



# Commission on Journals 2011

Crystallography  
**Journals**  
Online




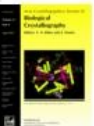






# IUCr templates and tools

(IUCr) Crystallography Journals Online - Mozilla

**Crystallography Journals Online**

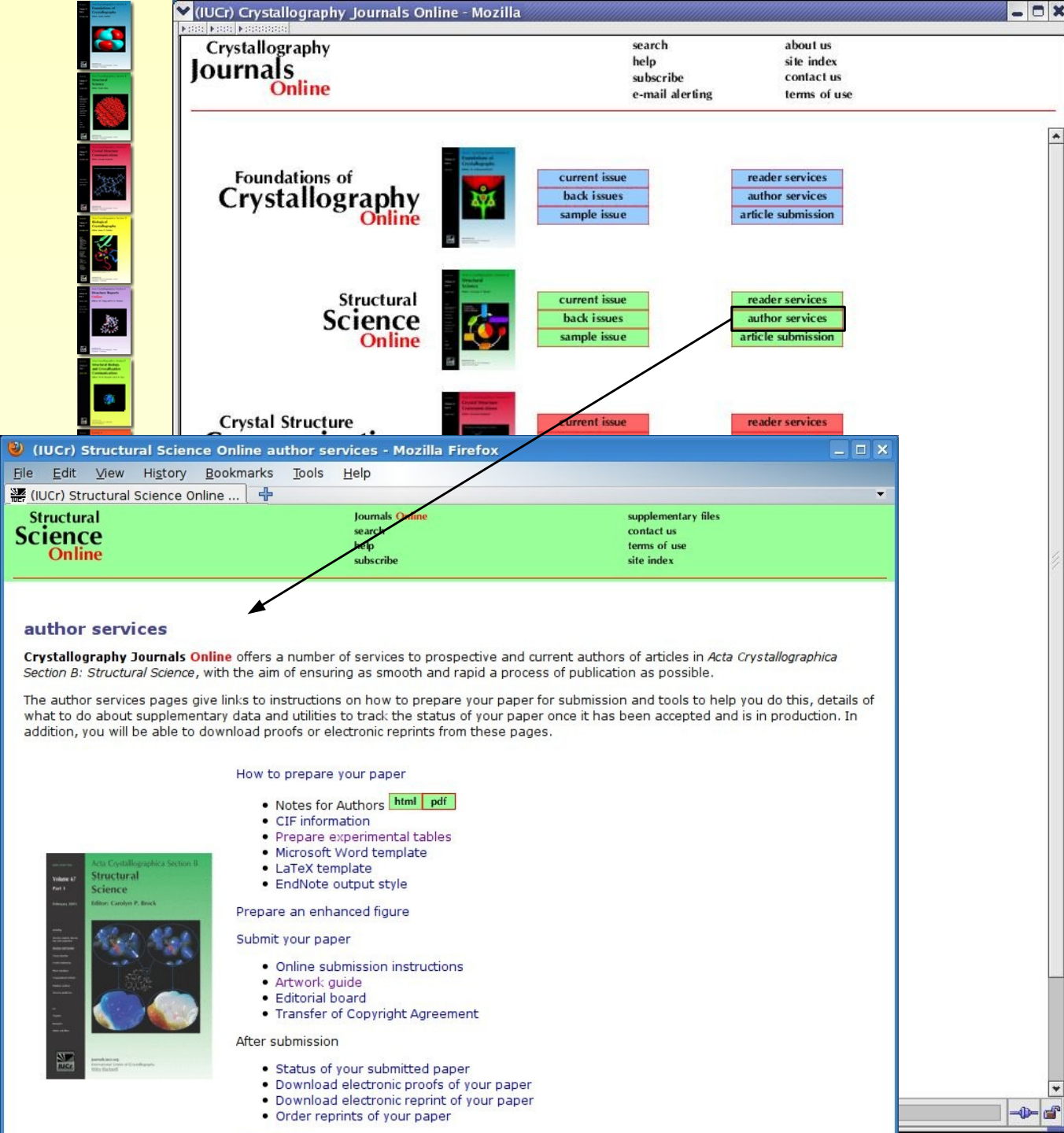
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<p><b>Foundations of Crystallography Online</b></p> 	<p>current issue back issues sample issue</p>	<p>reader services author services article submission</p>
<p><b>Structural Science Online</b></p> 	<p>current issue back issues sample issue</p>	<p>reader services author services article submission</p>
<p><b>Crystal Structure Communications Online</b></p> 	<p>current issue back issues sample issue</p>	<p>reader services author services article submission</p>
<p><b>Biological Crystallography Online</b></p> 	<p>current issue back issues sample issue</p>	<p>reader services author services article submission</p>
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<p><b>Applied Crystallography Online</b></p> 	<p>current issue back issues sample issue</p>	<p>reader services author services article submission</p>
<p><b>Synchrotron Radiation Online</b></p> 	<p>current issue back issues sample issue</p>	<p>reader services author services article submission</p>


Tools and author information available from:

- journals.iucr.org
- author services

Crystallography  
**Journals**  
Online



- Links include:
- WORD template
  - LaTeX template
  - CIF information
  - How to prepare experimental tables from CIF
  - PublBio



# Why templates and author tools?

- Provide a structured way of capturing articles
- Save authors' time if integrated with submission procedures
- Avoid rekeyboarding, particularly of data
- Improve efficiency and accuracy of journal production procedures by providing information in a format that can be easily processed
- Allow new features to be introduced to the journals, *e.g.* enhanced figures



# WORD Template

## Word styles and templates

IUCr

Author details	Check styles	Table tools	txt <body text style>	h1 <heading 1 style>	h2 <heading 2 style>	h3 <heading 3 style>	ack <acknowledgements>	ref <reference>	fig <figure caption>	th <table heading>	<table headnote> <table text> <table footnote>	<Appendix heading 1> <Appendix heading 2> <Appendix heading 3>	Help Info
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Tools

Styles

Authors who use **Microsoft Word** may prepare their papers for submission with the IUCr's Microsoft Word template, which enables authors to structure a manuscript for submission and publication.

### Current template

This template is packaged with a number of tools, including tools that allow tables of experimental data to be prepared easily.

- **Microsoft Word template for PC users (Word 2007 and 2010)**

### Older template versions

To download older template versions, use the right mouse button or use "Save As..."

- Microsoft Word template for PC users (Word 97-2003)
- Microsoft Word template for Macintosh users
- **README** file for Word 97-2003 users

### Additional information

The templates are undergoing development, so if you have any comments please send them to the IUCr (med@iucr.org).

Please note that the templates do not work with Microsoft Office 2008 for Mac.

Search term

Author  All journals   [Advanced search](#)

- Template for WORD 2007 and 2010
- Utilizes content management features of WORD
- Older templates available

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr

Author details Check styles Table tools

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< abstract >

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h2 < heading 2 style >

h3 < heading 3 style >

ack < acknowl- edgements >

ref < reference >

fig < figure caption >

th < table heading >

< table headnote >  
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< table footnote >

< Appendix heading 1 >  
< Appendix heading 2 >  
< Appendix heading 3 >

Help Info SGML Sgml Toggle highlights Misc

Current style: IUCr sans text grey

IUCr

Select journal \_\_\_\_\_

Select paper type \_\_\_\_\_

Click here to enter title

Click here to enter author details

Correspondence email:

**Keywords:** semicolon-separated list

**Synopsis**

One or two sentences appropriate for the journal's contents listing

**Abstract**

Click here to enter text.

**1. First level heading (style: IUCr heading 1)**

This is a main section (style: IUCr body text)

The main heading and paragraph styles can be applied using the IUCr tab, or using Word's style gallery. The heading styles automatically apply section numbering.

**1.1. Second level heading (style: IUCr heading 2)**

This is a subsection (style: IUCr body text)

**1.1.1. Third level heading (style: IUCr heading 3)**

This is a sub-subsection (style: IUCr body text)

**Acknowledgements** The acknowledgements should be in a single paragraph (style: IUCr acknowledgements; this style applies the heading).

Page: 1 of 2 Words: 272 English (U.K.) 100%

- Template packaged with tools:
- Interacts with external resources, e.g. World Directory
- Allows a personal database of author details to be collected
- Articles can be written in template or imported and marked up

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr

Author details Check styles Table tools

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h2 < heading 2 style >

h3 < heading 3 style >

ack < acknowl- edgements >

ref < reference >

fig < figure caption >

th < table heading >

< table headnote > < table text > < table footnote >

< Appendix heading 1 > < Appendix heading 2 > < Appendix heading 3 >

Help Info SGML Sgml Toggle highlights Misc

IUCr

Select journal

Select paper type

Acta Crystallographica Section A  
Acta Crystallographica Section B  
Acta Crystallographica Section D  
Acta Crystallographica Section F  
Journal of Applied Crystallography  
Journal of Synchrotron Radiation

Correspondence email:

**Keywords:** semicolon-separated list

**Synopsis**

One or two sentences appropriate for the journal's contents listing

**Abstract**

Click here to enter text.

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Page: 1 of 2 Words: 2/272 English (U.K.) 100%

- Use drop-down menu lists to select journal

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr

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< Appendix heading 1 >  
< Appendix heading 2 >  
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Help Info SGML Sgml Toggle highlights Misc

IUCr

Acta Crystallographica Section B

Select paper type  
research papers  
short communications  
lead articles  
feature articles  
letters to the editor  
scientific comment  
addenda and errata

Click here to enter title

Click here to enter author details

Correspondence email:

**Keywords:** semicolon-separated list

**Synopsis**  
One or two sentences appropriate for the journal's contents listing

**Abstract**  
Click here to enter text.

**1. First level heading (style: IUCr heading 1)**  
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**1.1.1. Third level heading (style: IUCr heading 3)**  
This is a sub-subsection (style: IUCr body text)

**Acknowledgements** The acknowledgements should be in a single paragraph (style: IUCr acknowledgements; this style applies the heading).

Page: 1 of 2 Words: 3/274 English (U.K.) 100%

- Select paper type
- Click to add title, keywords, synopsis and abstract

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr

Author details Check styles Table tools

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<Appendix heading 1> <Appendix heading 2> <Appendix heading 3>

Help Info Sgml Toggle highlights Misc

IUCr

Acta Crystallographica Section B

Select paper type

Click here to enter title

Click here to enter author details

Correspondence email:

Keywords: semicolon-separated list

Synopsis  
One or two sentences appropriate for the journal's contents list

Abstract  
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Page: 1 of 2 Words: 274 English (U.K.)

Update

Author 1

Use author from previous documents

Add author Move author Remove

Name

Title IUCr ID

Forename(s)

Surname

Qualifier (e.g. Jr, III)

E-mail

Correspondence author for publication

Primary contact author for this submission

Address

Use same address as

Department

Organization

Street/PO box

Town/city

State (province/country)

- Author details entered via menu
- Details formatted to journal style
- Information can be reused during submission

Document1 - Microsoft Word

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Help Info SGML Sgml Toggle highlights Misc

IUCr

Acta Crystallographica Section B

Select paper type

Click here to enter title

Click here to enter author details

Correspondence email:

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Use author from previous documents

Add author Move author Remove

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Title IUCr ID

Forename(s)

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Delhi</city><province></province><code>110012</code><country>India</country
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Page: 1 of 2 Words: 274

- Author details entered via menu
- Details formatted to journal style
- Information can be reused during submission
- Details stored as XML in zip file within document and in local database

Crystallography  
Journals  
Online

The screenshot shows the Microsoft Word interface with the IUcr template applied. The ribbon includes Home, Insert, Page Layout, References, Mailings, Review, View, MathType, Developer, Add-Ins, IUcr template, EndNote X2, Acrobat, and IUcr. The IUcr ribbon contains various style options like <keywords>, <synopsis>, <abstract>, <body text style>, <heading 1 style>, <heading 2 style>, <heading 3 style>, <acknowledgements>, <reference>, <figure caption>, <table heading>, <table footnote>, <table headnote>, <table text>, <table footnote>, <Appendix heading 1>, <Appendix heading 2>, and <Appendix heading 3>. The main document area shows the IUcr template with fields for title, author details, correspondence email, keywords, synopsis, and abstract. An 'Update' dialog box is open, showing the 'Author 1' tab with fields for Name, Title, Forename(s), Surname, Qualifier, E-mail, and Address. The dialog also includes checkboxes for 'Correspondence author for publication' and 'Primary contact author for this submission', and buttons for 'Add author', 'Move author', and 'Remove'.

- Author details entered *via* menu

- Details formatted to journal style

- Information can be reused during submission

- Details stored as XML in zip file within document and in local database

- Contact and corresponding authors can be distinguished

**Contact author** - the author who is the contact for submission, review and production

**Correspondence author(s)** - the author or authors for correspondence after publication (they get an asterisk and email address in the published paper)

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr

Author details Check styles Table tools

<keywords> <synopsis> <abstract>

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h2 <heading 2 style>

h3 <heading 3 style>

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ref <reference>

fig <figure caption>

th <table heading>

<table headnote> <table text> <table footnote>

<Appendix heading 1> <Appendix heading 2> <Appendix heading 3>

Help Info SGML Sgml Toggle highlights Misc

IUCr

Acta Crystallographica Section B

Select paper type

Click here to enter title

Click here to enter author details

Correspondence email:

Keywords: semicolon-separated list

Synopsis  
One or two sentences appropriate for the journal's contents list

Abstract  
Click here to enter text.

1. First level heading (style: IUCr heading 1)  
This is a main section (style: IUCr body text)

The main heading and paragraph styles can be applied using the style gallery. The heading styles automatically apply section numbering.

1.1. Second level heading (style: IUCr heading 2)  
This is a subsection (style: IUCr body text)

1.1.1. Third level heading (style: IUCr heading 3)  
This is a sub-subsection (style: IUCr body text)

Acknowledgements The acknowledgements should be in a single paragraph (style: IUCr acknowledgements; this style applies the heading).

Page: 1 of 2 Words: 274 English (U.K.)

Update

Author 1

Use author from previous documents

Add author Move author Remove

Name

Title IUCr ID 2662

Forename(s)

Surname

Qualifier (e.g. Jr, III)

E-mail

Correspondence author for publication

Primary contact author for this submission

Address

Use same address as

Department

Organization

Street/PO box

Town/city

State/province/country

Search WDC by IUCr ID

2662

Jillian Kaye Bradshaw  
International Union of Crystallography, 5  
Abbey Square, Chester, CH1 2HU, United  
Kingdom,  
jb@iucr.org  
[Use these details in the active author  
tab]

● Details can be retrieved from the World Directory

● In the future, author details could be picked up from services such as ORCID or from previous journal authors

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr

Author details Check styles Table tools

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Help Info SGML Sgml Toggle highlights Misc

Current style: IUCr sans text grey

# IUCr

Select journal \_\_\_\_\_

Select paper type \_\_\_\_\_

Click here to enter title

Click here to enter author details

Correspondence email:

**Keywords:** semicolon-separated list

**Synopsis**

One or two sentences appropriate for the journal's contents listing

**Abstract**

Click here to enter text.

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**Acknowledgements** The acknowledgements should be in a single paragraph (style: IUCr acknowledgements; this style applies the heading).

Page: 1 of 2 Words: 272 English (U.K.) 100%

- Mark up text with styles, e.g. first-, second- or third-level headings
- Styles also available from IUCr ribbon

Document1 - Microsoft Word

Table Tools

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr Design Layout

Author details Check styles Table tools

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th < table heading >

< table headnote > < table text > < table footnote >

< Appendix heading 1 > < Appendix heading 2 > < Appendix heading 3 >

Help Info SGML Sgml Toggle highlights Misc

Current style: IUCr table text

**References**

This is Word's reference management system, but if you usually use a different citation manager, please apply the IUCr references style to each reference.

**Table 1** This is a table heading (style: IUCr table caption; this style applies table numbering)

This is a table headnote (style: IUCr table headnote)

IUCr table text	IUCr table text	IUCr table text	IUCr table text
IUCr table text	IUCr table text	IUCr table text	IUCr table text

This is a table footnote (style: IUCr table footnote)

**Figure 1** Each figure caption should be a single paragraph (style: IUCr figure caption; this style applies the figure numbering).

**Appendix A.** First level appendix heading (style: IUCr appendix heading 1)

IUCr body text

**A1.** Second level appendix heading (style: IUCr appendix heading 2)

IUCr body text

**A1.1.** Third level appendix heading (style: IUCr appendix heading 3)

IUCr body text

Page: 2 of 2 Words: 274 English (U.K.) 100%

- Tables should be prepared using WORD's table editor with styles applied to caption, headnotes and footnotes
- Experimental tables can be prepared using **Table tools**

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr

Tools: Author details, Check styles, Table tools

Styles: <keywords>, <synopsis>, <abstract>, txt, h1, h2, h3, ack, ref, fig, th, <table headnote>, <table text>, <table footnote>, <Appendix heading 1>, <Appendix heading 2>, <Appendix heading 3>

References

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**Table 1** This is a table heading (style: IUCr table caption; this style applies table number).  
 This is a table headnote (style: IUCr table headnote).

IUCr table text	IUCr table text	IUCr table text	IUCr table text
IUCr table text	IUCr table text	IUCr table text	IUCr table text

This is a table footnote (style: IUCr table footnote).

**Figure 1** Each figure caption should be a single paragraph (style: IUCr figure caption; this style applies the figure numbering).

Appendix A. First level appendix heading (style: IUCr appendix heading 1)  
 IUCr body text

A1. Second level appendix heading (style: IUCr appendix heading 2)  
 IUCr body text

A1.1. Third level appendix heading (style: IUCr appendix heading 3)  
 IUCr body text

Page: 2 of 2 | Words: 274 | English (U.K.) | 100%

Use **Table tools** to prepare experimental tables from CIF for small molecule structures

For macromolecular structures use PDB code to import mmCIF to create table of experimental details

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr

Author details Check styles Table tools

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Help Info SGML Sgml Toggle highlights Misc

Current style: IUCr table caption

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**Table 1** This is a table head  
This is a table head  
IUCr table text  
IUCr table text  
This is a table foot

**Figure 1** Each figure applies the figure

**Appendix A.** First IUCr body text

**A1.** Second level IUCr body text

**A1.1.** Third level IUCr body text

Add to document Options... Save CIF Geometry tables

**Experimental details**

For all structures: monoclinic,  $P2_1/c$ . Experiments were carried out at 180 K with Mo  $\lambda$ K $\alpha$  radiation. Refinement was with 0 restraints.

	Id425_180k_22apr2011.int4	Id489	Id473
<b>Crystal data</b>			
Chemical formula	$C_{13}H_{14}N_2O_3$	$C_{13}H_{15}F_3N_2O_2$	$C_{17}H_{19}F_3N_2O$
$M_r$	246.26	312.29	324.34
$a, b, c$ (Å)	7.059 (3), 24.497 (10), 13.914 (6)	8.9941 (5), 11.2954 (6), 14.3536 (3)	12.1853 (5), 12.2242 (4), 10.6361 (3)
$\beta$ (°)	103.559 (6)	102.537 (3)	93.4529 (11)
$V$ (Å <sup>3</sup> )	2339.0 (16)	1423.44 (14)	1581.43 (3)
$Z$	8	4	4
$\mu$ (mm <sup>-1</sup> )	0.10	0.12	0.11
Crystal size (mm)	0.55 × 0.26 × 0.12	0.42 × 0.22 × 0.14	0.32 × 0.16 × 0.12
<b>Data collection</b>			
Diffractometer	Rigaku CrystalClear-SM Expert 2.0 14 diffractometer	KappaCCD diffractometer	KappaCCD diffractometer
Absorption correction	Multi-scan Higashi, 1995	Multi-scan from symmetry-related measurements, <i>SORTAV</i> (Blessing 1997)	Multi-scan from symmetry-related measurements, <i>SORTAV</i> (Blessing 1997)

Page: 2 of 2 Words: 274 English (U.K.) 100%

Each datablock from CIF appears as column in table

Document1 - Microsoft Word

Home Insert Page Layout References Mailings Review View MathType Developer Add-Ins IUCr template EndNote X2 Acrobat IUCr

Author details Check styles Table tools

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Table 1 This is a table head

IUCr table text

IUCr table text

This is a table foot

Figure 1 Each figure applies the figure

Appendix A. First IUCr body text

A1. Second level IUCr body text

A1.1. Third level IUCr body text

Rebuild table

Column heads: Datablock\_name

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- Id489
- Id473

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- Cell\_measurement\_reflections
- Cell\_measurement\_theta\_range
- Crystal\_shape
- Specimen\_colour
- Radiation\_source
- Monochromator
- Detector\_resolution
- Scan\_method
- Reflection\_theta\_range
- hkl\_range
- Structure\_factor\_coefficient
- Weighting\_scheme
- refine ls shift/su max

'Options...' include changing the order of structures in this table and including extra items.

Id489	Id473
$C_{15}H_{19}F_3N_2O_2$	$C_{17}H_{19}F_3N_2O$
312.29	324.34
8.9941 (5), 11.2954 (6), 14.3596 (9)	12.1853 (5), 12.2242 (4), 10.6361 (3)
102.597 (3)	99.4529 (11)
1423.44 (14)	1581.43 (9)
4	4
0.12	0.11
$0.42 \times 0.22 \times 0.14$	$0.32 \times 0.16 \times 0.12$
KappaCCD diffractometer	KappaCCD diffractometer
Absorption correction	Multi-scan Higashi, 1995
	Multi-scan multi-scan from symmetry-related measurement, SORAV (Blessing 1997)
	Multi-scan multi-scan from symmetry-related measurement, SORAV (Blessing 1997)

Page: 2 of 2 Words: 274 English (U.K.) 100%

Extra non-standard items present in CIF can be added to table

Datablocks can be selected for inclusion or exclusion

Several types of column headings can be selected

Small molecule, powder and incommensurate CIFs handled

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This is a table foot

Figure 1 Each figure applies the figure style

Appendix A. First IUCr body text

A1. Second level IUCr body text

A1.1. Third level IUCr body text

Experimental details

For all structures: monoclinic,  $P2_1/c$ . Experiments were carried out at 180 K with Mo  $K\alpha$  radiation. Refinement was with 0 restraints.

	18425_180k_22apr2011int4	18489	18473
<b>Crystal data</b>			
Chemical formula	$C_{13}H_{14}N_2O_3$	$C_{13}H_{19}F_3N_2O_2$	$C_{17}H_{19}F_3N_2O$
$M_r$	246.26	312.29	324.34
$a, b, c$ (Å)	7.059 (3), 24.497 (10), 13.914 (6)	8.9941 (5), 11.2954 (6), 14.3536 (9)	12.1853 (5), 12.2242 (4), 10.6361 (3)
$\beta$ (°)	103.559 (6)	102.537 (3)	99.4529 (11)
$V$ (Å <sup>3</sup> )	2339.0 (16)	1423.44 (14)	1581.43 (9)
Z	8	4	4
$\mu$ (mm <sup>-1</sup> )	0.10	0.12	0.11
Crystal size (mm)	0.55 × 0.26 × 0.12	0.42 × 0.22 × 0.14	0.32 × 0.16 × 0.12
<b>Data collection</b>			
Diffractometer	Rigaku CrystalClear-SM Expert 2.0 $\theta$ diffractometer	KappaCCD diffractometer	KappaCCD diffractometer
Absorption correction	Multi-scan Higashi, 1995	Multi-scan multi-scan from symmetry-related measurement, SORTAV (Blessing 1997)	Multi-scan multi-scan from symmetry-related measurement, SORTAV (Blessing 1997)

Page: 2 of 2 Words: 274 English (U.K.) 100%

- Once all items have been selected, the experimental table can be added to the document

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Figure 1 Each figure applies the figure IUCr body text

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A1.1. Third level IUCr body text

Selection of geometric parameters prior to creation of tables

Select/deselect a single parameter by clicking it; select/deselect a group of parameters by dragging the mouse over them.  
Move a single parameter by dragging its icon  
Move a group of parameters that have the same selection state by holding down the SHIFT key before dragging the icon of the first parameter in the group.  
Move a structure block by dragging its icon

Bonds Angles

3d425_180k_22apr2011.int4	3d489	3d473
⊙ O1—C8* 1.379(2)	⊙ O1—C7 1.378(2)	
⊙ O1—C2* 1.386(2)	⊙ O1—C1 1.3821(19)	
⊙ O1—C8 1.380(2)	⊙ N1—C7 1.315(2)	
⊙ O1—C2 1.380(2)	⊙ N1—C6 1.344(2)	
⊙ O2—C2* 1.216(2)	⊙ C7—C8 1.390(2)	
⊙ O2—C2 1.209(2)	⊙ O2—C1 1.215(2)	
⊙ C3—C4* 1.343(3)	⊙ C4—C5 1.366(2)	
⊙ C3—C2* 1.435(3)	⊙ C4—C8 1.416(2)	
⊙ C3—H3* 0.97(2)	⊙ C4—H4 0.9500	
⊙ C9—C8* 1.389(3)	⊙ F1—C15 1.327(2)	
⊙ C9—C5* 1.394(3)	⊙ C6—N2 1.357(2)	
⊙ C9—C4* 1.450(3)	⊙ C6—C5 1.433(2)	
⊙ N1—C8* 1.323(2)	⊙ F3—C15 1.331(2)	
⊙ N1—C7* 1.349(2)	⊙ C8—C3 1.435(2)	
⊙ C3—C4 1.348(3)	⊙ C2—C3 1.355(2)	

Page: 2 of 2 Words: 274 English (U.K.) 100%

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**Figure 1** Each figure applies the figure

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**A1.1.** Third level IUCr body text

Create tables Select... Hide non-selected geometry Change layout

Selection of geometric parameters prior to creation of tables

Select/deselect a single parameter by clicking it; select/deselect a group of parameters by dragging the mouse over them.  
Move a single parameter by dragging its icon  
Move a group of parameters that have the same selection state by holding down the SHIFT key before dragging the icon of the first parameter in the group.  
Move a structure block by dragging its icon

Bonds Angles

3d425_180k_22apr2011.tnt4	3d489	3d473
Select...	Select...	
⊙C8—O1—C2* 121.04(14)	⊙C7—O1—C1 122.18(13)	
⊙C8—O1—C2 121.43(14)	⊙C7—N1—O6 117.72(14)	
⊙C4—C3—C2* 122.71(17)	⊙N1—C7—O1 112.50(14)	
⊙C4—C3—H3* 123.1(12)	⊙N1—C7—C8 126.52(15)	
⊙C2—C3—H3* 114.2(11)	⊙O1—C7—C8 120.98(14)	
⊙C8—C9—C5* 115.18(17)	⊙C5—C4—C8 121.77(15)	
⊙C8—C9—C4* 119.15(17)	⊙C5—C4—H4 119.1	
⊙C5—C9—C4* 125.66(17)	⊙C8—C4—H4 119.1	
⊙C8—N1—C7* 116.81(16)	⊙N1—C6—N2 116.34(15)	
⊙C4—C3—C2 122.67(17)	⊙N1—C6—C5 122.03(15)	
⊙C4—C3—H2 122.1(13)	⊙N2—C6—C5 121.63(15)	
⊙C2—C3—H2 115.1(13)	⊙C7—C8—C4 114.64(15)	
⊙C3—C4—C9 118.65(17)	⊙C7—C8—C3 117.61(15)	
⊙C3—C4—C1 121.59(17)	⊙C4—C8—C3 127.74(15)	
⊙C9—C4—C1 119.75(16)	⊙C3—C2—C1 120.91(16)	

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- Can select which bonds and angles to include in table

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**Figure 1** Each figure applies the figure style

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**A1.** Second level IUCr body text

**A1.1.** Third level IUCr body text

Create tables Select... Hide non-selected geometry Change layout

If there is more than one structure, the layout can be switched between a 'side-by-side' view and a 'top-to-bottom' view.

**Selection of geometric parameters prior to creation of tables**

Select/deselect a single parameter by clicking it; select/deselect a group of parameters by dragging the mouse over them.

Move a single parameter by dragging its icon

Move a group of parameters that have the same selection state by holding down the SHIFT key before dragging the icon of the first parameter in the group.

Move a structure block by dragging its icon

**Bonds Angles**

Structure	Parameter	Value
Jd425_180k_22apr2011.int4	O1'-C8*	1.379(2)
	O1'-C2'	1.386(2)
	O1-C8	1.380(2)
	O1-C2	1.380(2)
	O2'-C2'	1.216(2)
	O2-C2	1.209(2)
	C3'-C4*	1.343(3)
	C3'-C2'	1.435(3)
	C3'-H3'	0.97(2)
	O9'-C8*	1.389(3)
	O9'-C5'	1.394(3)
	O9'-C4'	1.450(3)
	N1'-C8*	1.323(2)
	N1'-C7'	1.349(2)
C3-C4	1.348(3)	
Jd489	O1-C7	1.378(2)
	O1-C1	1.3821(19)
	N1-C7	1.315(2)
	N1-C6	1.344(2)
	C7-C8	1.390(2)
	O2-C1	1.215(2)
	C4-C5	1.366(2)
	C4-C8	1.416(2)
	C4-H4	0.9500
	F1-C15	1.327(2)
Jd473	C6-N2	1.357(2)
	C6-C5	1.433(2)
	F3-C15	1.331(2)
	C8-C3	1.435(2)
	C2-C3	1.355(2)

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- Can select which bonds and angles to include in table
- Layout can be changed to accommodate comparison tables

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< Appendix heading 1 > < Appendix heading 2 > < Appendix heading 3 >

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**Table 2 Data collection and refinement statistics**

Data collection	
Resolution range (Å)	49.43-2.9 (3.06-2.9) <sup>a</sup>
Unit cell	
(Å)	132.5, 196.7, 170.8
(°)	90.0, 92.8, 90.0
Space group	<i>P</i> 2 <sub>1</sub>
Redundancy	4.2 (4.2)
Reflections	805846
Unique reflections	193013
Completeness (%)	100 (99.9)
<i>R</i> <sub>merge</sub> (%)	12.0 (56.6)
<i>I</i> / <i>σ</i> <sub><i>I</i></sub>	10.7 (2.5)
Refinement	
Range (Å)	20.0-2.9
Reflections used	191418
$\frac{1}{2}R_{\text{free}}$	19.0/22.3
No. of atoms in the asymmetric unit	
Protein	63129
Ligand	645
Solvent	65
Rms deviations	
Bond lengths (Å)	0.014
Bond angles (°)	1.47
Average B	45.04
MolProbity validation	
Clashscore (all atom contacts)	4.2 (100 <sup>th</sup> percentile)
Poor rotamers (%)	3.91
Ramachandran (%)	
Favoured	96.28
Allowed	3.59
Disallowed	0.13
C <sup>β</sup> deviations > 0.25 Å	18
MolProbity score	1.90 (99 <sup>th</sup> percentile)

Use a CIF or mmCIF to create tables

Load CIF

Load a structure from the PDB archives to create tables

Fetch PDB CIF PDB code:

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- For macromolecular papers the PDB reference code can be used to upload an mmCIF

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**Table 2 Data collection and refinement statistics**

Data collection	
Resolution range (Å)	49.43-2.9 (3.06-2.9) <sup>a</sup>
Unit cell	
(Å)	132.5, 196.7, 170.8
(°)	90.0, 92.8, 90.0
Space group	
Redundancy	
Reflections	
Unique reflections	
Completeness (%)	
$R_{\text{merge}}$ (%)	
$I/\sigma I$	
Refinement	
Range (Å)	
Reflections used	
$R_{\text{free}}$	
No. of atoms in the asymmetric unit	
Protein	
Ligand	
Solvent	
Rms deviations	
Bond lengths (Å)	
Bond angles (°)	
Average B	
MolProbity validation	
Clashscore (all atom contacts)	
Poor rotamers (%)	
Ramachandran (%)	
Favoured	96.28
Allowed	3.59
Disallowed	0.13
C $\beta$ deviations > 0.25 Å	18
MolProbity score	1.90 (99 <sup>th</sup> percentile)

Add following table to document

**Sample information**

Macromolecule details	
Database code(s)	PDB code: 2XQ1; UNP code: CATA_PICAN
Component molecules	Peroxisomal catalase (EC number: 1.11.1.6), protoporphyrin IX containing Fe, water
Macromolecular assembly	
Mass (Da)	
Source organism	FICHIA ANGUSTA
Crystallization and crystal data	
Crystallization method	.
Temperature (K)	.
Apparatus	.
Atmosphere	.
Pressure (kPa)	.
Crystal growth time	.
Seeding	.
Additional details	. 0.2 M magnesium formate, 20% (W/V) PBG 3350
Crystallization solutions	
Crystal data	

Add all tables to document

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Tables generated containing Sample information

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**Table 2 Data collection and refinement statistics**

**Data collection**

Resolution range (Å)	49.43-2.9 (3.06-2.9) <sup>a</sup>
Unit cell	
(Å)	132.5, 196.7, 170.8
(°)	90.0, 92.8, 90.0
Space group	
Redundancy	
Reflections	
Unique reflections	
Completeness (%)	
<sup>a</sup> R <sub>merge</sub> (%)	
<i>I</i> / <i>σ</i>	

**Refinement**

Range (Å)	
Reflections used	
<sup>b</sup> R <sub>refined</sub>	
No. of atoms in the asymm.	
Protein	
Ligand	
Solvent	

**Rms deviations**

Bond lengths (Å)	
Bond angles (°)	

Average B

**MolProbability validation**

Clashscore (all atom c)	
Poor rotamers (%)	
Ramachandran (%)	
Favoured	96.28
Allowed	3.59
Disallowed	0.13
C <sup>β</sup> deviations > 0.25 Å	18
MolProbability score	1.90 (99 <sup>th</sup> percentile)

Crystal data

Crystal shape	NONB
Crystal size (mm)	7 × 7 × 7 mm
Matthews coefficient, V <sub>M</sub> (Å <sup>3</sup> Da <sup>-1</sup> )	2.49
Solvent content (%)	50.14

Unit-cell data

Crystal system, space group	P2 <sub>1</sub>
a, b, c (Å)	132.52, 196.68, 170.85
α, β, γ (°)	90, 92.85, 90
No. of molecules in unit cell, Z	

Add all tables to document

Add following table to document

**Data collection and structure solution statistics**

Values for the outer shell are given in parentheses.

Diffraction source	Synchrotron; ESRF beamline ID14-1
X-ray beam size	.
Sampling protocol	
Diffraction protocol	Single wavelength
Monochromator	Diamond (111), Ge(220)
Collimation	.

Tables generated containing

Sample information

Data collection and structure solution statistics

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**Table 2 Data collection and refinement statistics**

**Data collection**

Resolution range (Å)	49.43-2.9 (3.06-2.9) <sup>a</sup>
Unit cell	
(Å)	132.5, 196.7, 170.8
(°)	90.0, 92.8, 90.0
Space group	
Redundancy	
Reflections	
Unique reflections	
Completeness (%)	
<sup>a</sup> R <sub>average</sub> (%)	
<i>I</i> / <i>σ</i>	
<b>Refinement</b>	
Range (Å)	
Reflections used	
<sup>b</sup> R <sub>free</sub>	
No. of atoms in the asymmetric unit	
Protein	
Ligand	
Solvent	
<b>Rms deviations</b>	
Bond lengths (Å)	
Bond angles (°)	
Average B	
<b>MolProbity validation</b>	
Clashscore (all atoms)	
Poor rotamers (%)	
Ramachandran (%)	
Favoured	96.28
Allowed	3.59
Disallowed	0.13
C <sup>α</sup> deviations > 0.25 Å	18
MolProbity score	1.90 (99 <sup>th</sup> percentile)

**Structure refinement and model validation**

Values for the outer shell are given in parentheses.

Refinement software	REFMAC5.5.0109
Refinement on	
σ cutoff	
Resolution range (Å)	20.00-2.90 (2.974-2.900)
No. of reflections used in refinement	(13850)
No. of reflections above σ cutoff in final cycle	191418
Final overall R factor	0.191
Atomic displacement model	
Overall average B factor (Å <sup>2</sup> )	42.5
No. of protein atoms	63129
No. of ligand atoms	645
No. of solvent atoms	65
Total No. of atoms	63839
No. of refined parameters	
Non-crystallographic symmetry restraints	
Bulk solvent model	MASK
Final R <sub>work</sub>	0.19059 (0.298)
No. of reflections for R <sub>work</sub>	976 (69)

Page: 16 of 17 Words: 4,993 English (U.K.) 130%

Tables generated containing

Sample information

Data collection and structure solution statistics

Structure refinement and model validation

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**References**

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**Table 1** This is a table heading (style: IUCr table caption; this style applies table numbering)

This is a table headnote (style: IUCr table headnote)

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IUCr table text	IUCr table text	IUCr table text	IUCr table text

This is a table footnote (style: IUCr table footnote)

**Figure 1** Each figure caption should be a single paragraph (style: IUCr figure caption; this style applies the figure numbering).

**Appendix A.** First level appendix heading (style: IUCr appendix heading 1)

IUCr body text

**A1.** Second level appendix heading (style: IUCr appendix heading 2)

IUCr body text

**A1.1.** Third level appendix heading (style: IUCr appendix heading 3)

IUCr body text

Page: 2 of 2 Words: 274 English (U.K.) 100%

- Figure captions should be listed
- Insert appendices if appropriate
- Headings, tables, figure captions etc. are automatically numbered in journal style

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Chen, J. (2003). *Citations and References*. New York: Cortoso Press.  
 Haas, J. (2005). *Creating a Formal Publication*. Boston: Proseware, Inc.  
 Kramer, J. D. (2006). *How to Write Bibliographies*. Chicago: Adventure Works Press.

Works Cited

Works Cited

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References

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IUCr figure caption; this style applies the figure numbering).

Appendix A. First level appendix heading (style: IUCr appendix heading 1)

IUCr body text

A1. Second level appendix heading (style: IUCr appendix heading 2)

IUCr body text

A1.1. Third level appendix heading (style: IUCr appendix heading 3)

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Page: 2 of 2 Words: 272 English (U.K.) 100%

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< keywords > < synopsis > < abstract >

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< Appendix heading 1 > < Appendix heading 2 > < Appendix heading 3 >

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Update Citations and Bibliography

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Bibliography

Chen, J. (2003). *Citations and References*. New York: Cortoso Press.

Haas, J. (2005). *Creating a Formal Publication*. Boston: Proseware, Inc.

Kramer, J. D. (2006). *How to Write Bibliographies*. Chicago: Adventure Works Press.

Works Cited

Works Cited

Chen, J. (2003). *Citations and References*. New York: Cortoso Press.

Haas, J. (2005). *Creating a Formal Publication*. Boston: Proseware, Inc.

Kramer, J. D. (2006). *How to Write Bibliographies*. Chicago: Adventure Works Press.

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Paul P. Ewald, *Acta Crystallographica*

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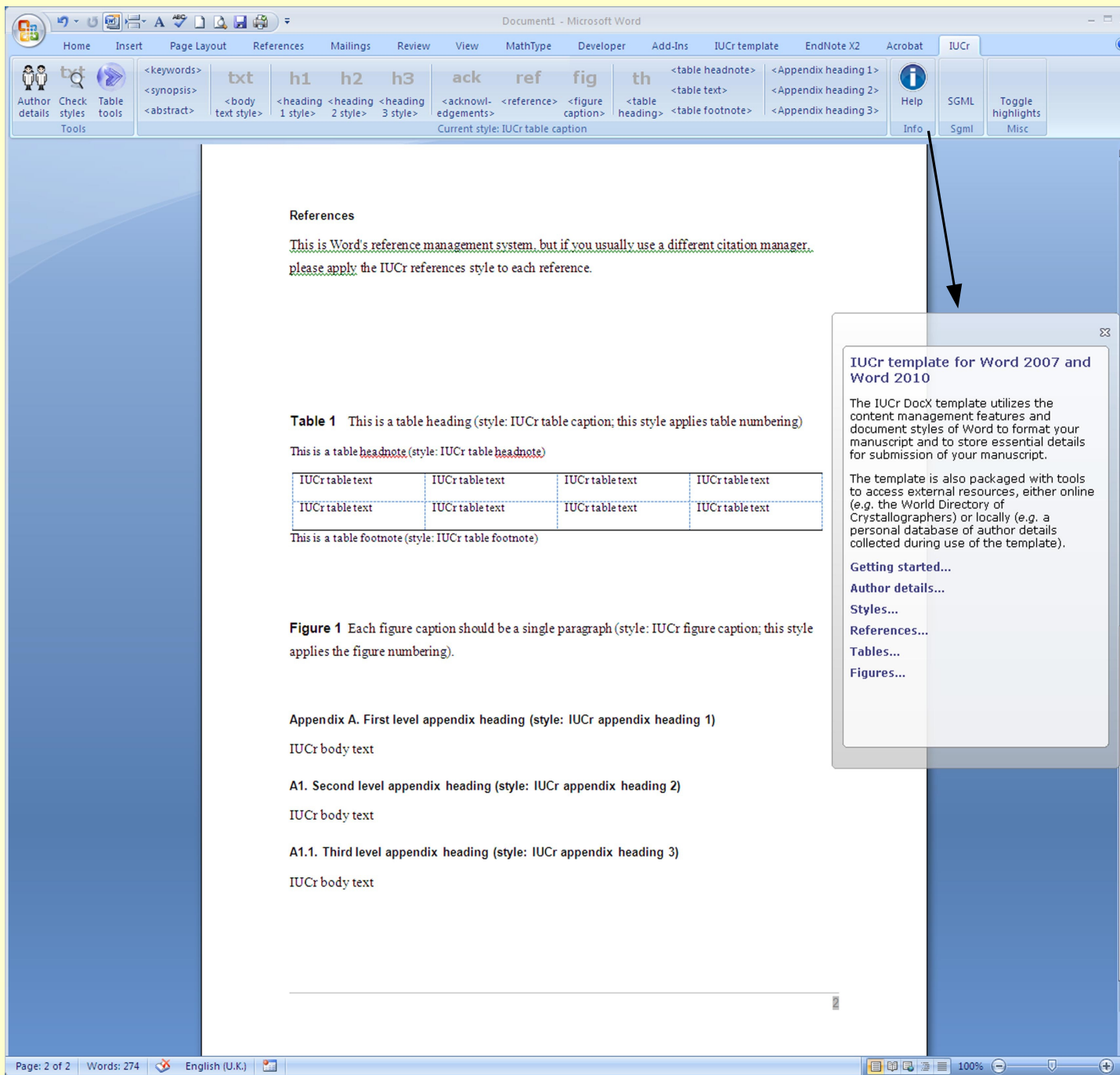
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h2 <heading 2 style>

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fig <figure caption>

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<Appendix heading 3>

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**Structural characterization of  $\text{LaTi}_2\text{Al}_9\text{O}_{19}$  and critical review of  $\text{La}_3\text{Ti}_5\text{Al}_{15}\text{O}_{37}$  crystal structure**

Marta Kasunič,<sup>a</sup> Anton Meden,<sup>a</sup> Srečo D. Škapin,<sup>b</sup> Danilo Suvorov<sup>b</sup> and Amalija Golobič<sup>a\*</sup>

<sup>a</sup>Faculty of Chemistry and Chemical Technology, University of Ljubljana, Aškerčeva 5, 1000 Ljubljana, Slovenia, and <sup>b</sup>Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia. E-mail: amalija.golobic@fkkt.uni-lj.si

**Synopsis** A crystal structure of  $\text{LaTi}_2\text{Al}_9\text{O}_{19}$  determined by X-ray powder diffraction is presented together with its dielectric properties. A critical review of a crystal structure, published as  $\text{La}_3\text{Ti}_5\text{Al}_{15}\text{O}_{37}$ , is also included.

**Abstract** The non-perovskite compound  $\text{LaTi}_2\text{Al}_9\text{O}_{19}$  was synthesized and structurally characterized by means of conventional X-ray powder diffraction. The plausibility of the obtained crystal structure, which is isostructural with  $\text{SrTi}_3\text{Al}_9\text{O}_{19}$ , was confirmed by bond valence sums calculations. Dielectric properties of the studied compound at 1 MHz were measured as well. Critical review of the crystal structure of  $\text{La}_3\text{Ti}_5\text{Al}_{15}\text{O}_{37}$ , which is referred as the most complex structure solved *ab initio* from XRPD till now, is also given.

**Keywords:** XRPD; structure determination;  $\text{La}_2\text{O}_3\text{-TiO}_2\text{-Al}_2\text{O}_3$  ternary system;  $\text{LaTi}_2\text{Al}_9\text{O}_{19}$ ;  $\text{La}_3\text{Ti}_5\text{Al}_{15}\text{O}_{37}$ .

**1. Introduction**

In order to stabilize  $\text{La}_2\text{TiO}_5$  and consequently to prepare new compounds, possibly with promising microwave and dielectric properties that would be applicable as components in various electronic circuits, the ternary system  $\text{La}_2\text{O}_3\text{-TiO}_2\text{-Al}_2\text{O}_3$  has been extensively studied (Škapin *et al.*, 1993; Suvorov *et al.*, 1998). Until this work, crystal structures of several ternary oxides were determined: (1) A-site deficient perovskites  $\text{La}_{0.683}\text{Al}_{0.05}\text{Ti}_{0.95}\text{O}_3$  (Yoshioka, 1994; Ali *et al.*, 2001),  $\text{La}_{0.7}\text{Al}_{0.1}\text{Ti}_{0.9}\text{O}_3$  and  $\text{La}_{0.71}\text{Al}_{0.15}\text{Ti}_{0.85}\text{O}_3$  (Yoshioka, 1994), (2) a perovskite compound with vacancies distributed among all sites,  $\text{La}_{0.9}\text{Al}_{0.465}\text{Ti}_{0.465}\text{O}_{2.9}$  (Slater & Irvine, 1999) and (3)

The title, authors and addresses contain hiddentext. Before editing, reveal the hiddentext by pressing

Page: 1 of 14 Words: 3,876 English (U.K.) 100%

- In the in-house template, used in the Editorial Office, styles show up as colour-coded text
- Author markup can therefore be quickly checked



# LaTeX template

## LaTeX style file and templates

Authors who use **LaTeX** may prepare their papers for submission with a set of customised macros. The macros allow an author to structure a manuscript in the style of the journal, and to present mathematical equations in a portable form. A LyX template is also available for users of this LaTeX-compatible graphical document editor.

### prerequisites

1. LaTeX2e, version 1997/12/01 or later.
2. The *iucr* macro package.
3. Optionally, BibTeX for citation handling.

See *availability* below for sources.

### general notes on the use of the *iucr* package

A paper prepared in LaTeX format should declare a document of class *iucr*; that is, the first non-comment line of the file should be of the form

```
\documentclass{iucr}
```

Additional options will normally be specified with this command. The most common option is `preprint`, to produce a single double-spaced version of the paper suitable for review purposes. Use this option for the hard-copy version of the paper. The Co-editor:

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

Since the journals are not typeset directly from LaTeX (but from another language, SGML, into which the LaTeX file is translated), it is usually appropriate to prepare the manuscript **solely** in this 'preprint' mode.

For camera-ready conference papers the preprint option may be omitted, and the paper should be made up according to the style of the journal, including the proper placement of figures and tables. See the specific instructions for preparing camera-ready papers in such cases.

For papers containing long mathematical equations, it is helpful if the author processes the paper without the preprint option, so that the equations may be adjusted to fit properly into the narrow columns of the journal.

### special instructions for Acta Crystallographica Section B

A submission to Acta Crystallographica Section B often comprises one or more sets of crystal structure data in CIF format for the body of the manuscript. For such papers the following applies:

1. Standard experimental tables (*i.e.* those containing data that can be encoded in a CIF - experimental details, geometry, displacement parameters) will be typeset from the CIF.
2. All other parts of the paper including non-standard tabular information may be presented in LaTeX format. Manuscripts should be prepared for submission to a Coeditor with the document class invocation:
 

```
\documentclass[preprint]{iucr}
\journalcode{B}
```
3. Authors should provide a preprint version to the Coeditor for review. This has double line spacing and one column. They should also send hard-copy versions of the figures, and the CIF file (by email or on diskette). When the preprint is accepted, the author will be asked to send final electronic versions to the editorial office in Chester.
4. Electronic versions of the figures should preferably be PostScript files, with one figure per page. However, there is an option for calling figures into the LaTeX file so that they can be printed in the hard-copy review manuscript.

When accepted for publication, the final version to be submitted to the editorial office should be prepared with the invocation

```
\documentclass[dj]{iucr}
\journalcode{B}
```

• LaTeX template instructions and files (**template and IUCr class file**) from author services

```
-----
% Template file for the submission of papers to IUCr journals in LaTeX2e
% using the iucr document class
% Copyright 1999-2011 International Union of Crystallography
% Version 1.4a (17 April 2011)
-----
\documentclass{iucr}           % DO NOT DELETE THIS LINE

%-----
% Information about the type of paper
%-----
\paperprocode{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
% LA - lead article
% FE - feature articles
% ST - structural communications
% XC - crystallization communications
% (Following categories rarely in LaTeX)
% AA - abstracts
% AD - addenda and errata
% BC - books received
% BR - book reviews
% CA - cif applications
% CE - current events
% CI - inorganic compounds
% 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
```

# Use of LaTeX

- Easy to create complex mathematical equations
- Indicates structure of document which is useful in translating for production
- However, authors can essentially redefine any command, sometimes making the use of LaTeX challenging within submission and production systems

```
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\papertype{FA}                % Indicate type of article
% FA - research papers (full article)
% SC - short communications
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% FE - feature articles
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% AA - abstracts
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% 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
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% 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
% SR - software reviews
% TE - teaching and education

\paperlang(english)           % Can be english, french, german or russian
%-----
% Information about journal to which submitted
%
```

# LaTeX templates

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% Information about the type of paper
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\paperprodcode{a000000}       % Replace with production code if known
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                             % SC - short communications
                             % LA - lead article
                             % FE - feature articles
                             % ST - structural communications
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                             % (Following categories rarely in LaTeX)
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                             % CO - organic compounds
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                             % 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
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                             % LE - letters to the editor
                             % LN - laboratory notes
                             % ME - forthcoming meetings/short courses
                             % MR - meeting reports
                             % MN - notes and news
                             % NP - new commercial products
                             % OB - obituaries
                             % SR - software reviews
                             % TE - teaching and education

\paperlang(english)          % Can be english, french, german or russian
%-----
% Information about journal to which submitted
%
```

- Authors strongly encouraged to use IUCr template (in **preprint mode**) – will closely match target sgml file for production
- Other styles (e.g. REVTeX) can be handled but more editorial intervention needed to create effective sgml translation

# BibTeX

```
1 :
2 @Book{          knuth84,
3   author       = "Donald E. Knuth",
4   title        = "The \TeX{}book",
5   publisher    = {Addison-Wesley},
6   year        = 1984
7 }
8
9 @Book{          lamport86,
10  author       = "Leslie Lamport",
11  title        = "{\LaTeX{}} A Document Preparation System",
12  publisher    = {Addison-Wesley},
13  year        = 1986
14 }
15
16 @Book{          NocedalWright2000,
17  author       = "Nocedal, J., and Wright, S.",
18  title        = "Numerical Optimization",
19  address     = "New York",
20  publisher    = {Springer},
21  year        = 2000
22 }
23
24 @book(Saad-book2,
25   author="Y. Saad", title={Iterative Methods for
26   Sparse Linear Systems, 2nd edition},
27   Publisher="SIAM", address="Philadelphia, PA", year="2003")
28
29
30 @Article{       pauling89,
31  author       = {Pauling, L.},
32  title        = {},
33  journal      = {Proc. Natl Acad. Sci},
34  volume      = {86},
35  pages       = "8595--8599",
36  year        = 1989
37 }
38
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41  title        = {},
42  journal      = {Acta Cryst.},
43  volume      = {D51},
44  pages       = "663--681",
45  year        = 1995
46 }
47
48 @Article{       kabsch93,
49  author       = {Kabsch, W.},
50  title        = {},
51  journal      = {J. Appl. Cryst.},
52  volume      = {26},
53  pages       = "795--800",
54  year        = 1993
55 }
56
57 @Article{       kabsch2010,
```

- LaTeX submissions usually have an associated bibliography (BibTeX) file
- BibTeX files contain structured information and allow references to be automatically formatted in journal style (provided the quality of information in the BibTeX file is reasonable)



# Other tools (ask for a demonstration)

## pubCIF

- Standalone tool for editing CIFs and previewing them in journal style
- Used mainly for submissions to Sections C and E
- pubCIF engine underlies WORD template and pubBio
- Popular, well established and widely distributed; used by most C and E Co-editors

## Enhanced figure toolkit

- Available as a standalone tool or within the submission system
- Creates standard figures for inclusion in the “archived” journal and corresponding 3D interactive figures
- Easy to use, but not yet adopted by the majority of authors
- Interactive figures can be created from small molecule and macromolecular CIFs

## Chemistry toolkit

Work is in progress on a chemistry toolkit, to allow chemical connectivity information and diagrams to be created from CIFs on a routine basis

## Other toolkits

What else should we be working on?

Over to Louise for info on publBIO

