer listings

One specific change of typeface is the use of a fixed-pitch typewriter-style font to indicate verbatim output from a computer program or file. Short pieces of in-line verbatim text should be marked with the macro `\verb`. This differs from most L^AT_EX macros in that the argument should *not* be enclosed in matching braces or square brackets (`{}`, `[]`), but should instead be delimited by a repetition of the *same* arbitrary character – any character may be chosen provided it does not itself occur within the verbatim text. A good choice is the double-quote mark `"`: `\verb"verbatim text"`

Longer (multi-line) listings should be described in the *verbatim* environment:

```
\begin{verbatim}
\subsection{Computer listings}
```

```
One specific change of typeface is the use of
a fixed-pitch typewriter-style font to indicate
verbatim output from a computer program or file.
Short pieces of in-line verbatim text should be
marked with the macro \verb"\verb". This
\end{verbatim}
```

1.1.5.5. Footnotes

The use of footnotes in the main body of the chapter is discouraged, but where their use is unavoidable they may normally be handled with the standard L^AT_EX `\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), man-

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.

```
... 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.
```

In some Volumes of the *International Tables* series, authors' affiliations are given in the form of an unnumbered footnote in the first column of the opening page of a chapter. These may be handled by using `\fntext` *without* a numerical argument. Alternatively, the custom *affiliationnote* environment may be used.

```
\begin{affiliationnote}
J. Soape, Baskerville Lodge, Dartmoor, Devon, England;
A. N. Author, 3 Watery Way, Full Fathom 5, Atlantis.
\end{affiliationnote}
```

1.1.6. Mathematics

The standard L^AT_EX 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.*

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Table 1.1.8.1. *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			

1.1.8.2. Figures

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

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

If PostScript figures 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%):

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

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

Some special commands are available for typesetting extracts from Crystallographic Information Files (CIFs) and for describing entries in CIF dictionaries.

A CIF data name such as `_cell_length_a` is typeset with the command `\cifname{_cell_length_a}`. A listing as extracted from a CIF may be placed in a *ciflisting* environment:

```
\begin{ciflisting}
_cell_length_a          10.452(3)
_cell_length_b          11.664(4)
_cell_length_c          15.641(4)
_cell_angle_alpha       94.37(2)
_cell_angle_beta        89.75(2)
_cell_angle_gamma       111.87(2)
\end{ciflisting}
```

produces

```
_cell_length_a          10.452(3)
_cell_length_b          11.664(4)
_cell_length_c          15.641(4)
_cell_angle_alpha       94.37(2)
_cell_angle_beta        89.75(2)
_cell_angle_gamma       111.87(2)
```

A CIF dictionary entry is handled within the *cifdefblock* or *boxedcifdefblock* environments (the latter encloses the definition in a box). The entry should be formatted in the style of the CIF dictionaries produced by the IUCr *ciftex* program and published *e.g.* in the CIF specification paper of Hall, Allen & Brown [*Acta Cryst.* (1991), **A45**, 655–685]. Here is an example, showing the macros available for the purpose:

```
\begin{boxedcifdefblock}
\cifname{_atom_site_attached_hydrogens}
\ciftype{numb}
\cifdefinition{The number of hydrogen atoms
attached to the atom at this site excluding
any H atoms for which coordinates (measured
or calculated) are given.}
%
\cifattributes{Appears in list containing
\cifname{_atom_site_label}. Where no value
is given, the assumed value is '0'. The
permitted range is 0  $\rightarrow$  4.}
%
\cifexamples{Example(s): '2' (water oxygen),
'1' (hydroxyl oxygen), '4' (ammonium nitrogen).}
%
\cifcat{atom_site}
\end{boxedcifdefblock}
```

which produces

<code><i>_atom_site_attached_hydrogens</i></code>	<i>(numb)</i>
The number of hydrogen atoms attached to the atom at this site excluding any H atoms for which coordinates (measured or calculated) are given.	
Appears in list containing <code><i>_atom_site_label</i></code> . Where no value is given, the assumed value is '0'. The permitted range is 0 \rightarrow 4.	
Example(s): '2' (water oxygen), '1' (hydroxyl oxygen), '4' (ammonium nitrogen).	
	<code>[<i>atom_site</i>]</code>

.1.9 Appendix 1.1.1

Obtaining the IUCr L^AT_EX package

The L^AT_EX 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/it` 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

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

itdocumentation.ltx, this document;

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

iucr.bib, a Bib_TE_X bibliography file for this document;

iucrit.bst, the IUCr Bib_TE_X style file for *International Tables*.

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

```
% latex itdocumentation.ltx
% bibtex itdocumentation
% latex itdocumentation.ltx
% latex itdocumentation.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.

A1.1.1.1. *Compatibility*

The *iucr* package has been designed for L^AT_EX_{2 ϵ} and will only work with that format. The development version of L^AT_EX was LaTeX2e <1998/12/01> patch level 1 as distributed on the T_EX User Group T_EXLive4 CD-ROM (see <http://www.tug.org/texlive/> for details).

A1.1.1.2. *Ancillary packages*

The *iucr* macros also use a number of public packages that are distributed with L^AT_EX (*e.g.* *nfss*, *multicol*, *dvips*, *float*, *harvard*, *tabularx*). If these are not available on your system, they may be found in the **templates/latex/utilities** subdirectory of the ftp server 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 1.1.2 Marking up appendices

A1.1.2.1. *Placement*

Appendices are regarded in the IUCr DTD as an integral part of the *body matter* of the chapter, 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.

A1.1.2.2. *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 1.1.3 The **ittemplate.ltx** template file

Below is given a complete listing of the template file **ittemplate.ltx**. The article that you are now reading was constructed using version 0.6 of the template, and you may find it useful to examine its source code (it is available as the file **itdocumentation.ltx** in the IUCr macro distribution package).

```
%-----
% Template file for the submission of chapters to the IUCr series
% International Tables for Crystallography in LaTeX2e
% using the iucr document class
% Copyright 1998=2016 International Union of Crystallography
% Version 0.6 (14 January 2016)
%-----

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

%-----
% Information about the part and chapter number
%-----
\part{1}                          % Replace with part number if known
\parttitle{PART TITLE}           % Replace with part title if known
\chapter{1}                       % Replace with chapter number if known

\begin{document}                 % DO NOT DELETE THIS LINE

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

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

\title{Title of chapter}
%\shorttitle{Short Title}
```

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```
% Use \author for all authors' names.

\author{Forename}{Surname}
\author{F.}{Family Name}

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

%\shortauthor{Soape and Author}

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

\keyword{keyword}

\maketitle % DO NOT DELETE THIS LINE

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

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

\section{Section title}

Text text
text text text text text text.

\subsection{Title}

Text text
text text text text text text.

\subsubsection{Title}

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.

\subsection{Title}

Text text
text text text text text text.

\subsubsection{Title}

Text text
text text text text text text.

\sectioniv{Title}

Text text
text text text text text text.

\sectionv{Title}

Text text
text text text text text text.

%-----
% The back matter of the paper - references
%-----
```

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```

\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
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

```

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, Loic Bertrand, Gunnar Thorkildsen, Chris Cousins, Thomas Proffen, Christian Anders Cumbaa, Bud Bridges and other users who provided valuable feedback during the development of the macros and associated templates.

(This block generated from the references environment.

Parthé, E. & Gelato, L. (1984). *Acta Cryst.* **A40**, 169–183.
 Rauch, H. & Petrascheck, D. (1976). *Grundlagen für ein Laue-Neutroneninterferometer Teil 1: Dynamische Beugung*. Report AIAU 74405b. Atominstytut der Österreichischen Universitäten, Austria.

(This block generated by Bib \TeX .)

Knuth, D. E. (1984). *The \TeX book*. Addison-Wesley.
 Lamport, L. (1986). *\LaTeX : A Document Preparation System*. Addison-Wesley.
 Parthé, E. & Gelato, L. (1984). *The standardization of inorganic crystal-structure data*. *Acta Cryst.* **A40**, 169–183.
 Pauling, L. (1989). *Icosahedral quasicrystals of intermetallic compounds are icosahedral twins of cubic crystals of three kinds, consisting of large (about 5000 atoms) icosahedral complexes in either a cubic body-centered or a cubic face-centered arrangement or smaller (about 1350 atoms) icosahedral complexes in the β -tungsten arrangement*. *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. Atominstytut der Österreichischen Universitäten, Austria.