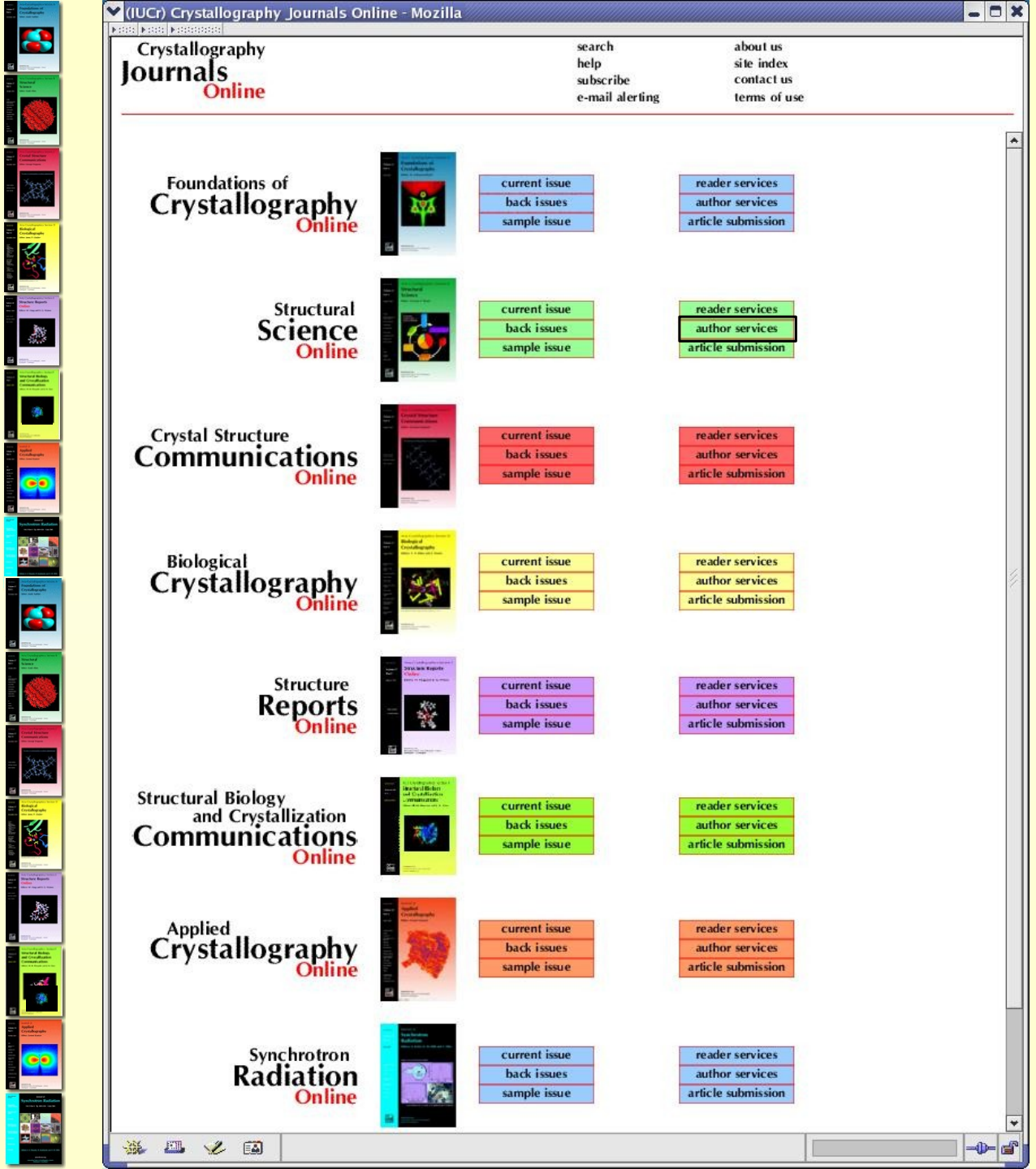
Commission on Journals 2011

2013 international year of crystallography

Crystallography Journals Online

IUCr templates and tools

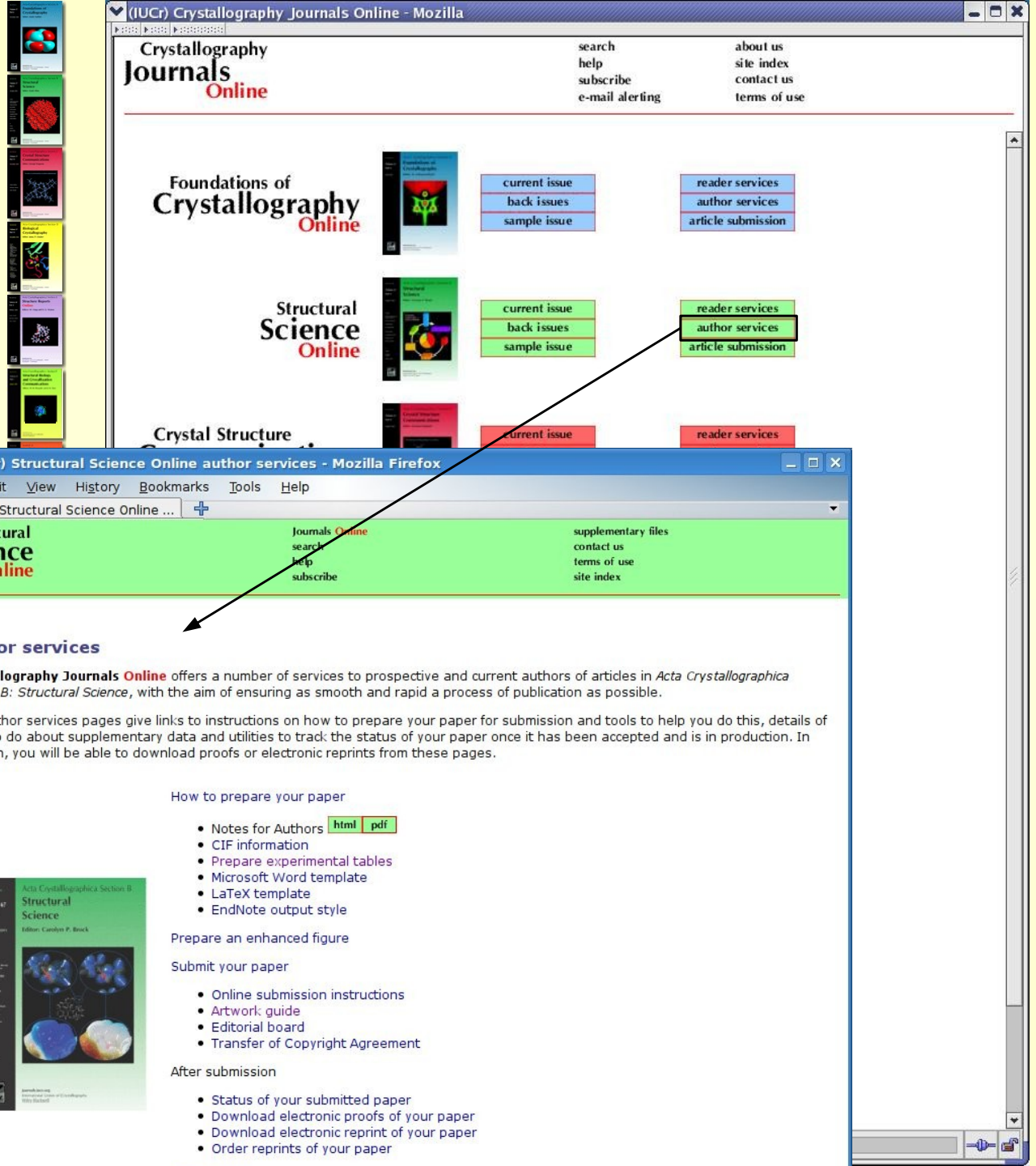
Crystallography Journals Online



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

Crystallography Journals Online

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

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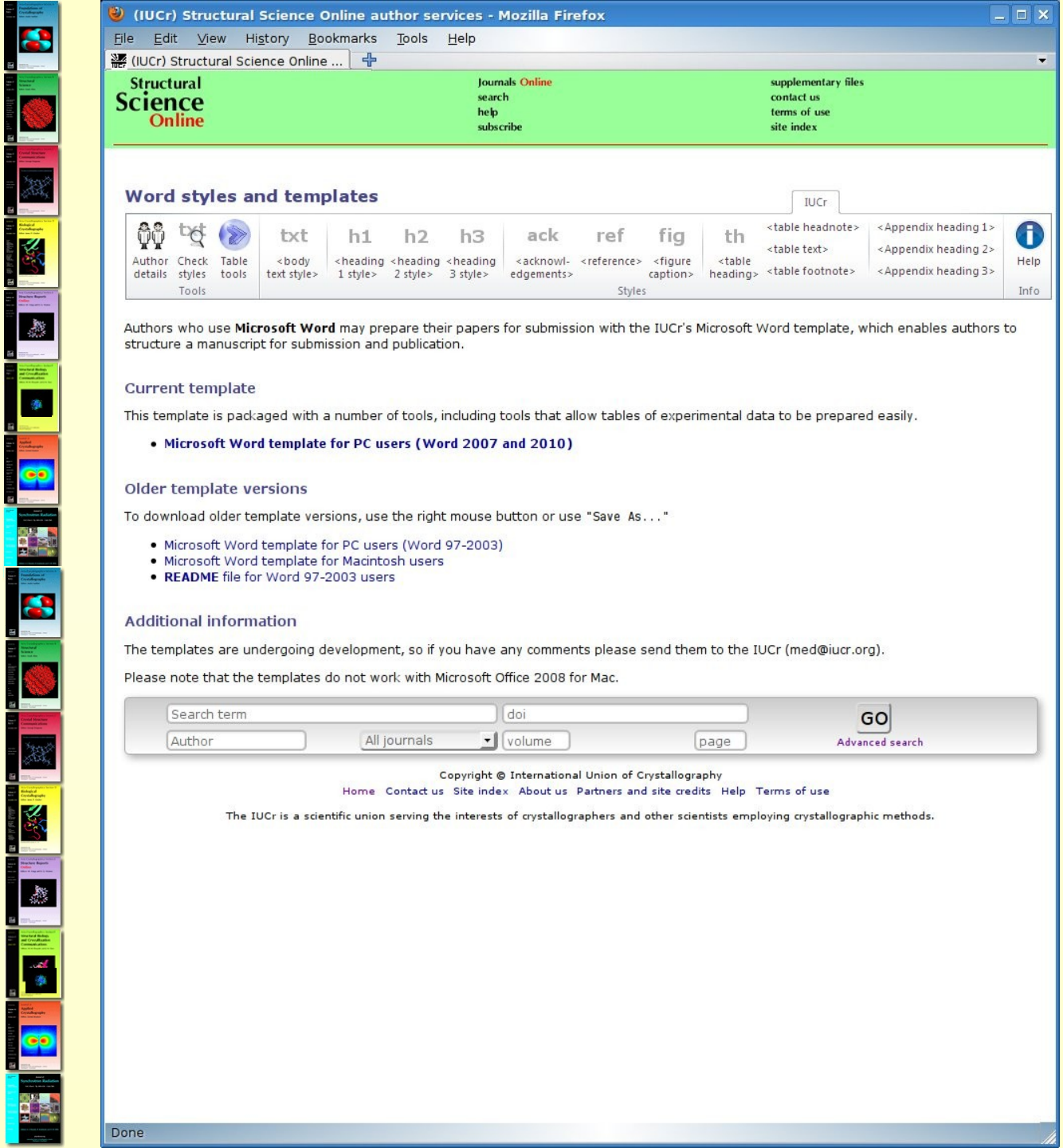
WORD Template

Crystallography Journals Online



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

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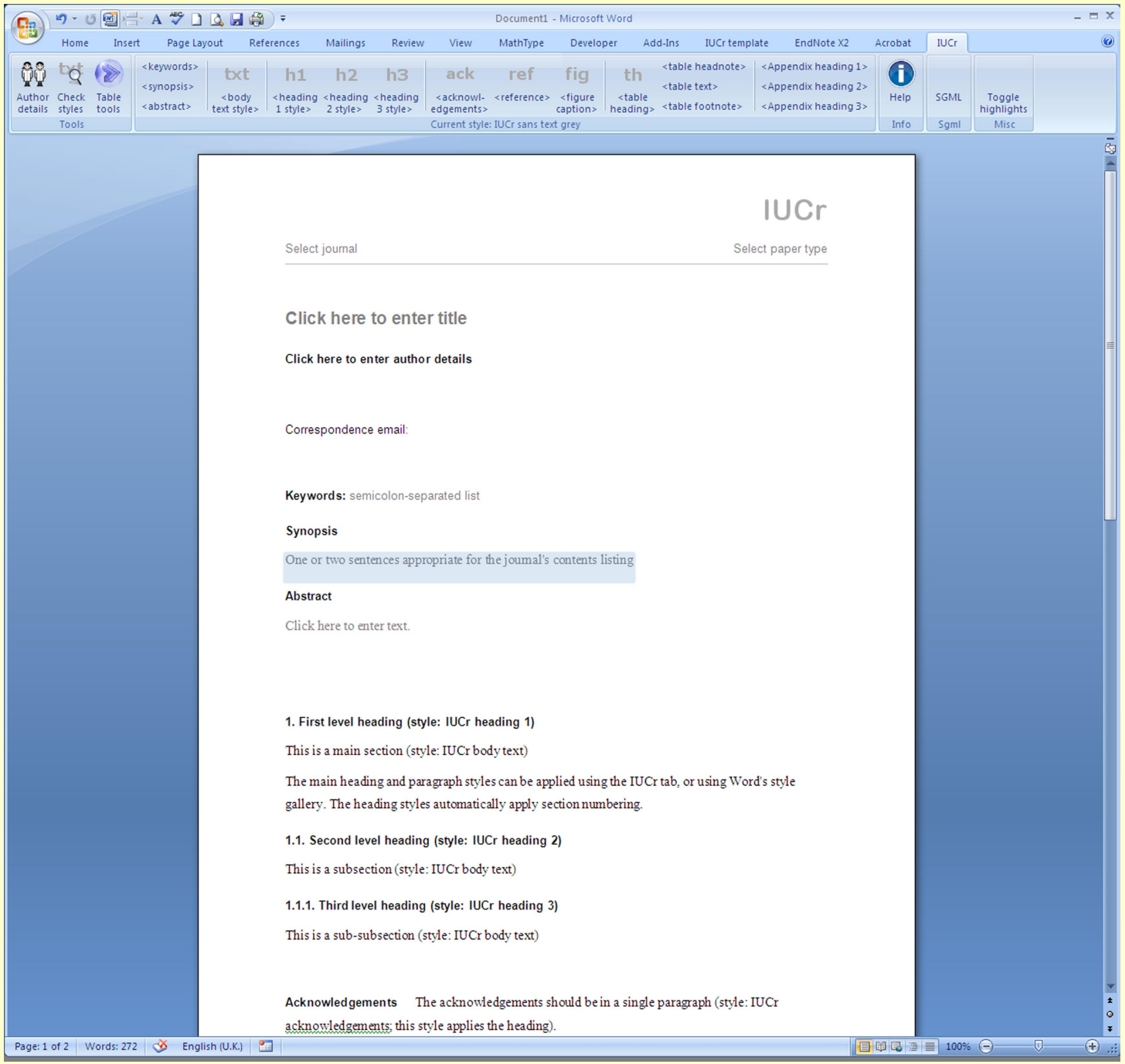

- Template packaged with tools:
- Interacts with external resources, *e.g.* World Directory
- Allows a personal database of author details to be collected
- Articles can be written in template or imported and marked up

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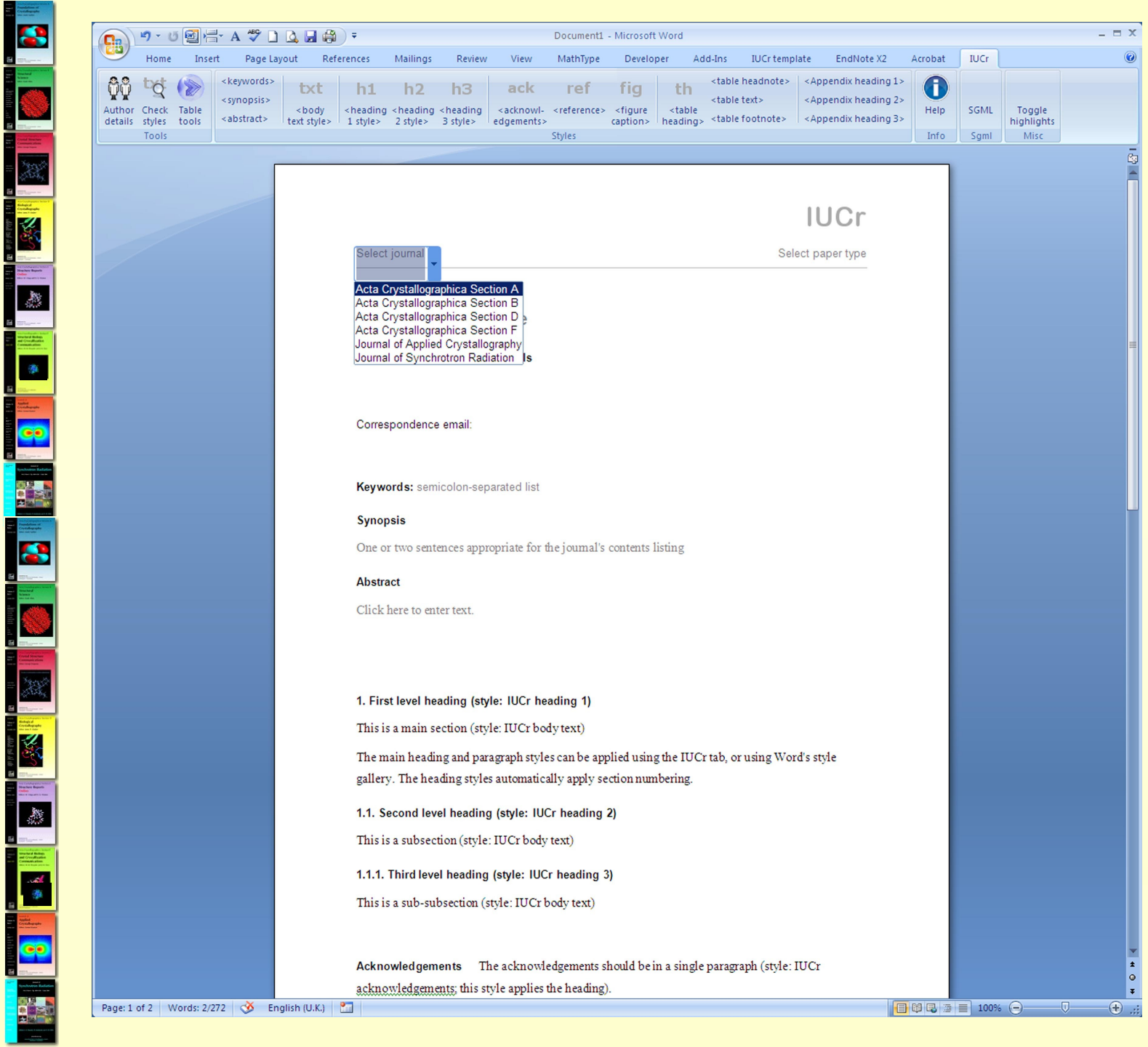
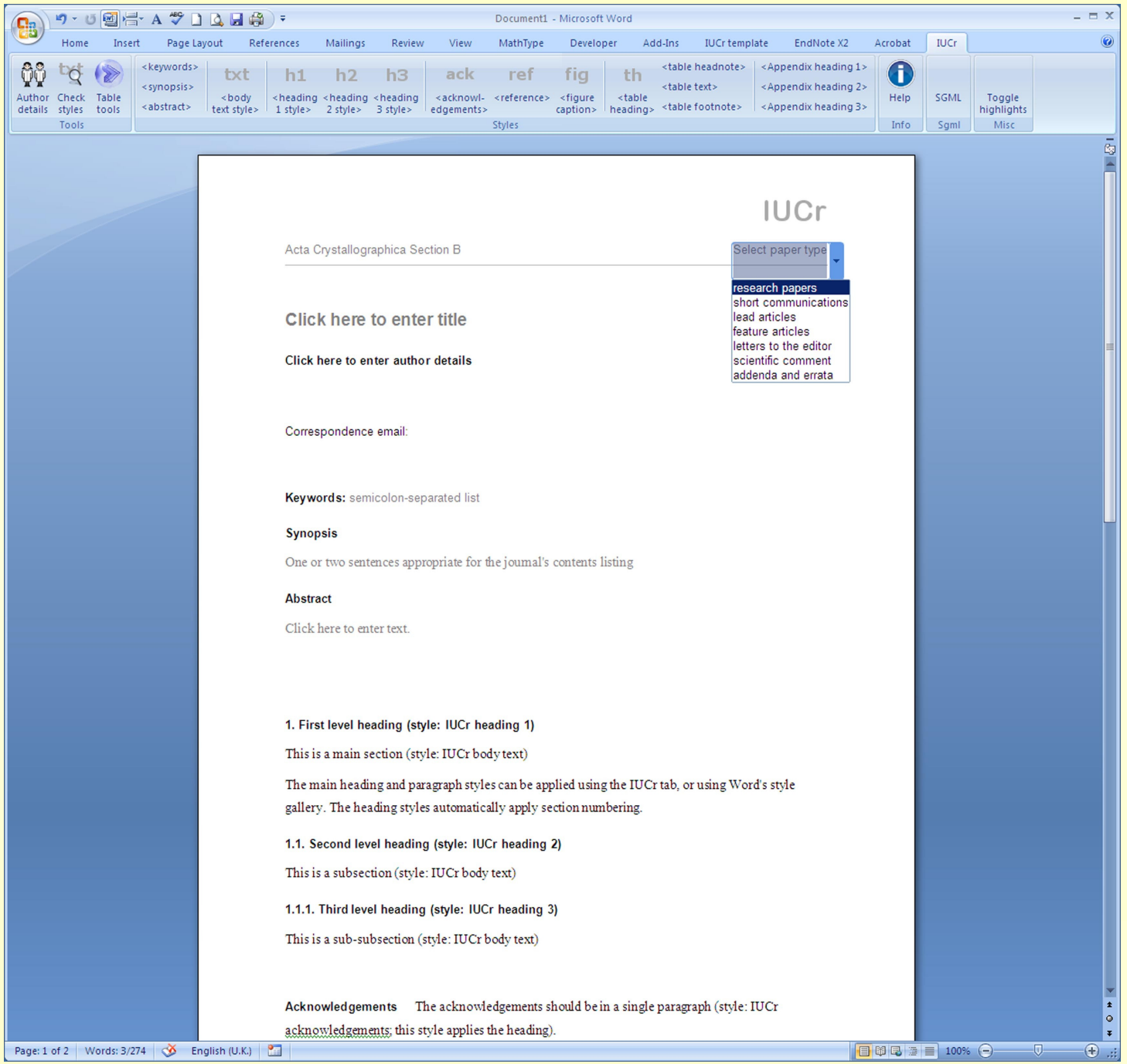


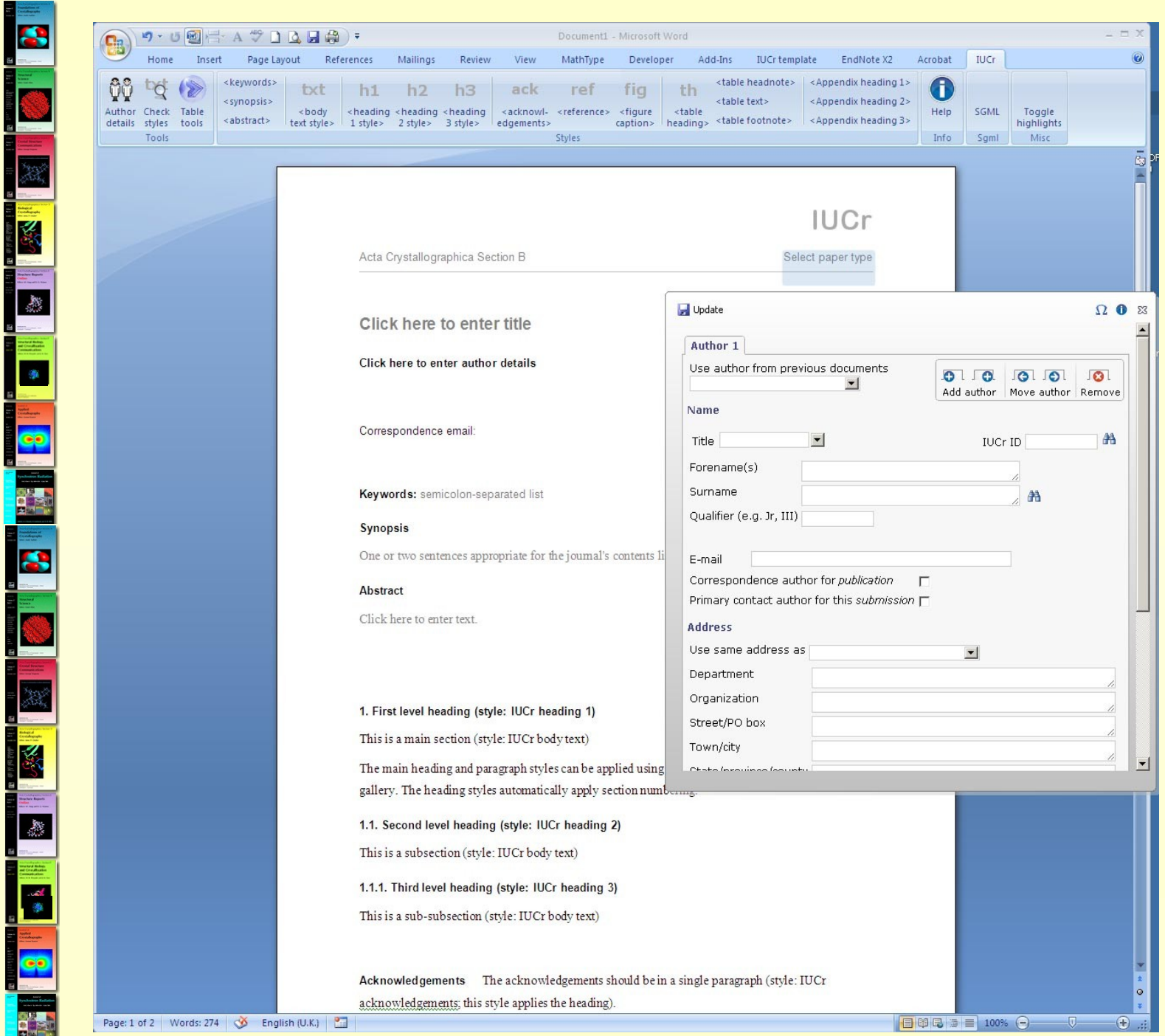
- Use drop-down menu lists to select journal

Crystallography Journals Online



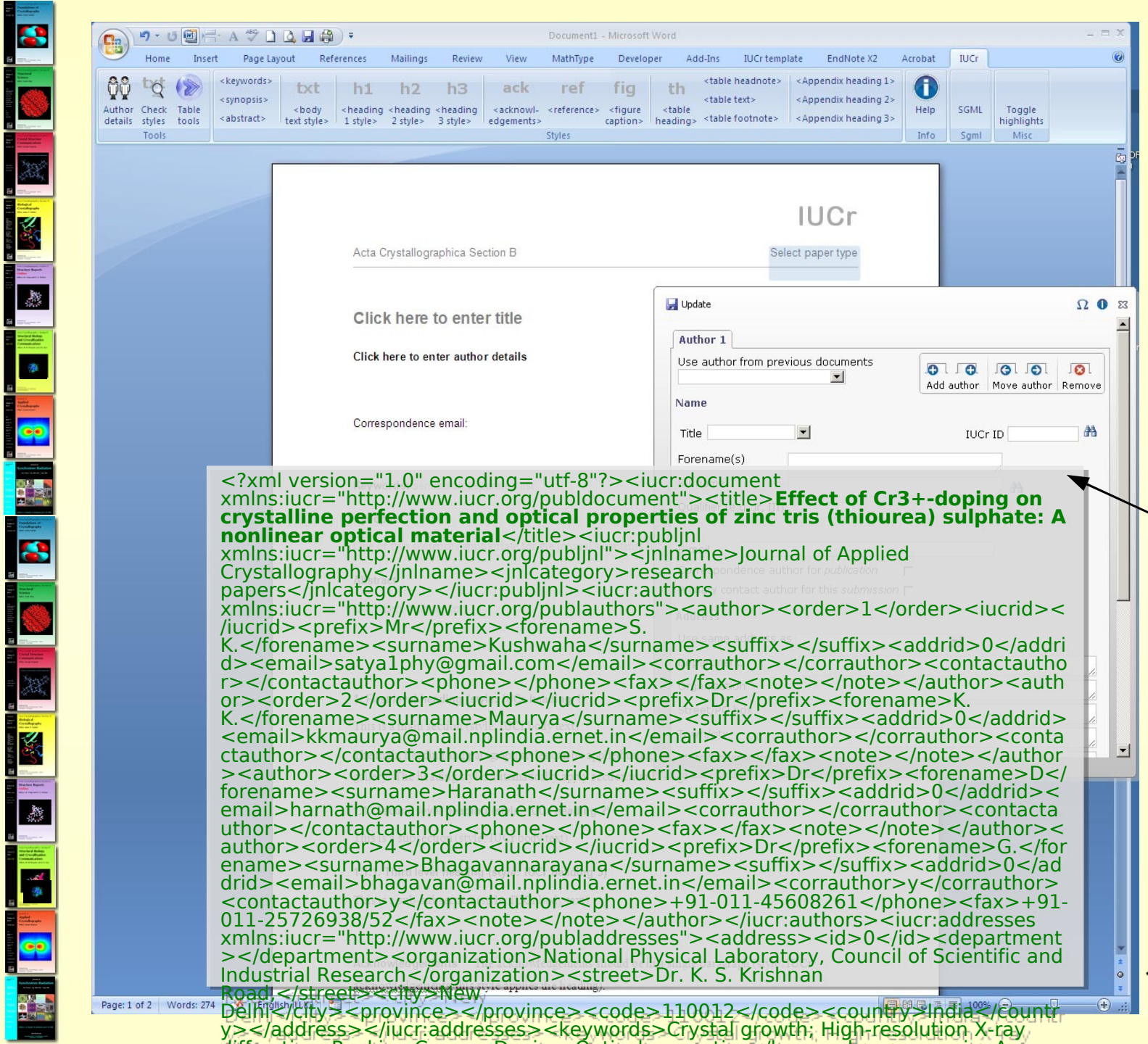
- Select paper type
- Click to add title, keywords, synopsis and abstract

Crystallography Journals Online



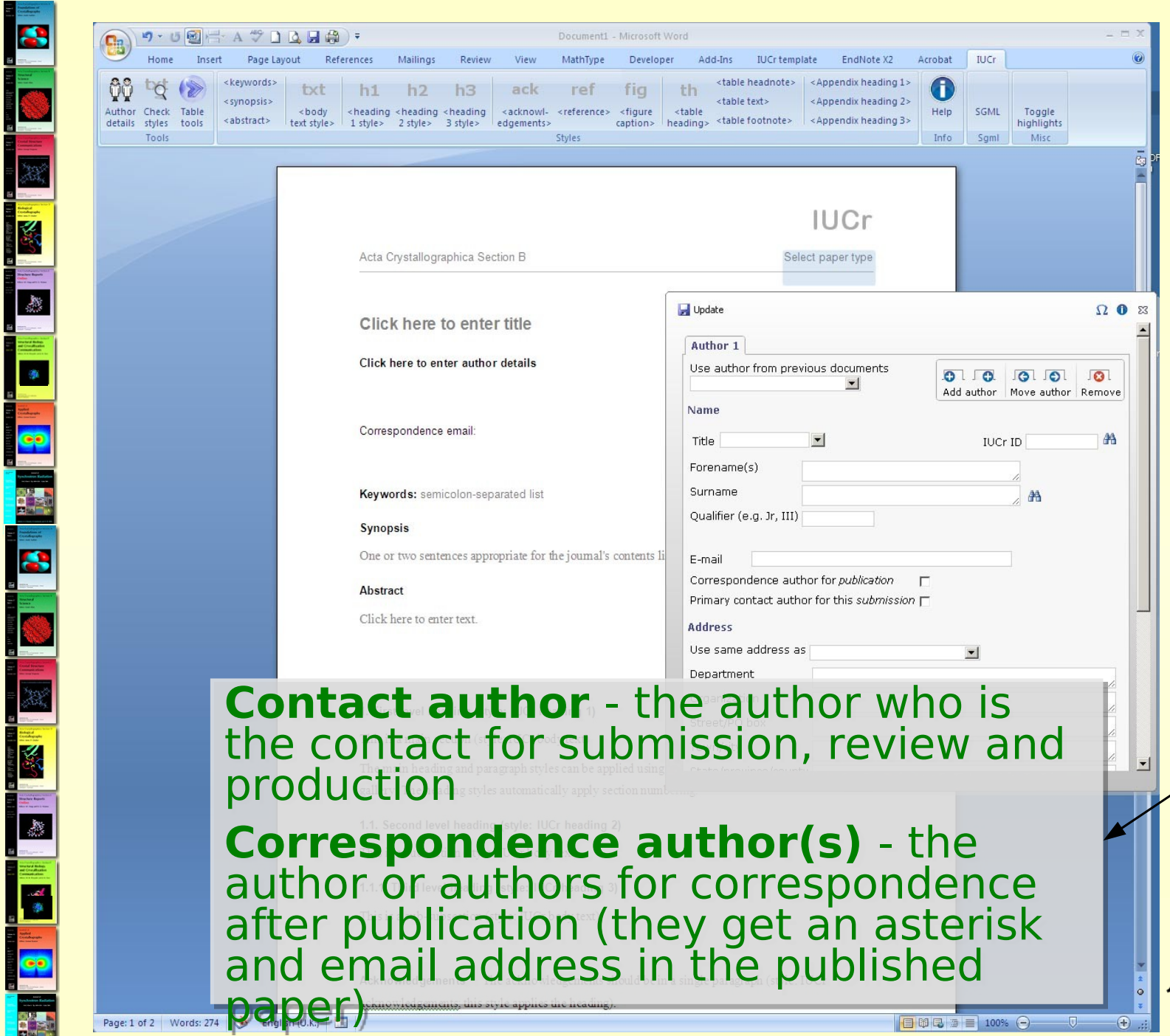
- Author details entered *via* menu
- Details formatted to journal style
- Information can be reused during submission

Crystallography Journals Online



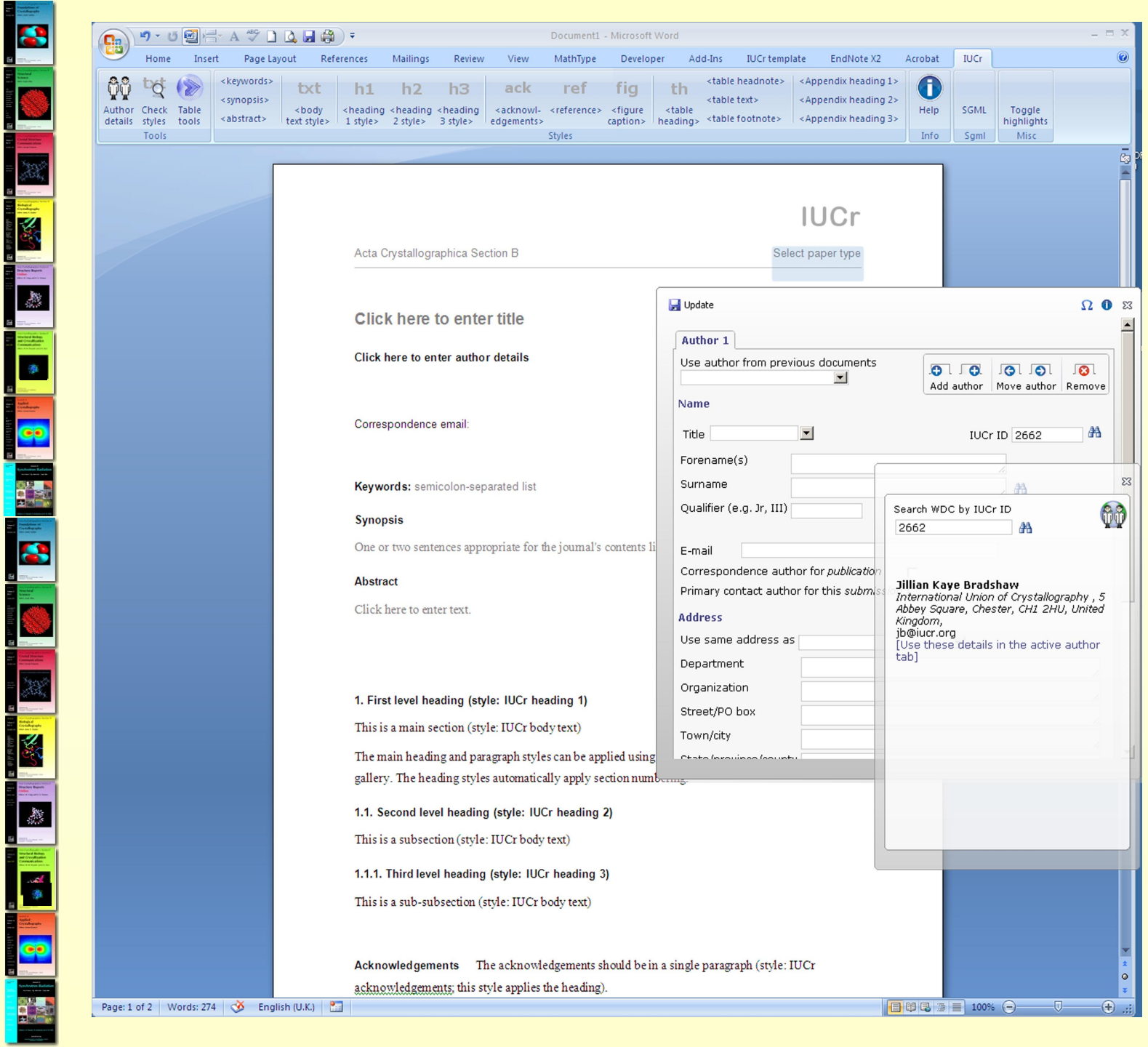
- Author details entered *via* menu
- Details formatted to journal style
- Information can be reused during submission
- Details stored as XML in zip file within document and in local database

Crystallography Journals Online



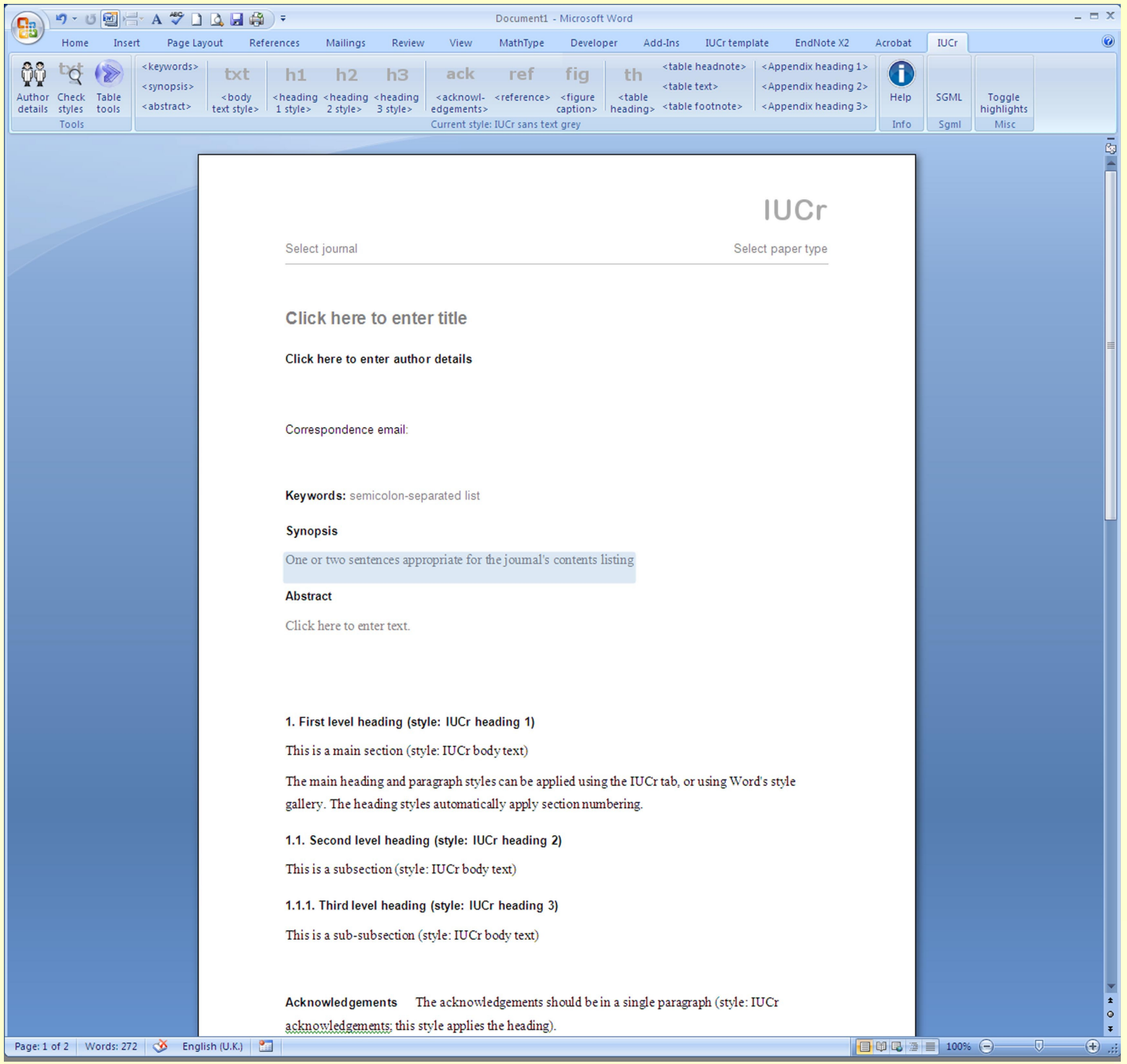
- Author details entered *via* menu
- Details formatted to journal style
- Information can be reused during submission
- Details stored as XML in zip file within document and in local database
- Contact and corresponding authors can be distinguished

Crystallography Journals Online



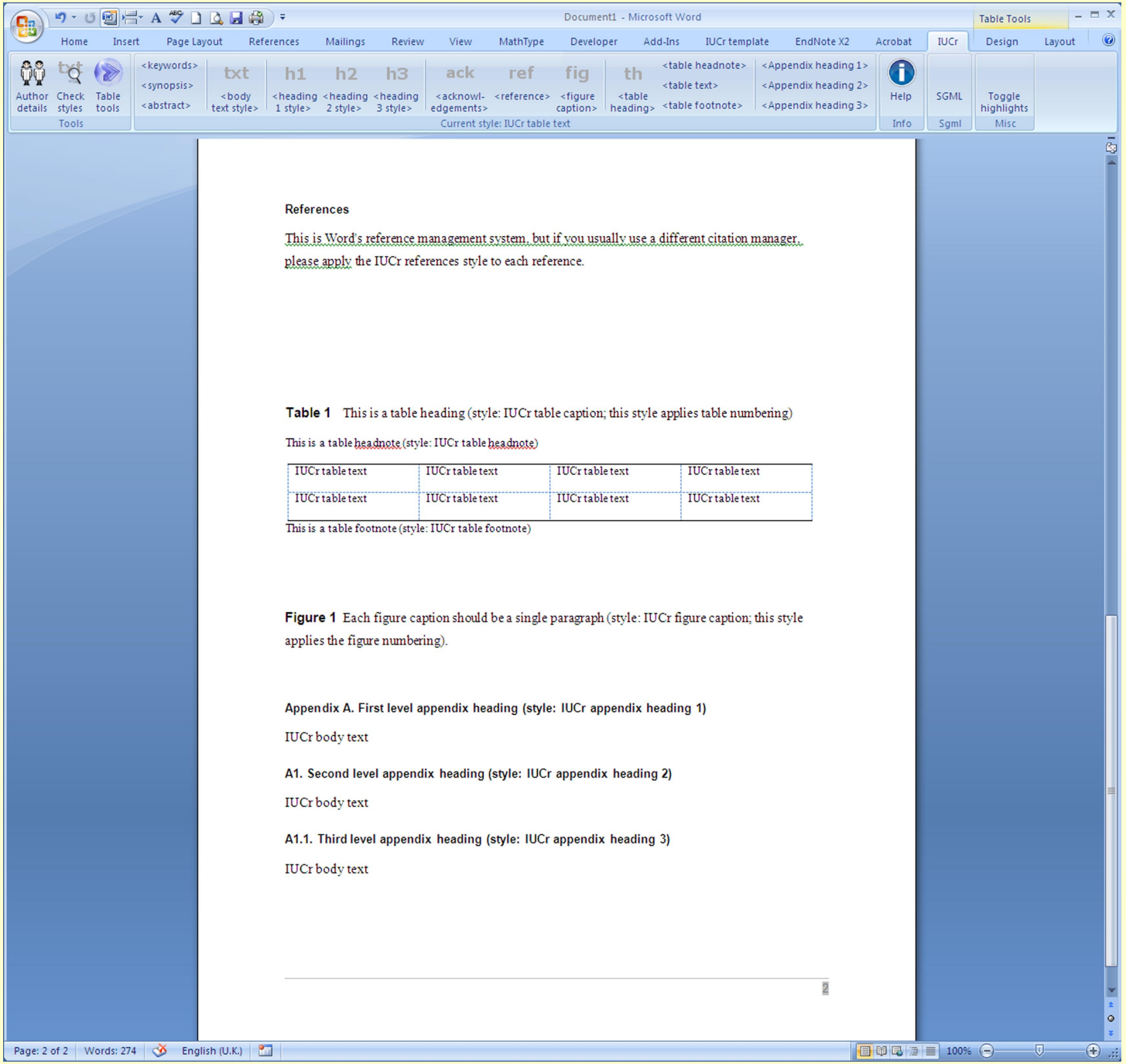
- Details can be retrieved from the World Directory
- In the future, author details could be picked up from services such as ORCID or from previous journal authors

Crystallography Journals Online



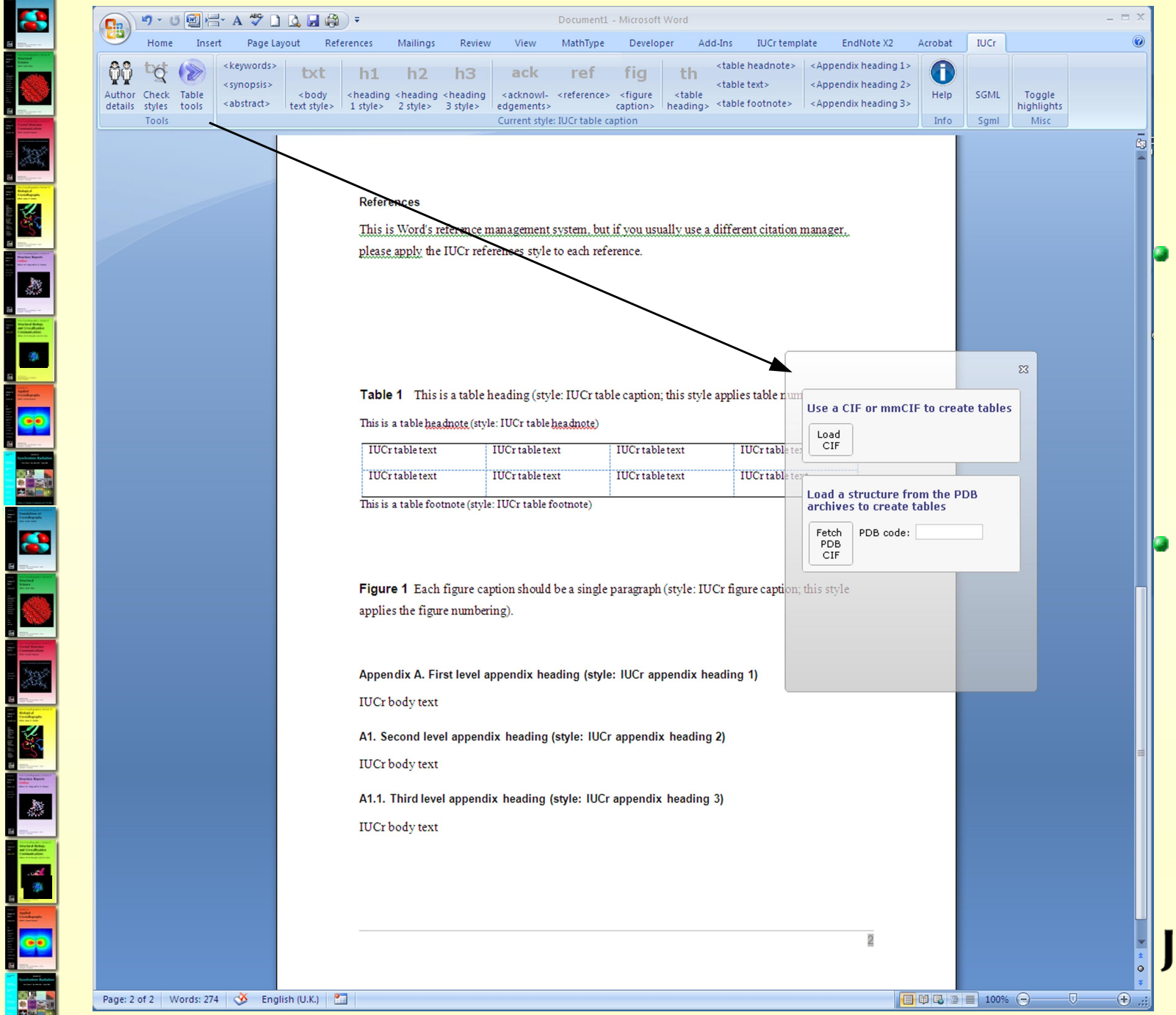
- Mark up text with styles, *e.g.* first-, second- or third-level headings
- Styles also available from IUCr ribbon

Crystallography Journals Online



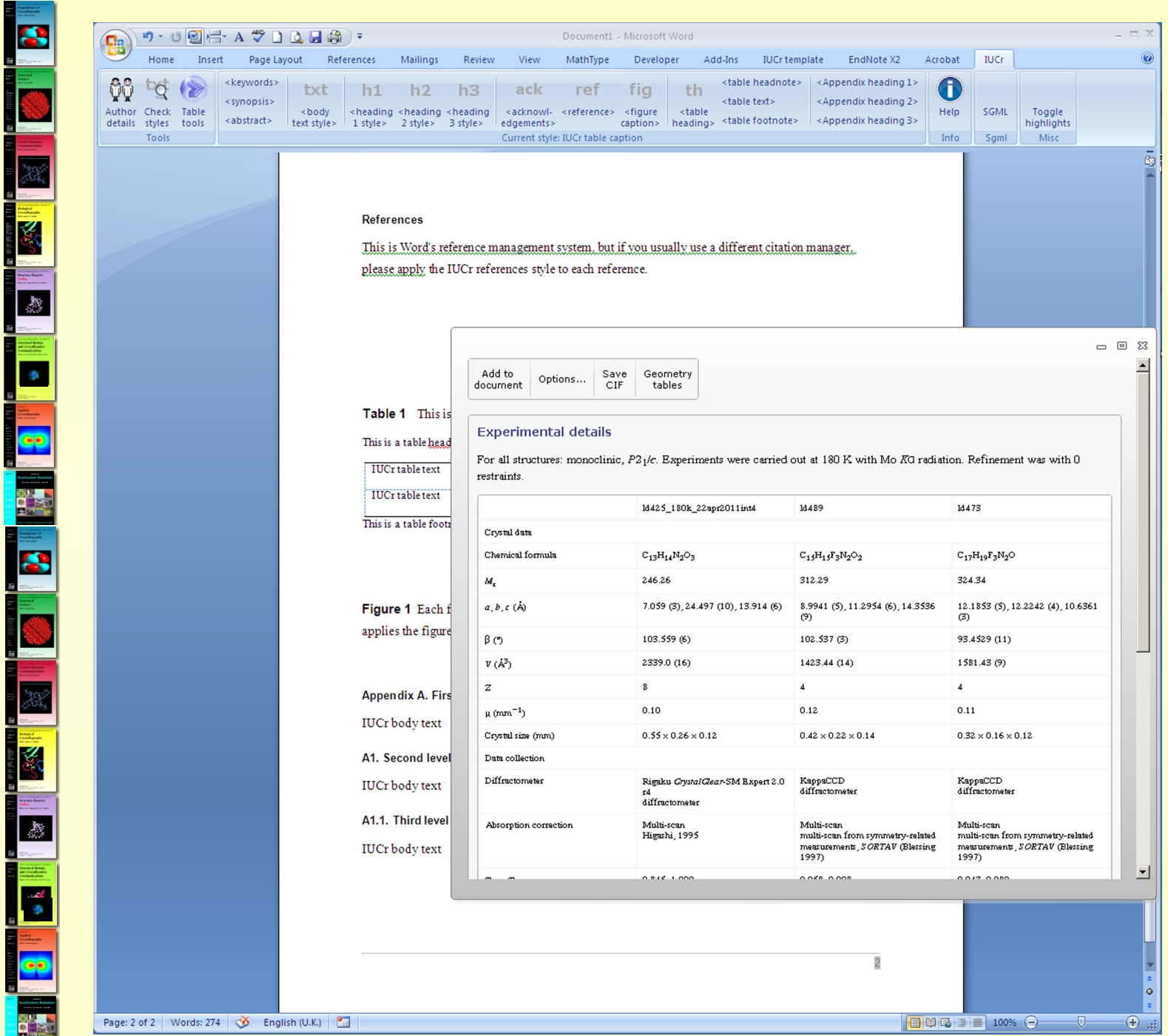
- Tables should be prepared using WORD's table editor with styles applied to caption, headnotes and footnotes
- Experimental tables can be prepared using **Table tools**

Crystallography Journals Online



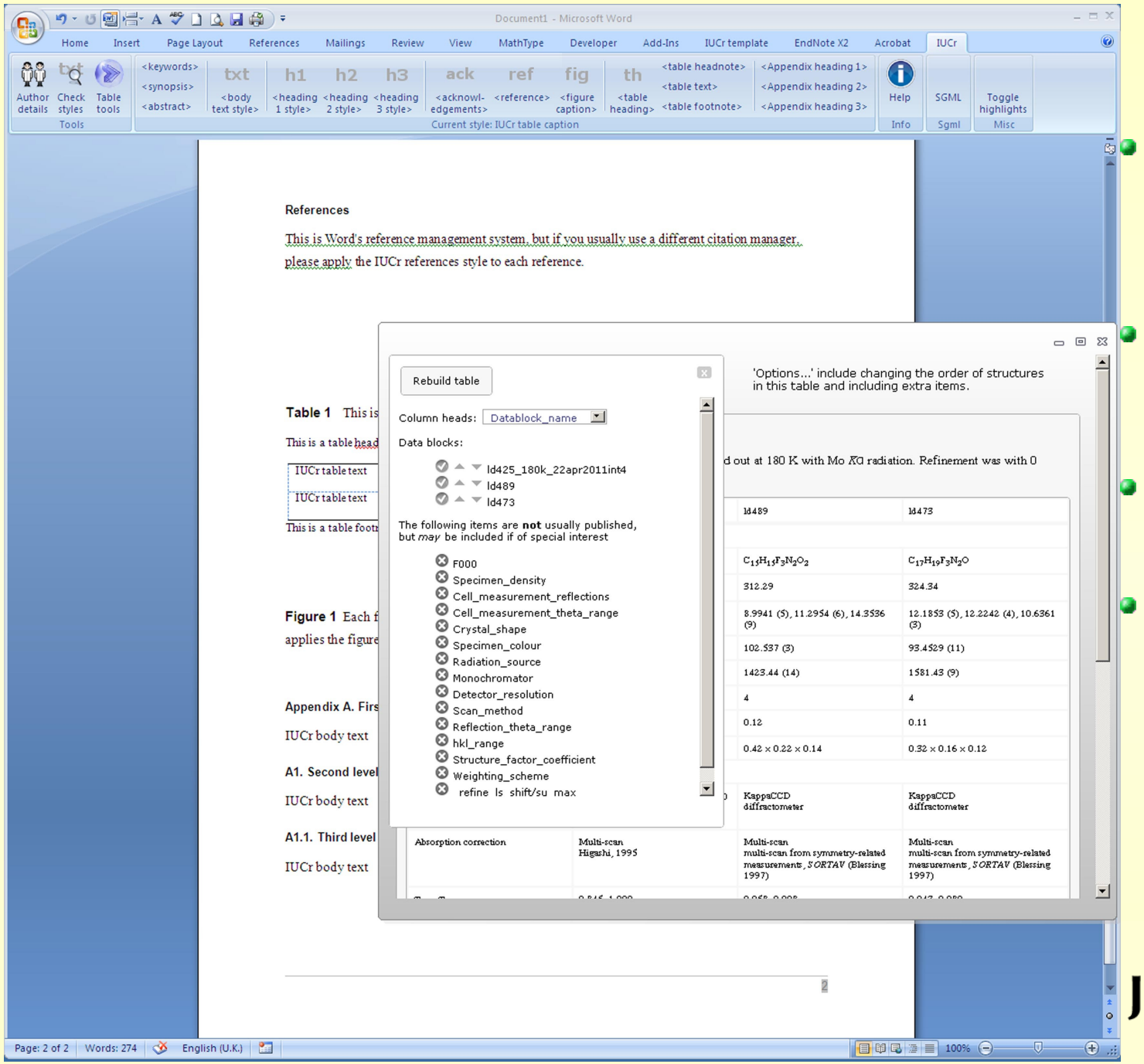
- Use **Table tools** to prepare experimental tables from CIF for small molecule structures
- For macromolecular structures use PDB code to import mmCIF to create table of experimental details

Crystallography Journals Online



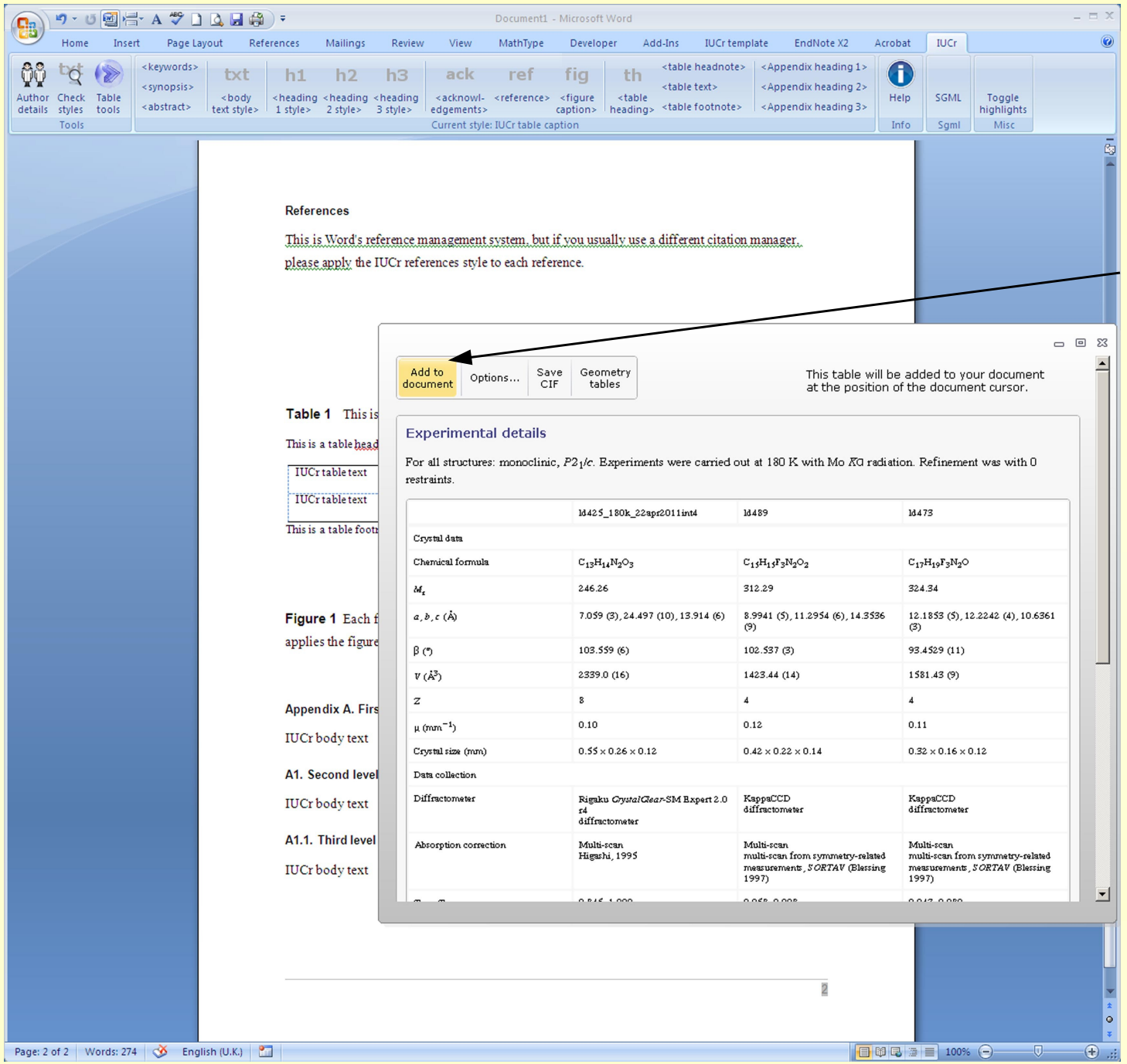
- Each datablock from CIF appears as column in table

Crystallography Journals Online



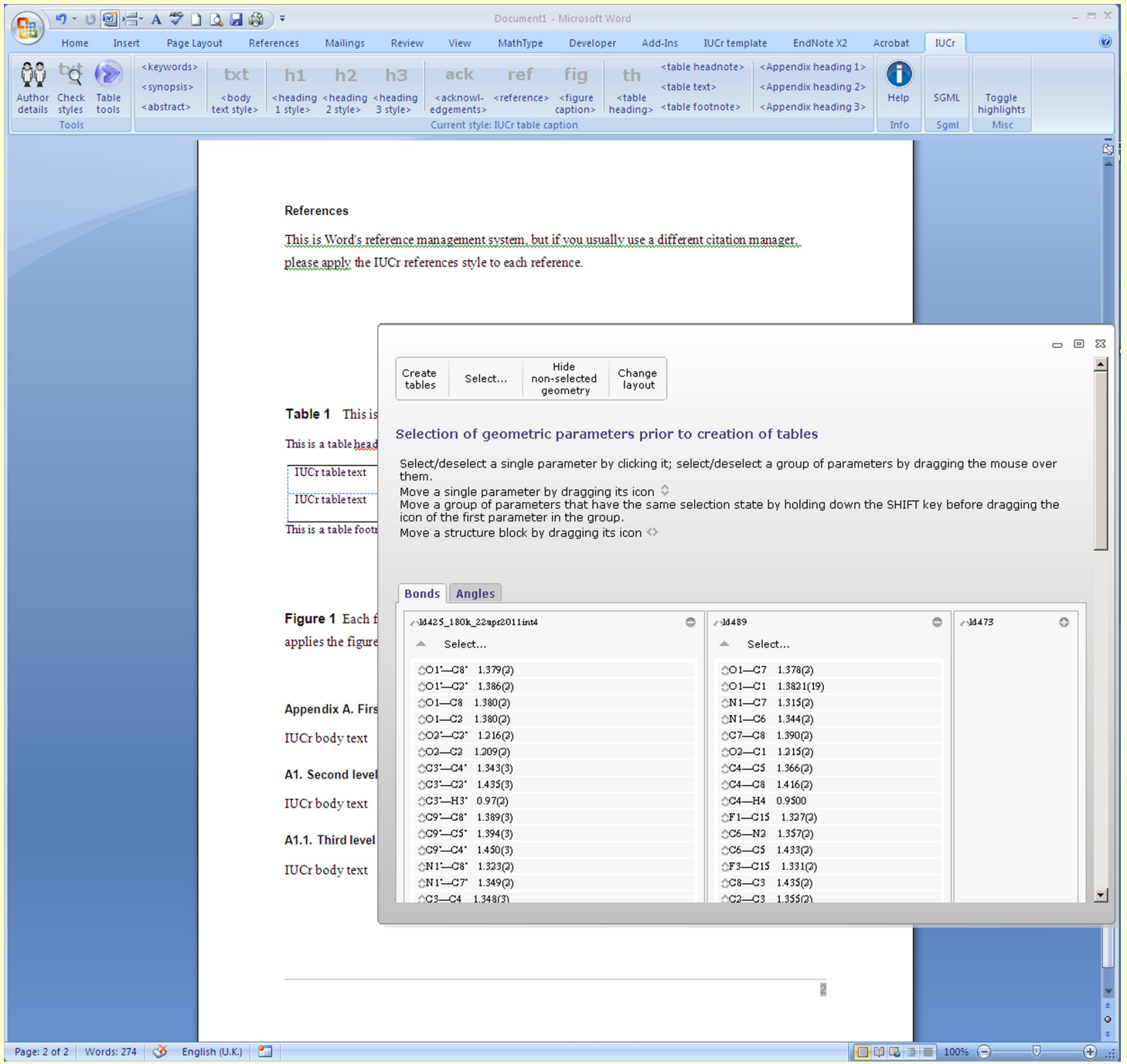
- Extra non-standard items present in CIF can be added to table
- Datablocks can be selected for inclusion or exclusion
- Several types of column headings can be selected
- Small molecule, powder and incommensurate CIFs handled

Crystallography Journals Online



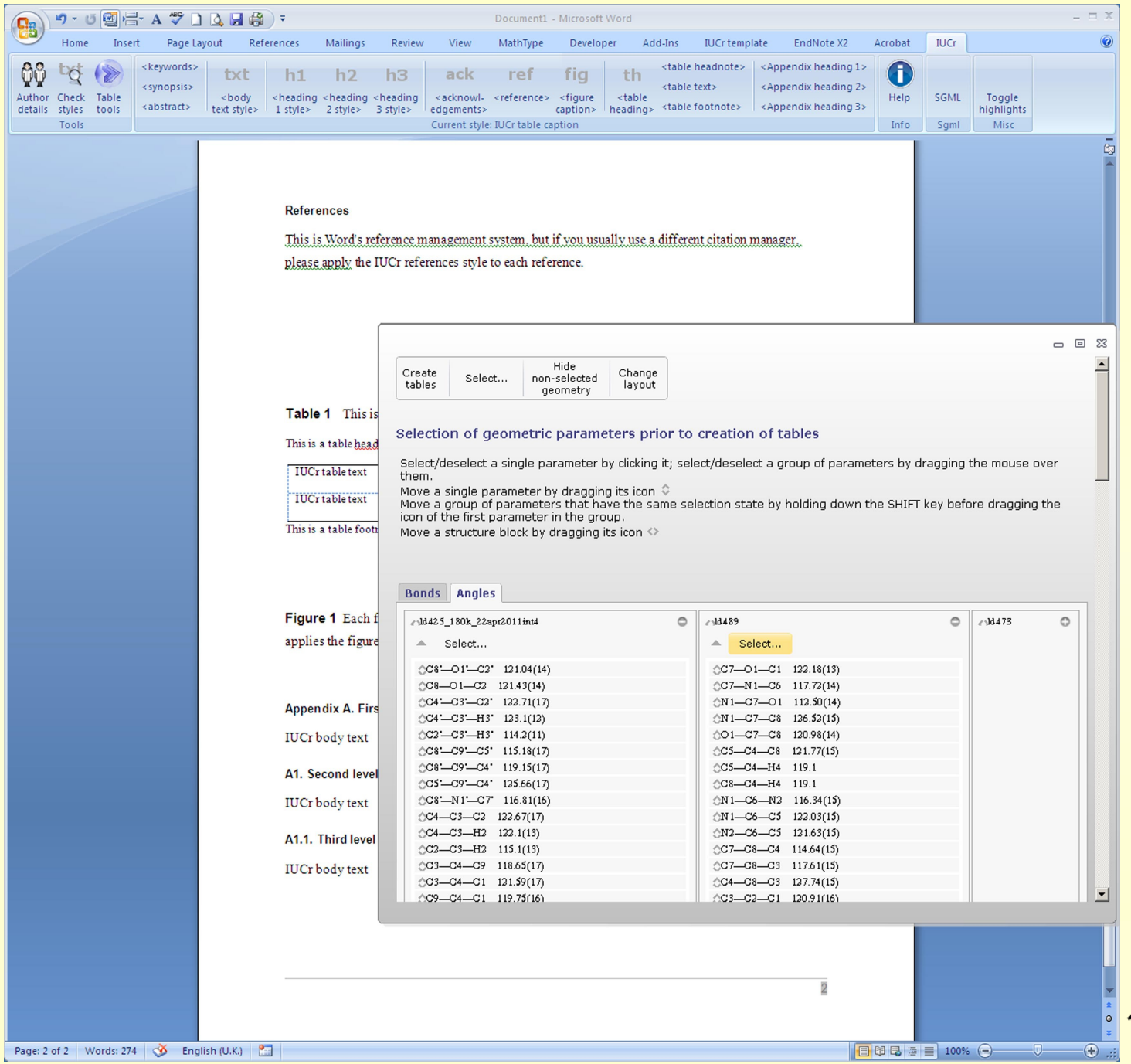
- Once all items have been selected, the experimental table can be added to the document

Crystallography Journals Online



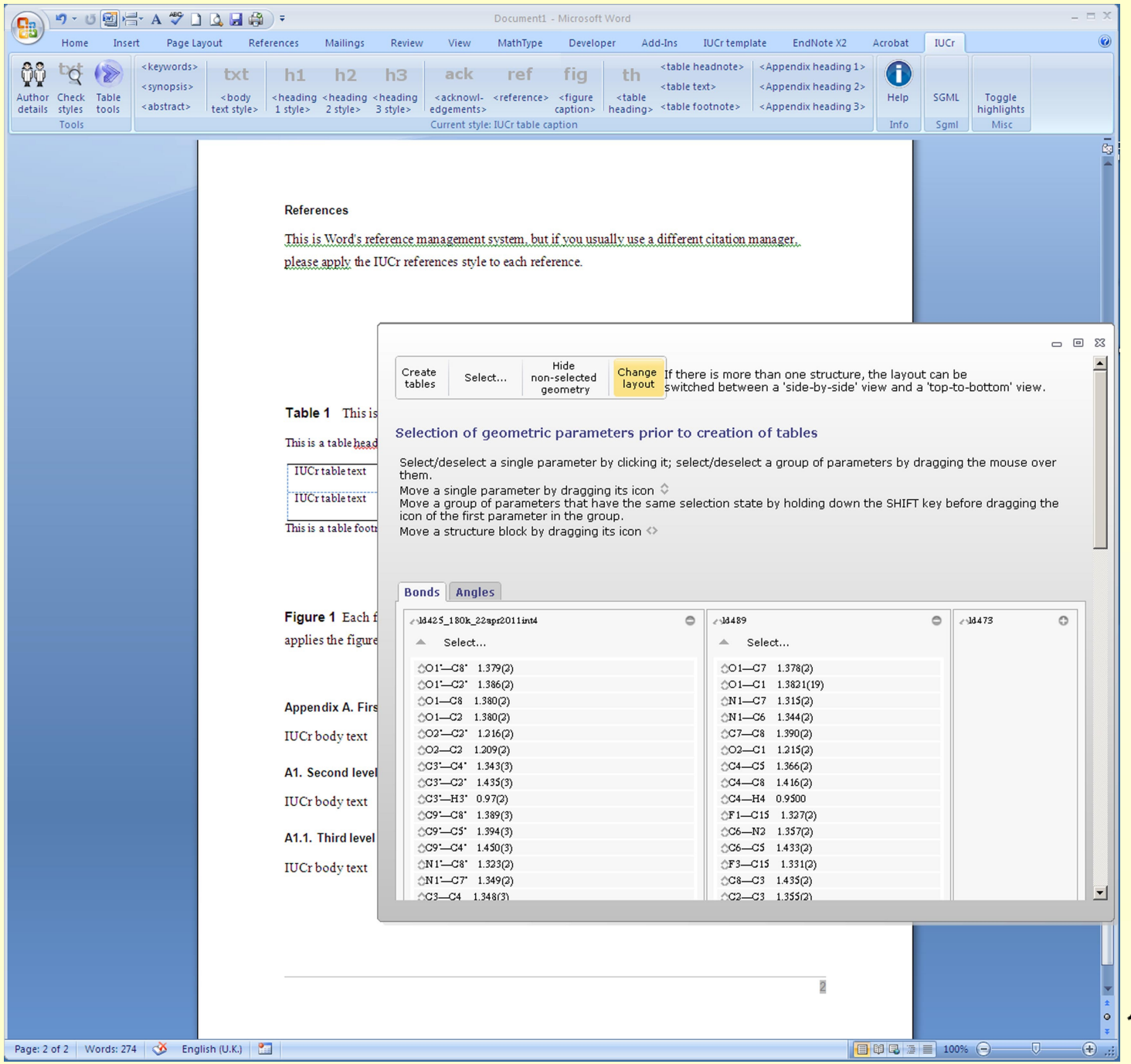
- Can also create geometry tables from CIF

Crystallography Journals Online



- Can also create geometry tables from CIF
- Can select which bonds and angles to include in table

Crystallography Journals Online



- Can also create geometry tables from CIF
- Can select which bonds and angles to include in table
- Layout can be changed to accommodate comparison tables

Crystallography Journals Online

be5173.doc.copy.docx - Microsoft Word

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

Author details | Check styles | Table tools | <keywords> <synopsis> <abstract> | <body text style> | <heading 1 style> <heading 2 style> <heading 3 style> | <acknowl-edgements> <reference> <figure caption> | <table heading> <table headnote> <table text> <table footnote> | <Appendix heading 1> <Appendix heading 2> <Appendix heading 3> | Help | SGML | Toggle highlights

Tools | Current style: Heading 3 | Info | Sgml | Misc

Table 2 Data collection and refinement statistics

Data collection	
Resolution range (Å)	49.43-2.9 (3.06-2.9)[a]
Unit cell	
(Å)	132.5, 196.7, 170.8
(°)	90.0, 92.8, 90.0
Space group	$P2_1$
Redundancy	4.2 (4.2)
Reflections	805846
Unique reflections	193013
Completeness (%)	100 (99.9)
[b]R_{merge} (%)	12.0 (56.6)
$I/\sigma I$	10.7 (2.5)
Refinement	
Range (Å)	20.0-2.9
Reflections used	191418
[c]R/R_{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 (100th percentile)
Poor rotamers (%)	3.91
Ramachandran (%)	
Favoured	96.28
Allowed	3.59
Disallowed	0.13
C^β deviations > 0.25 Å	18
MolProbity score	1.90 (99th 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: 2xq1

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

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

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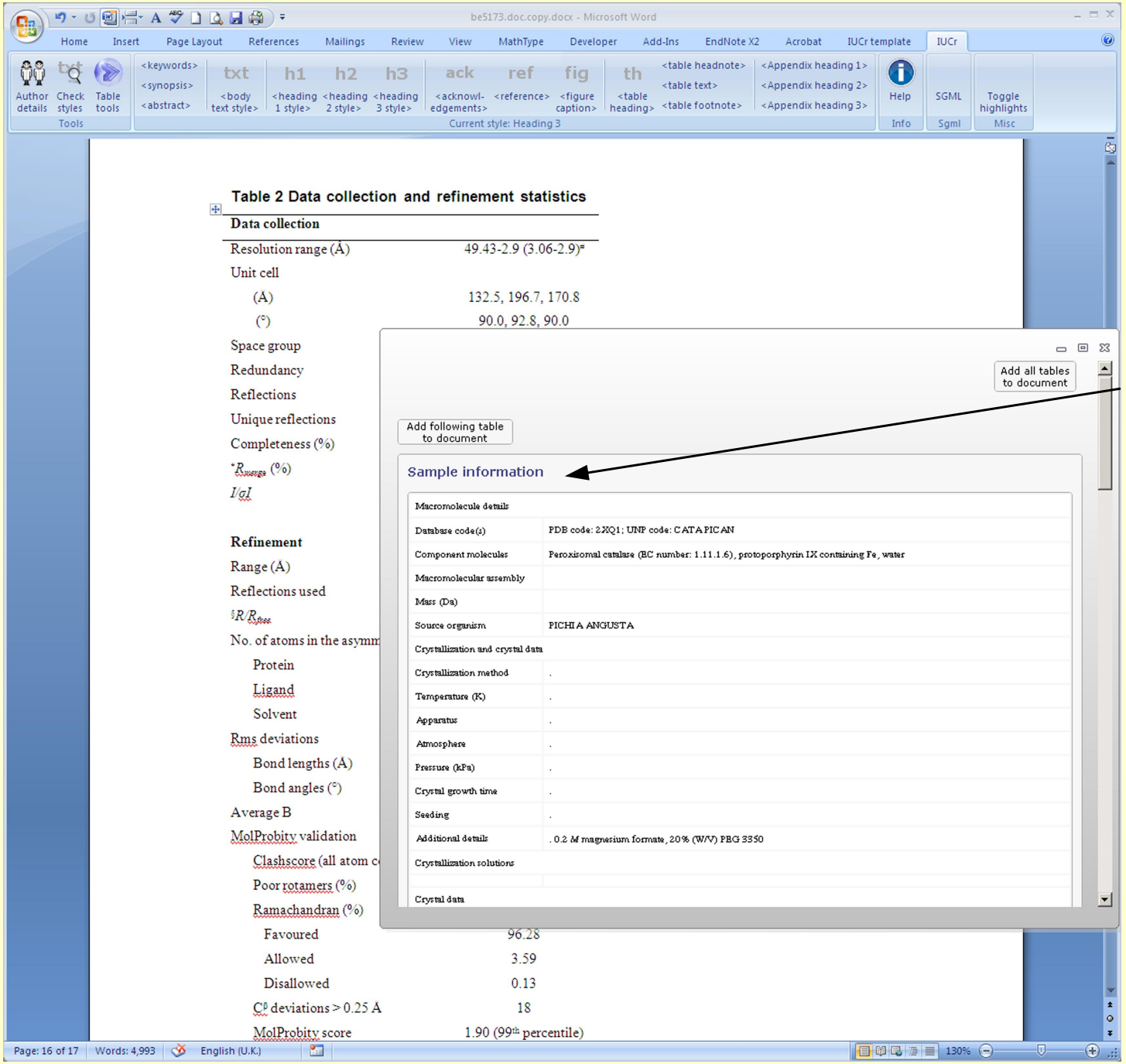

- Tables generated containing
- Sample information

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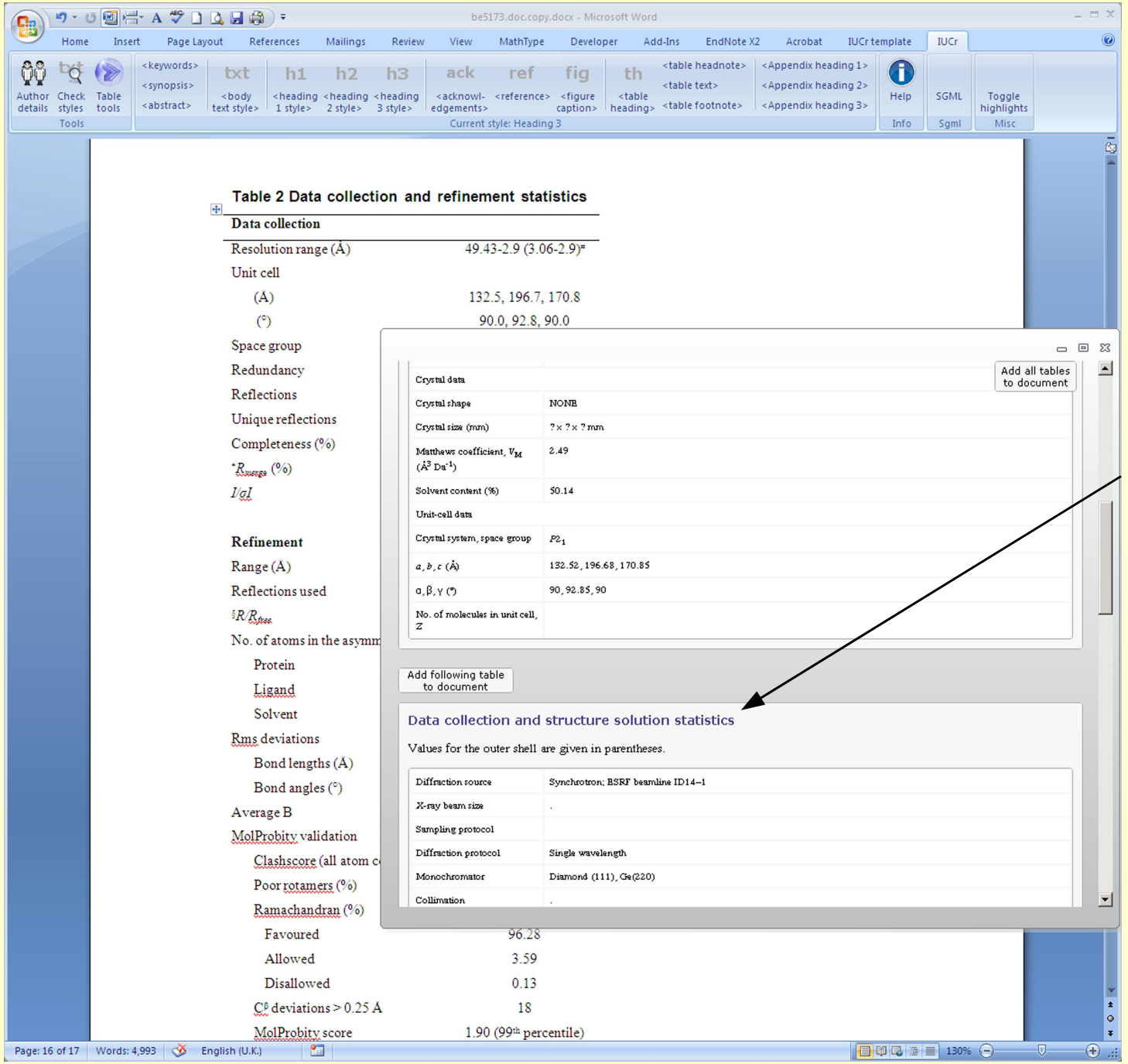
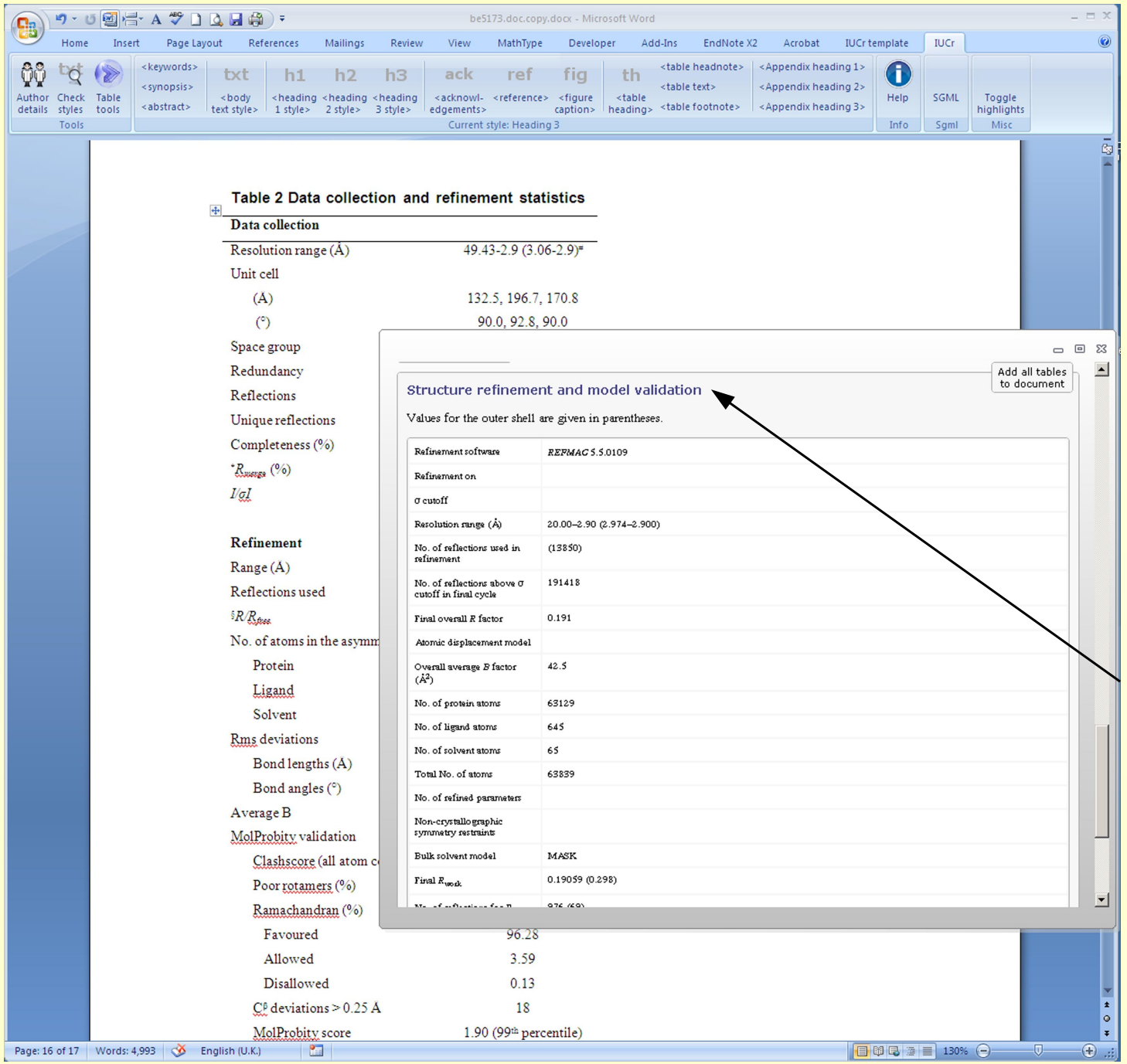


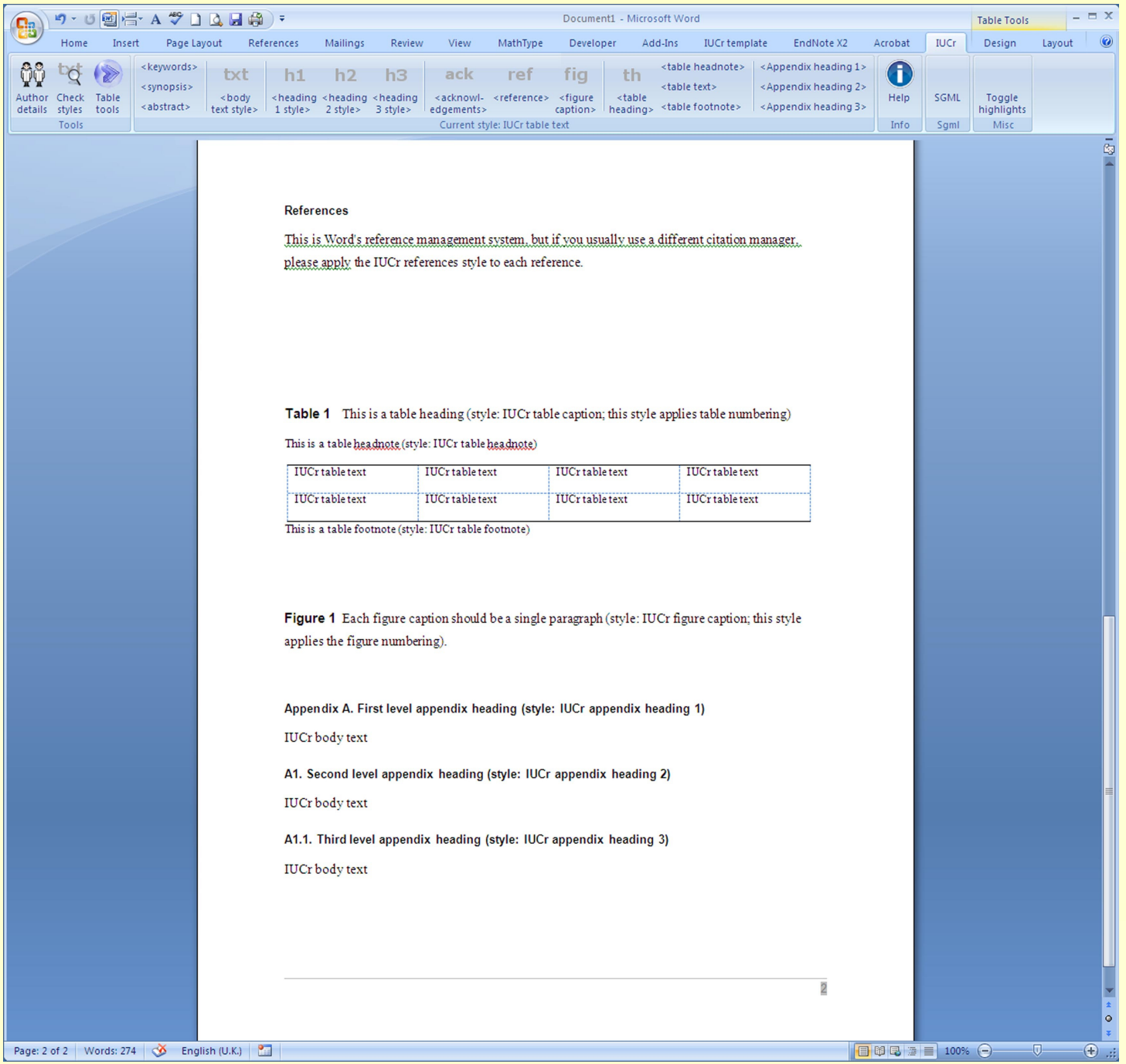
- Tables generated containing
- Sample information
- Data collection and structure solution statistics

Crystallography Journals Online



- Tables generated containing
- Sample information
- Data collection and structure solution statistics
- Structure refinement and model validation

Crystallography Journals Online



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

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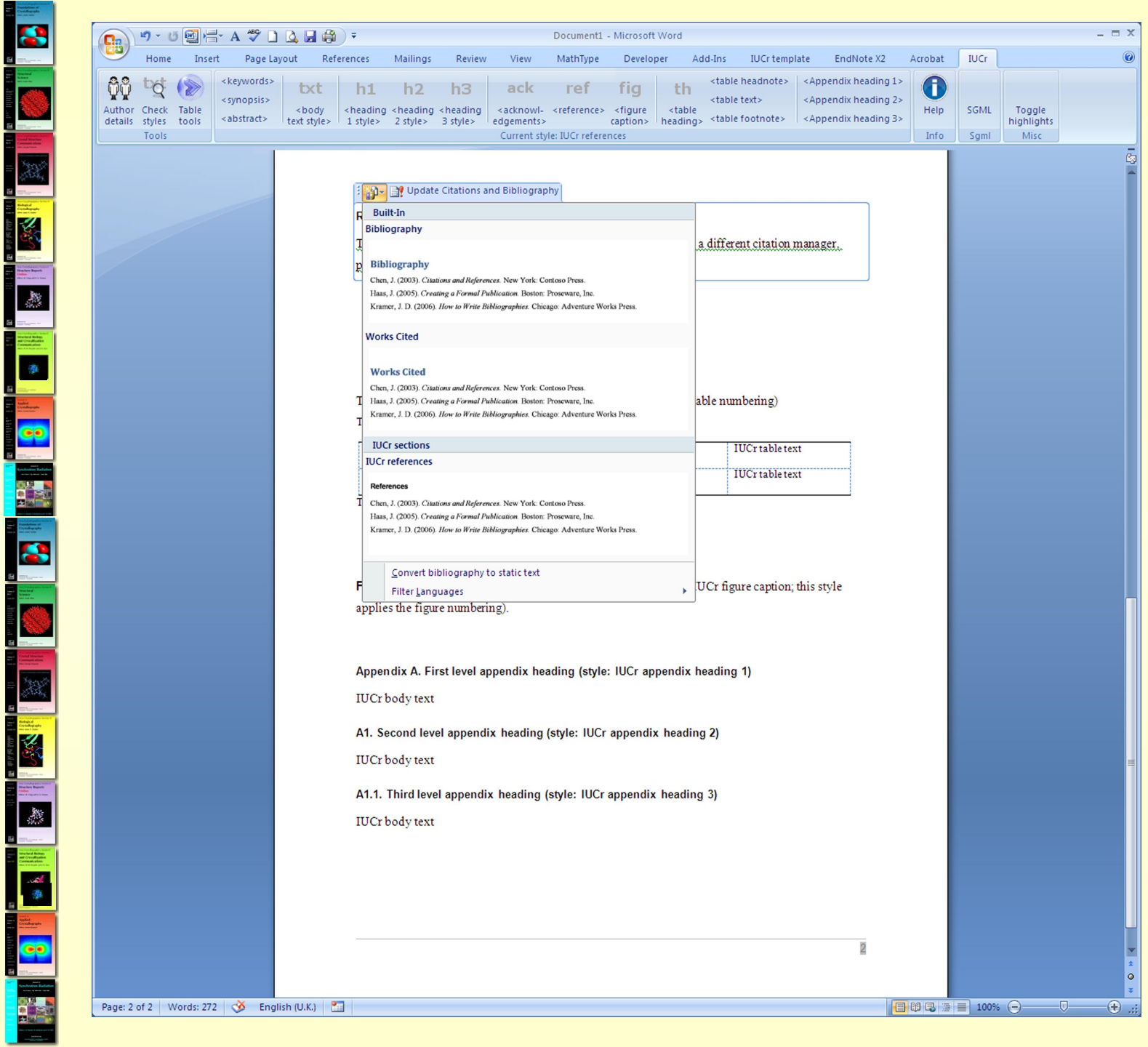
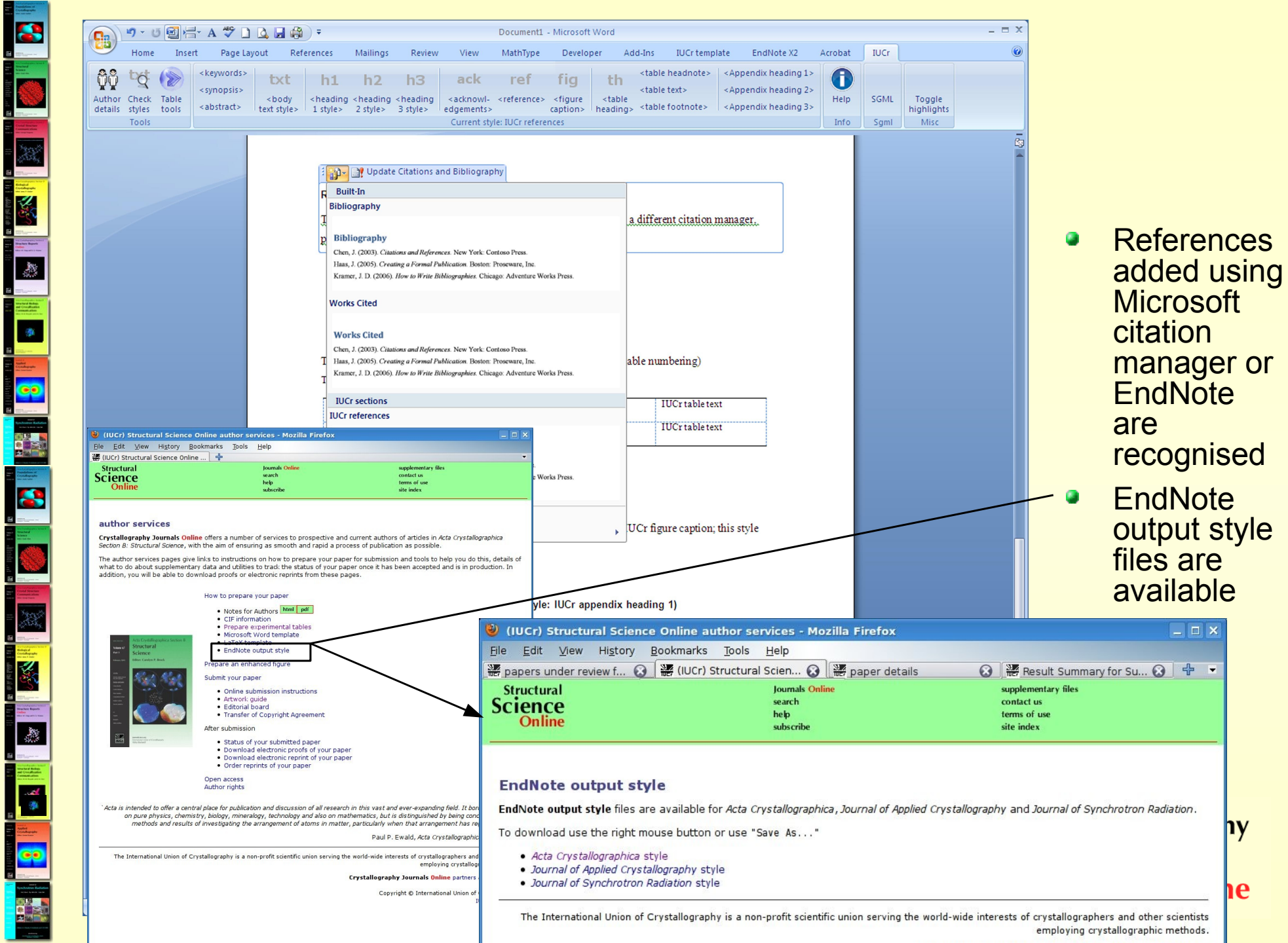
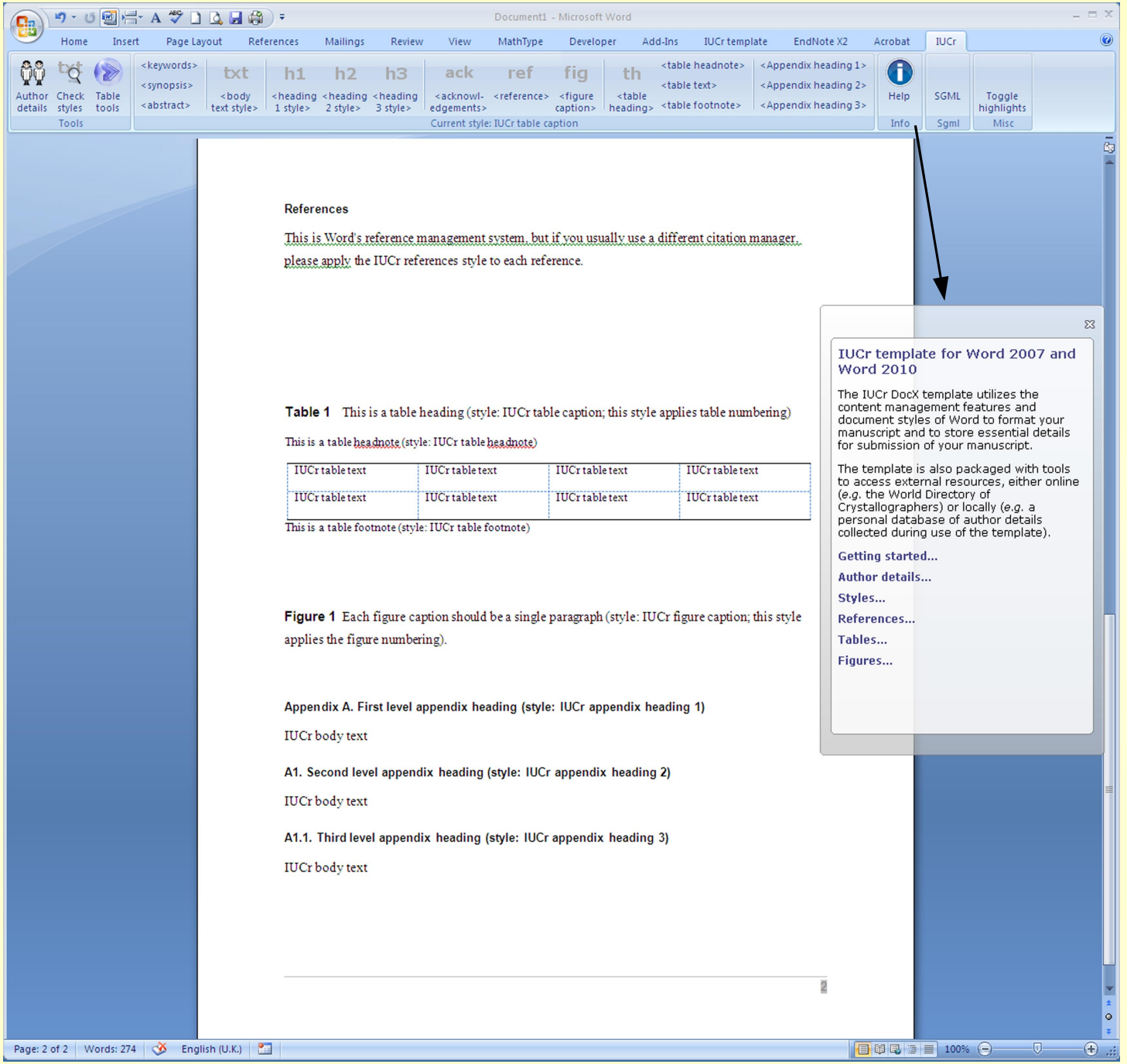


- References added using Microsoft citation manager or EndNote are recognised

Crystallography Journals Online



- References added using Microsoft citation manager or EndNote are recognised
- EndNote output style files are available



- Help accessible at any time
- Template is designed to be easy to use and to save time
- Mac version available in autumn
- Simple OpenOffice template also available

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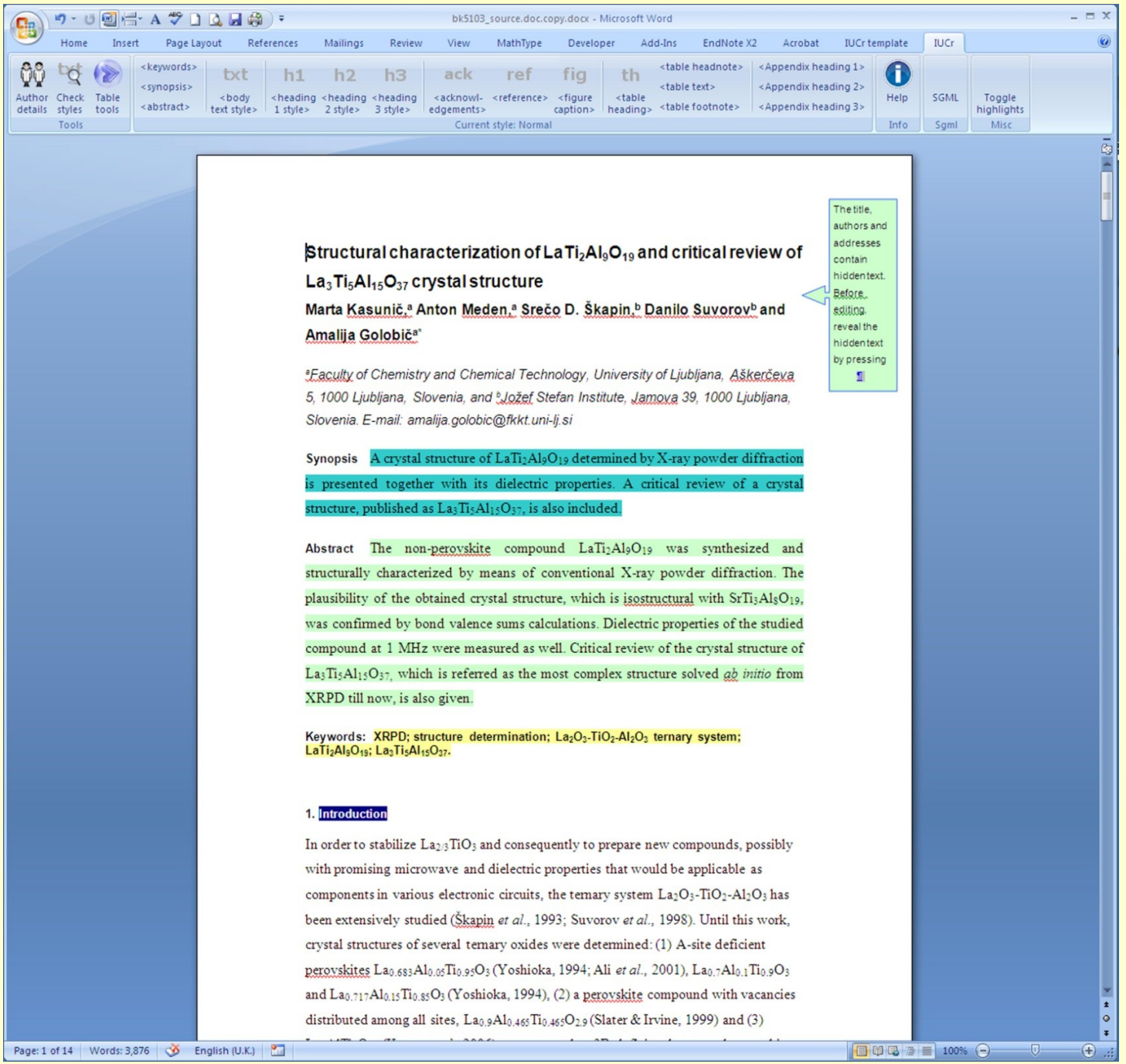


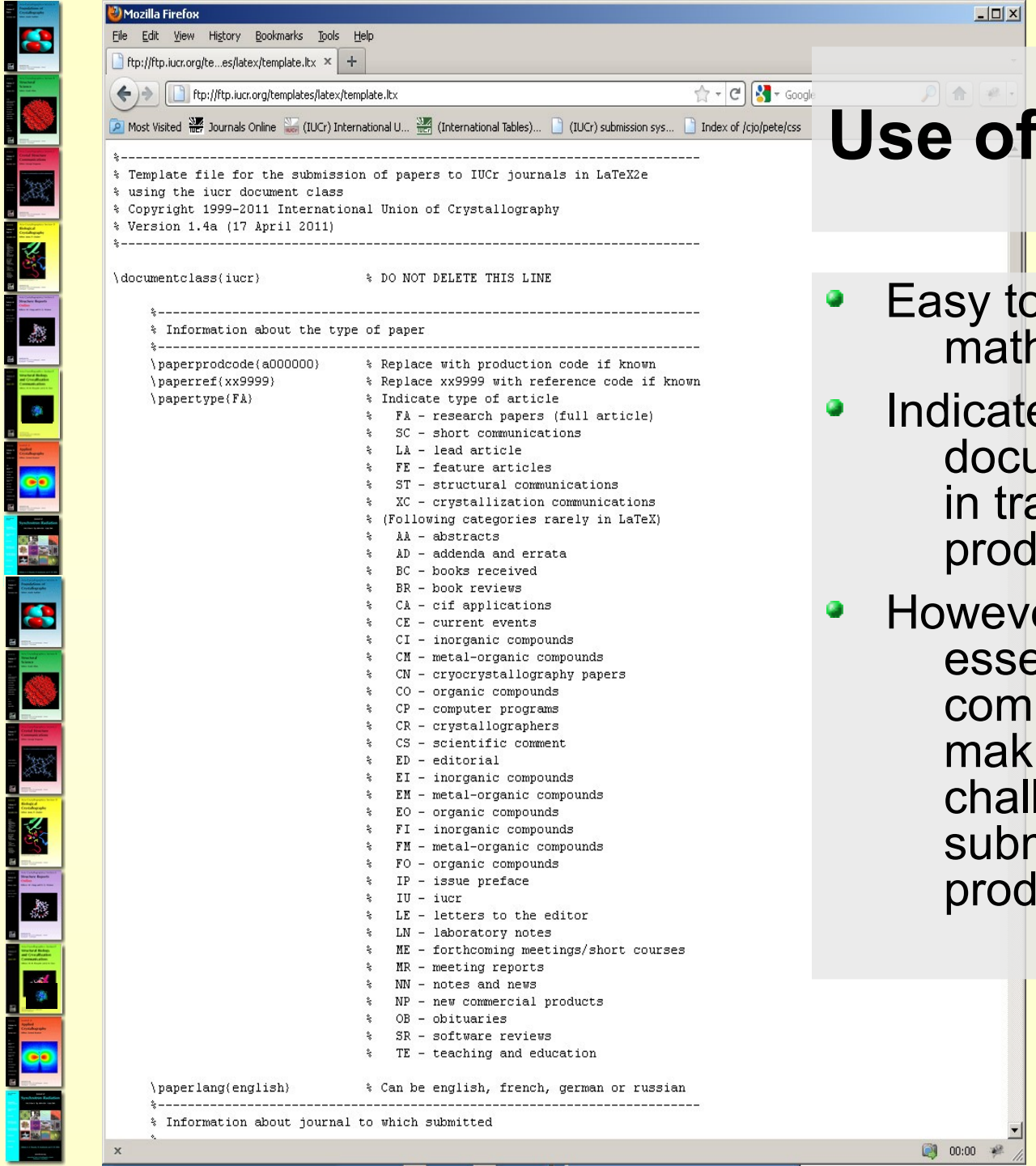
- In the in-house template, used in the Editorial Office, styles show up as colour-coded text
- Author mark-up can therefore be quickly checked

Crystallography Journals Online

LaTeX template

Crystallography Journals Online

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



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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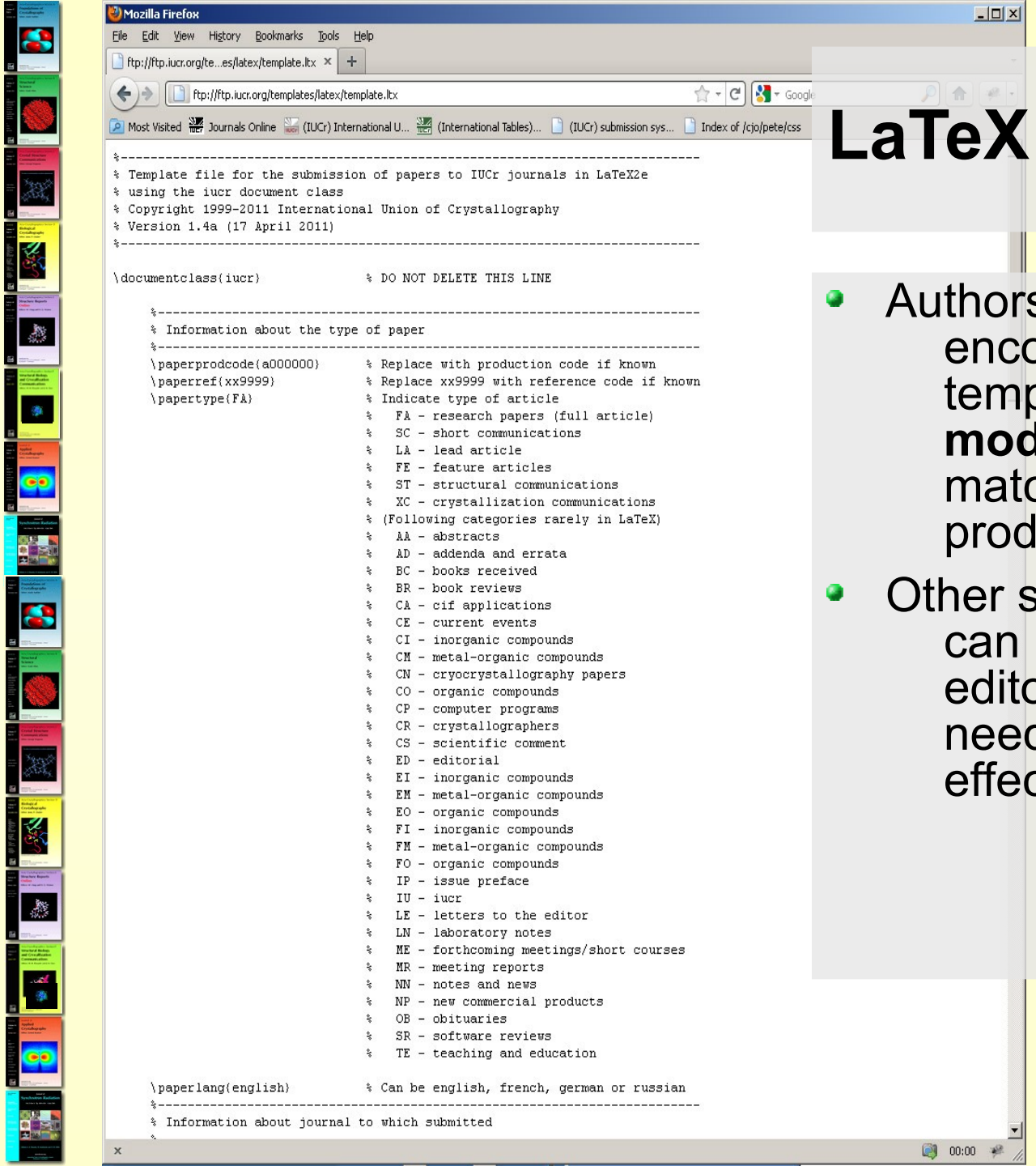

LaTeX templates

- 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

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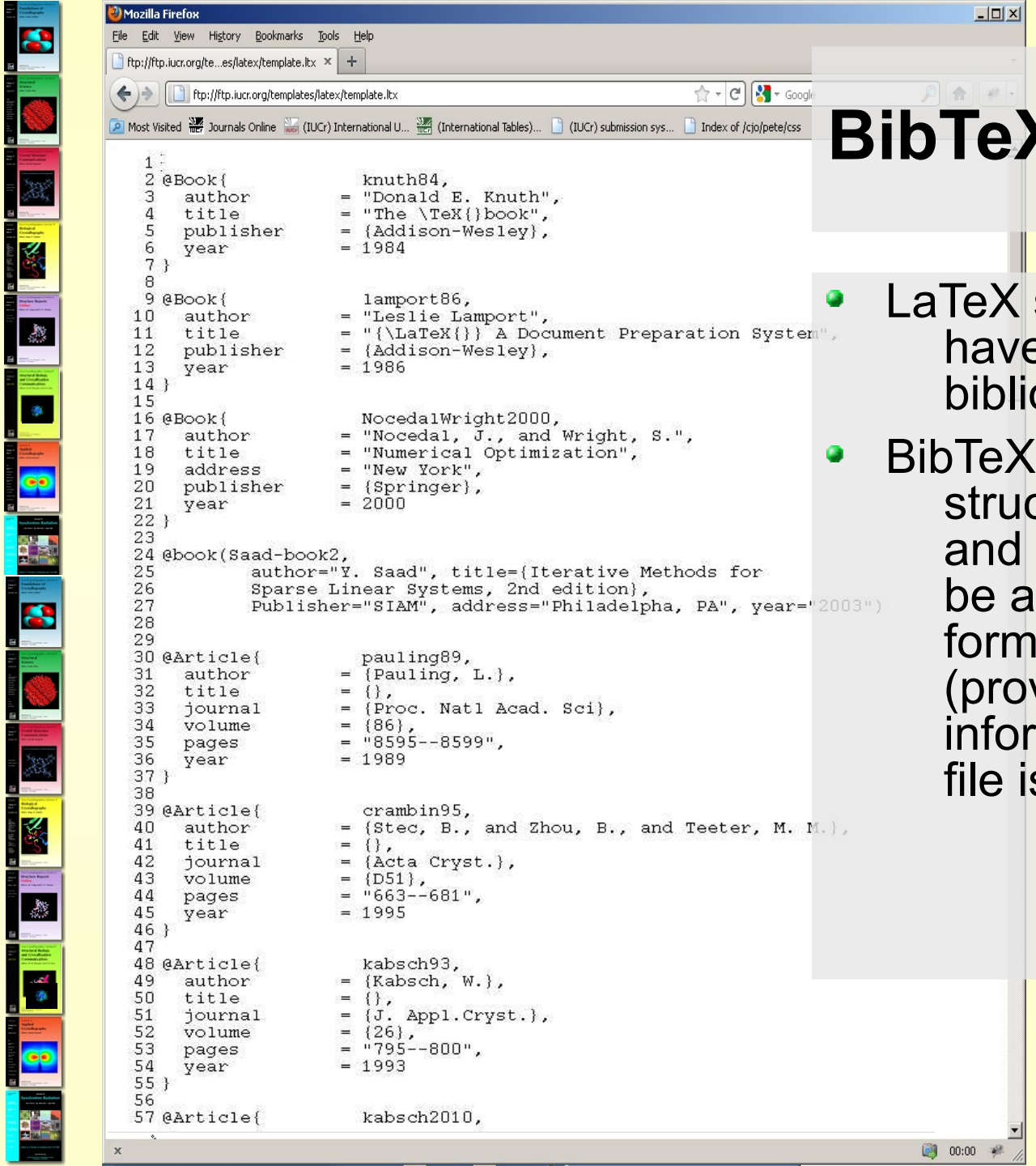

BibTeX

- 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)

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Other tools (ask for a demonstration)

publCIF

- Standalone tool for editing CIFs and previewing them in journal style
- Used mainly for submissions to Sections C and E
- publCIF engine underlies WORD template and publBio
- 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?

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Over to Louise for info on publBIO

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