



Commission on Journals 2011

Crystallography
Journals
Online



Figure and scheme preparation for publication

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(IUCr) Artwork guide

artwork guide

The aim of this guide is to help you prepare your electronic artwork for submission to IUCr journals. By following the recommendations in this guide, you will be helping us to achieve the highest possible standards of reproduction.

1. General points to consider
2. Preferred file formats
3. Figure sizing
4. Composite images
5. Fonts, labelling
6. Number formats
7. Colour
8. Cropping
9. Notes on particular types of figures
10. General guide to digital images
11. Checklist
12. Useful resources
13. FAQs

1. General points to consider

All figures should be submitted electronically via the submission system. Figures should be numbered sequentially in the order in which they are referred to in the text. Captions to figures should be provided separately in the manuscript file. Please submit one file per figure.

Please aim to keep lettering on figures to a minimum, and ensure you use SI units (*e.g.* K) throughout.

Only those figures that are necessary to illustrate the techniques or results described will be published; any others will be deposited.

For any figures that have been published previously, please ensure you obtain permission from the copyright holder prior to submitting your article to us. Please also forward a copy of the permission letter to the IUCr.

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2. Preferred file formats

The IUCr recommends that only the following file formats are used for electronic artwork submission:

- EPS (Encapsulated PostScript, .eps), PS (PostScript, .ps)
- TIFF (Tagged Image File Format, .tif)
- HPGL (Hewlett Packard Graphics Language, .hpg)

We recommend that you **do not use** the following file formats, because they may result in lower standards of reproduction:

- JPEG (Joint Photographic Expert Group Image File, .jpg)
- GIF (Graphic Image File, .gif)
- PDF (Portable Document File, .pdf)
- MS Office (Word, Excel, PowerPoint) (.doc, .rtf, .xls, .ppt)

EPS, PS (resolution independent unless there is an embedded bitmap/halftone)

Line weights should be between 0.35 and 1.5pt at final size. Please ensure that fonts are embedded. For embedded images, please follow the guidelines for TIFF below.


TIFF

Colour images should have a resolution of at least 400 d.p.i. (dots per inch) at final size.

Monochrome images (black line art on a white background) and greyscale images should have a minimum resolution of 600 d.p.i. at final size.

Done

- Online artwork guide available from author services page



Figures – general

- All figures submitted electronically, ideally at start of submission
- All figures have caption; schemes do not
- Figures numbered in order they are cited in the text
- Grids and shadings to be avoided (and coloured backgrounds)
- Specialised symbols (*e.g.* open circles, closed triangles) should either be avoided in the caption or given as words
- Consider how final figure will appear in print – should fit one page
- Any special instructions for figure handling should be sent to the Editorial Office on acceptance



Image formats

- Recommended formats in Notes for Authors
 - Encapsulated Postscript or PostScript (.eps, .ps) (resolution independent unless there is an embedded bitmap, in which case minimum 600 d.p.i.)
 - Tiff (.tif, minimum resolution 600 d.p.i. final size)
 - HPGL (.hpg) (resolution independent)
- Less recommended
 - MS Office (WORD, Powerpoint, Excel) (.doc, .rtf, .ppt, .xls) (potential loss of image quality, loss of fonts, movement of labelling)
 - PDF (.pdf) (potential loss of image quality)
 - JPEG (.jpg) (uses lossy compression methods – loss of features, ghost effects)
 - GIF (low resolution and limited to 256 colours)
 - PNG (limited colour range in certain circumstances)
- However, PDF and PNG may be necessary for certain LaTeX distributions

Resolution and image formats

This one is saved as an EPS file

vector format
EPS file

This is an example of a 600-dpi image

600 dpi
TIFF file

This is an example of a 72-dpi image

72 dpi
TIFF file

This is an example of a 72-dpi image

72 dpi
JPEG file
(medium quality)

Black and white line images should be a minimum of 600 d.p.i. at final size

Resolution and image formats



400 dpi
TIFF file

72 dpi
TIFF file

72 dpi
JPEG file
(medium quality)

Greyscale and colour images should be a minimum of 400 d.p.i. at final size

What is considered to be a figure, table or scheme?

Table 2. Calculated apatite lattice parameters.

Sample	$a(\text{\AA})$	$c(\text{\AA})$
GI744/1	9.376(3)	6.888(4)
GI744/2	9.382(7)	6.889(0)
SAR1	9.369(4)	6.886(9)
HAI08	9.385(0)	6.884(3)
988	9.446(7)	6.884(9)
LI95	9.443(9)	6.884(2)
LI95A	9.430(2)	6.883(3)
ELISH	9.449(5)	6.883(6)
ELISH2	9.448(3)	6.884(5)
HAI03	9.404(0)	6.877(9)
C57	9.438(8)	6.879(3)
KH1	9.449(8)	6.872(3)

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TABLE?**

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HAI08	9.385(0)	6.884(3)
988	9.446(7)	6.884(9)
LI95	9.443(9)	6.884(2)
LI95A	9.430(2)	6.883(3)
ELISH	9.449(5)	6.883(6)
ELISH2	9.448(3)	6.884(5)
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Calculated apatite lattice parameters.

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GI744/1	9.376 (3)	6.888 (4)
GI744/2	9.382 (7)	6.889 (1)
SAR1	9.369 (4)	6.886 (9)
HAI08	9.385 (1)	6.884 (3)
988	9.446 (7)	6.884 (9)
LI95	9.443 (9)	6.884 (2)
LI95A	9.430 (2)	6.883 (3)
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**FIGURE OR
TABLE?**

What is considered to be a figure, table or scheme?

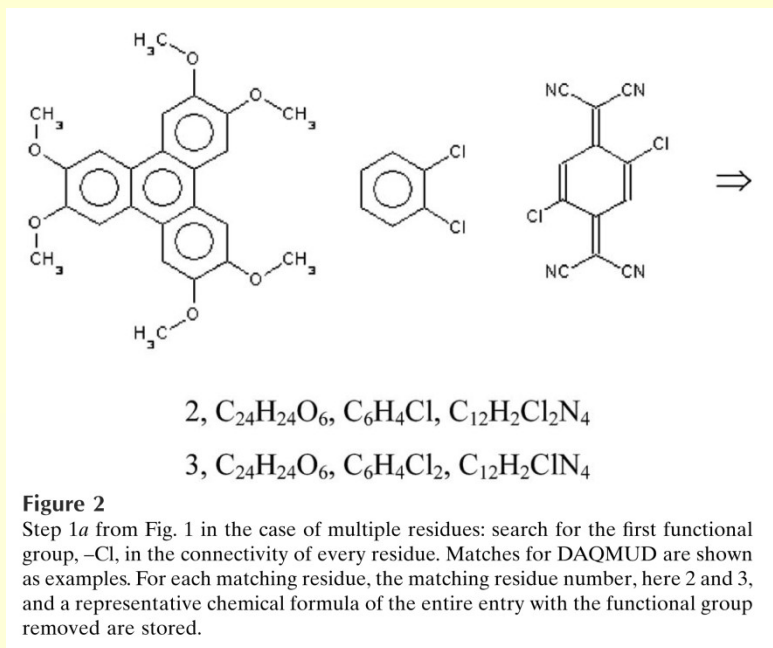
Table 2. Calculated apatite lattice parameters.

Sample	$a(\text{\AA})$	$c(\text{\AA})$
GI744/1	9.376(3)	6.888(4)
GI744/2	9.382(7)	6.889(0)
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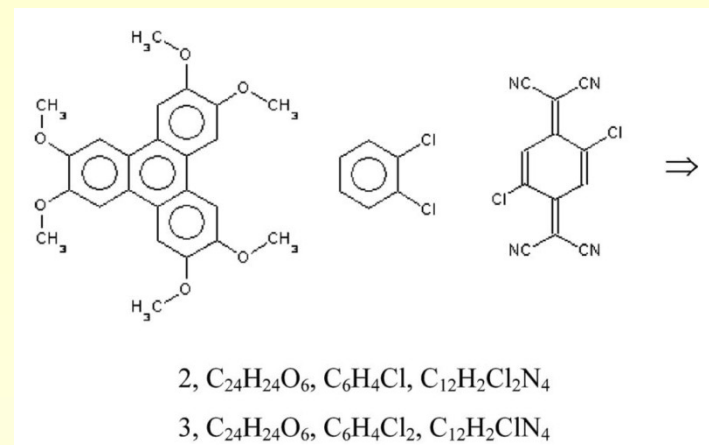
FIGURE OR TABLE

Sample	$a(\text{\AA})$	$c(\text{\AA})$
GI744/1	9.376(3)	6.888(4)
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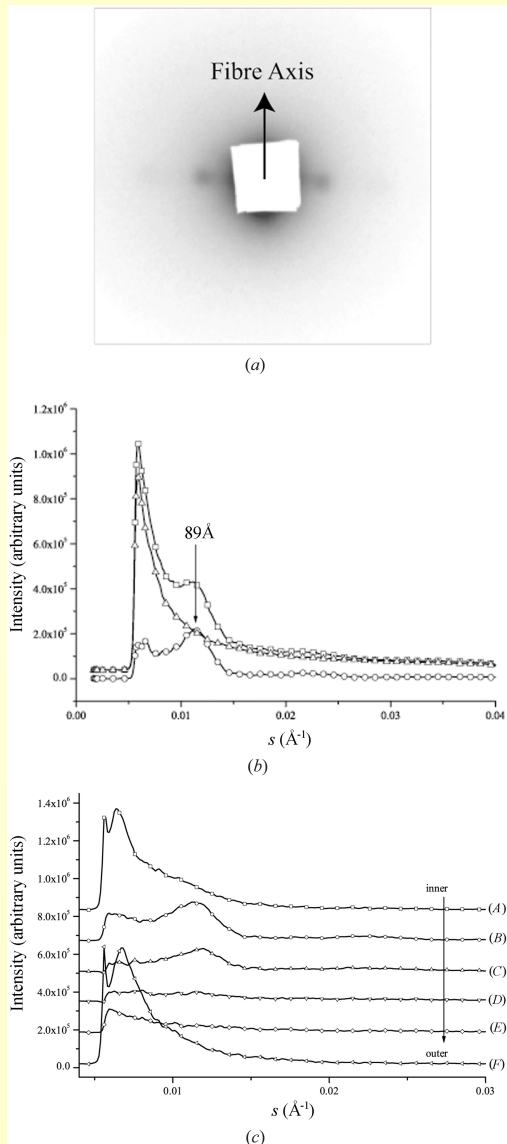


FIGURE



SCHEME

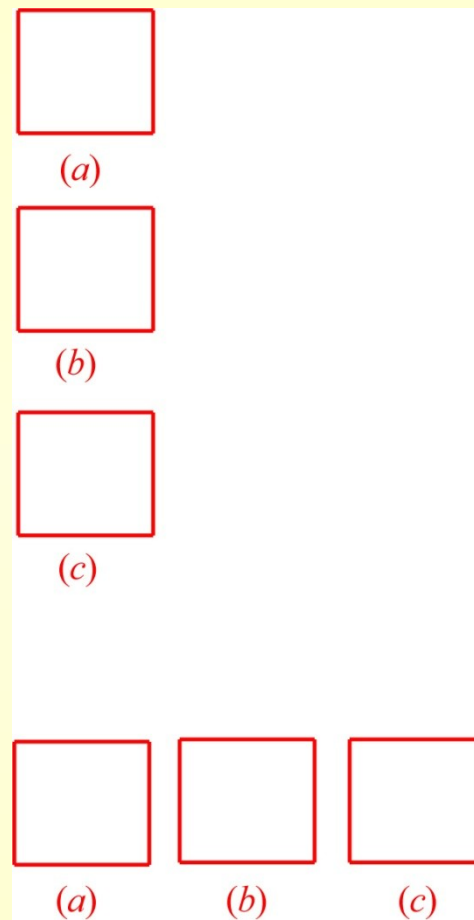
Composite figures



- Parts of figures (a), (b) etc.; labelling should be in 8pt Times and Times Italic at final size
- Ask authors to revise figures if labelling too small

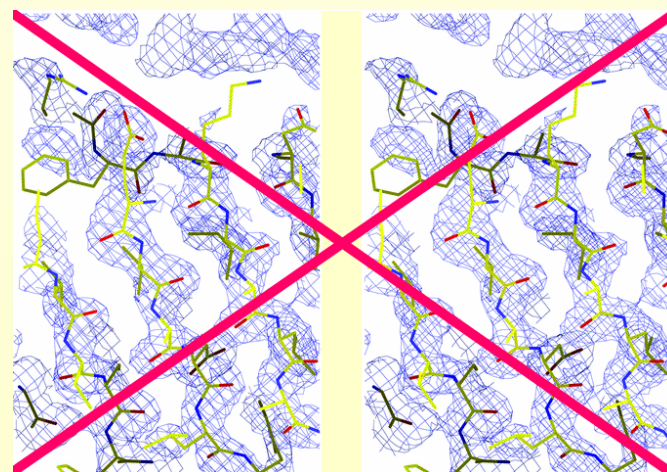
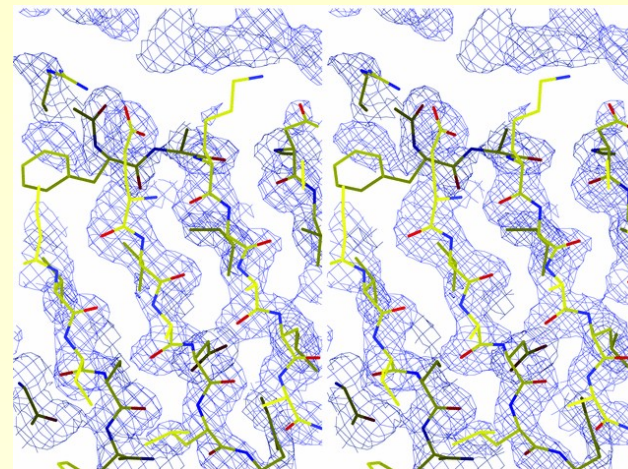
Arrangement of composite figures

- Vertical or horizontal arrangements are OK
- The overall width and height of the journal page should be considered
- Composite figures (together with their caption) should fit on one page – if more space is needed, ask authors to split figure into two
- Large amounts of white space should be avoided



Stereoviews

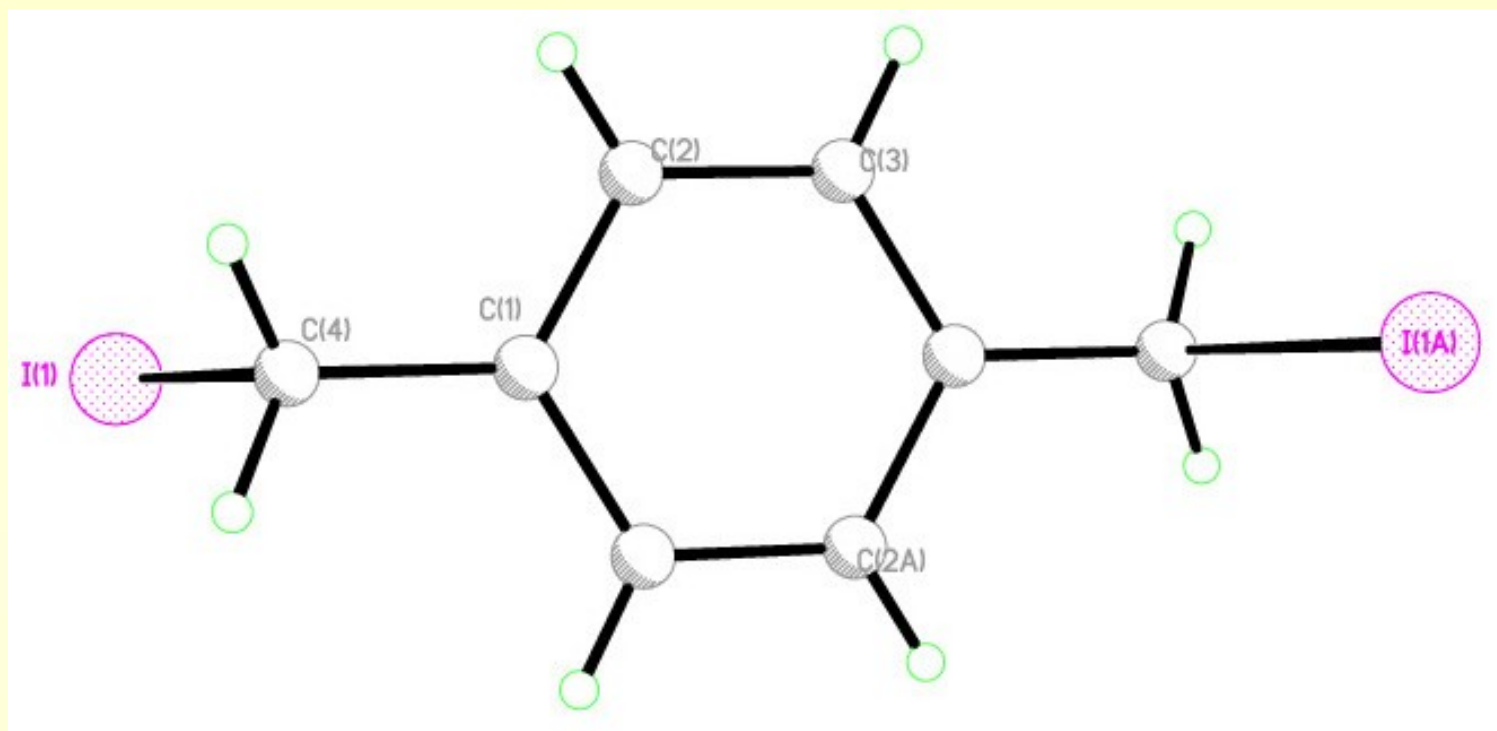
- Left and right views should be within a single figure
- Atom labelling should be on both left and right views in stereo perspective




Cropping images

- Images should be cropped before submission
- Information such as 'Figure 1' that will not be part of the final figure should be omitted
- Images should not be boxed
- Labels for parts of a figure should ideally be centred below the figure

Labelling of structural diagrams



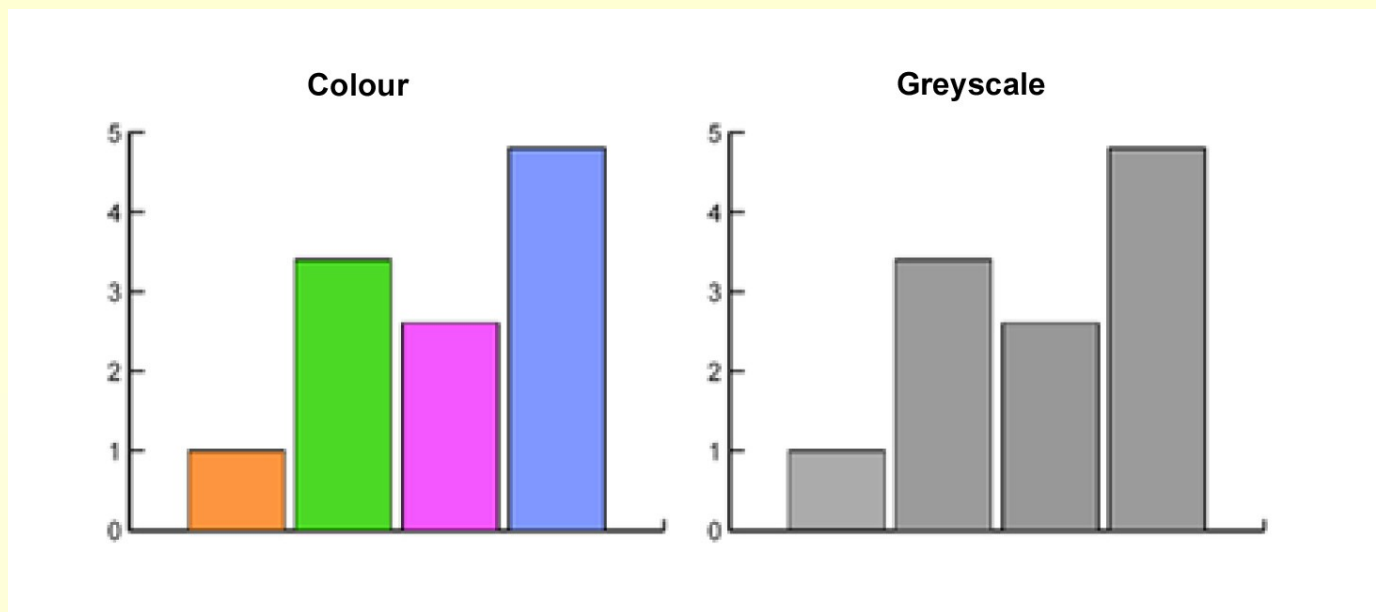
- Atoms should be shown as ellipsoids not spheres
- Atom numbers should usually not be in parentheses
- Atom labels should not intersect with bonds or ellipsoids



Sizing of artwork

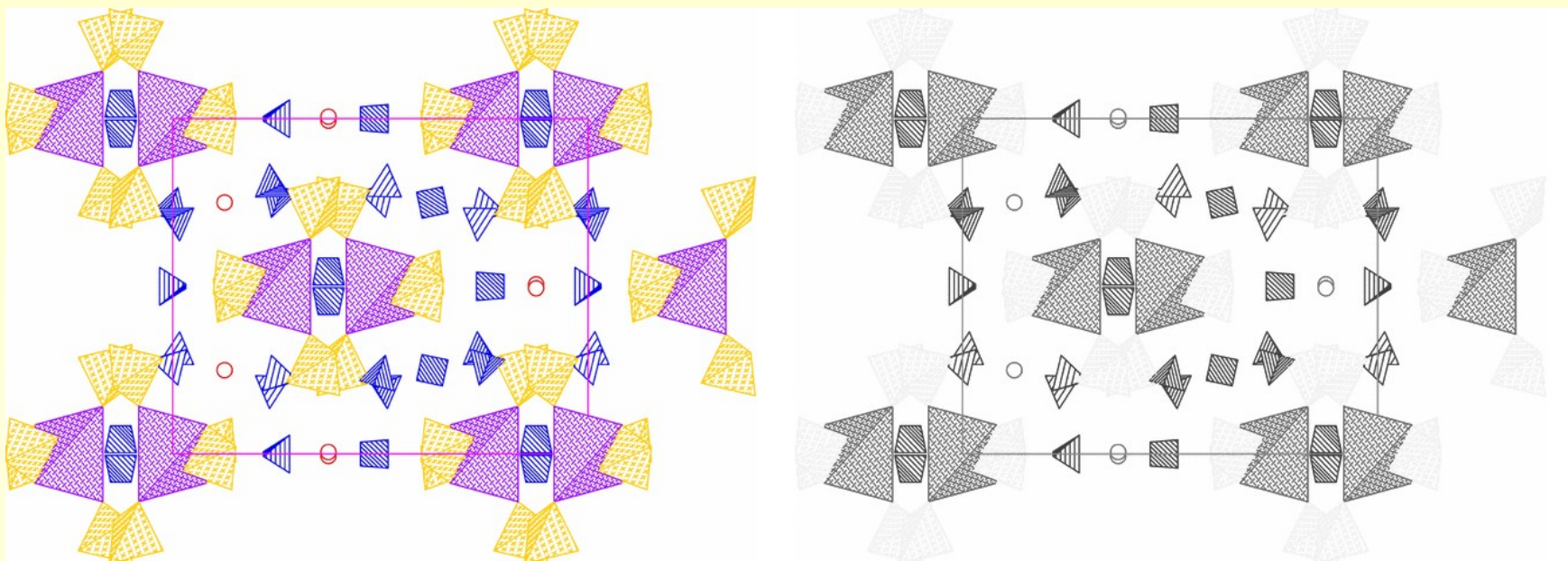
- Most artwork will be sized to fit a single column which is 21.5 picas (8.85 cm) wide
- In exceptional circumstances diagrams will be sized to fit 1.5 columns (12 cm) or double column width (18 cm)
- Submitted artwork should generally be the same size or larger than the published size

Colour and greyscale



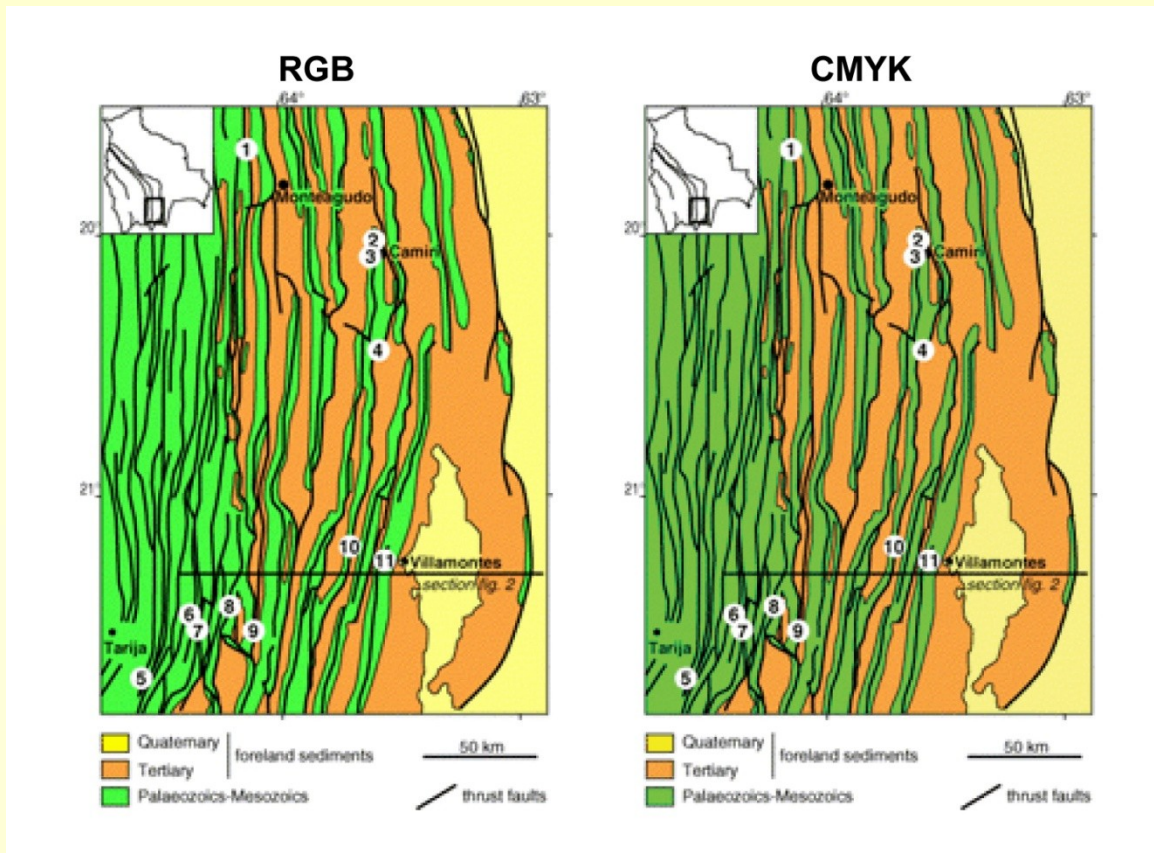
- In the printed journal colour figures may be printed as greyscale, but appear in colour online
- Colours should be distinct when converted

Colour and greyscale



- Colours should not disappear when converted – authors to revise figures where pale colours are used

RGB and CMYK colour



- Colour figures are converted to CMYK for printing
- If accurate colour reproduction is required, figures should be submitted as CMYK

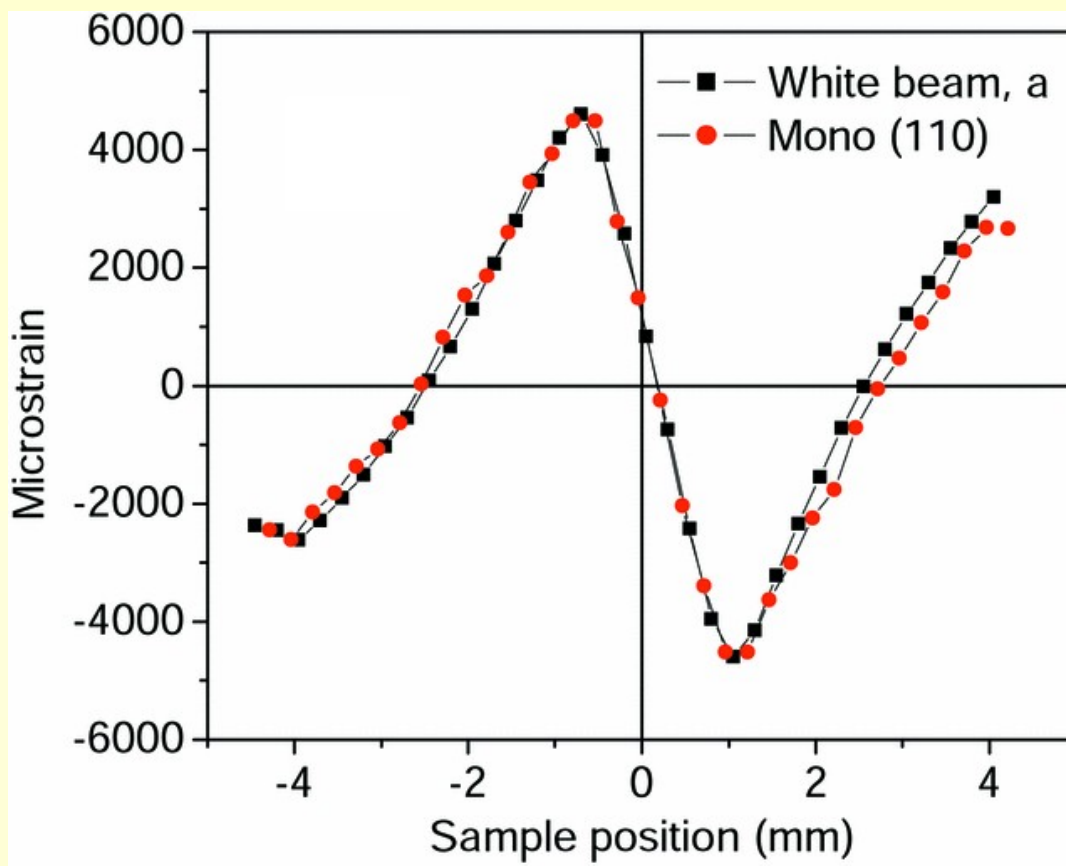
RGB

Red, Green, Blue

CMYK

Cyan, Magenta, Yellow (and Black)

Use of colour



- Colour is very expensive to print
- Colour to be used only when absolutely necessary
- Figure captions to be colour independent











Online submission system

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Structural Science Online		current issue back issues sample issue	reader services author services article submission
Crystal Structure Communications Online		current issue back issues sample issue	reader services author services article submission
Biological Crystallography Online		current issue back issues sample issue	reader services author services article submission
Structure Reports Online		current issue back issues sample issue	reader services author services article submission
Structural Biology and Crystallization Communications Online		current issue back issues sample issue	reader services author services article submission
Applied Crystallography Online		current issue back issues sample issue	reader services author services article submission
Synchrotron Radiation Online		current issue back issues sample issue	reader services author services article submission

Where to submit?

- journals.iucr.org
- Or from author services on journal home page

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The service is easy and straightforward to use, and requires you to supply

- the text of your article as a single file
- your full contact details
- details of your article
- details of the authors of your article (surnames, forenames and e-mail addresses of all authors)
- high-resolution graphics files for each figure and chemical scheme, and supplementary data (including a CIF and structure factor or Rietveld data files for structural papers), together with any other supplementary files you wish to submit

If you have not used this service before, please first read the detailed online submission instructions. Context-sensitive help is available by holding your mouse over underlined text in the submission forms or by clicking on the help icons

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- the text of your article as a single file
- your full contact details
- details of your article
- details of the authors of your article (surnames, forenames and e-mail addresses of all authors)
- high-resolution graphics files for each figure and chemical scheme, and supplementary data (including a CIF and structure factor or Rietveld data files for structural papers), together with any other supplementary files you wish to submit

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- Submission tips are also available

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- the text of your article as a single file
- your full contact details
- details of your article
- details of the authors of your article (surnames, forenames and e-mail addresses of all authors)
- high-resolution graphics files for each figure and chemical scheme, and supplementary data (including a CIF and structure factor or Rietveld data files for structural papers), together with any other supplementary files you wish to submit

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Submission tips can be found by holding your mouse over underlined text [submit your article](#)

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Done

- Full submission instructions are available
- Submission tips are also available
- Context-sensitive help also available

What needs to be ready before submission?

- Article text prepared as a single file
- Figures and schemes as separate graphics files
- A CIF for articles reporting a crystal structure
- Structure factor/powder data file for each datablock in the CIF
- Any other supplementary data as separate file
- Full contact details (e-mail address, mailing address, telephone and fax numbers)
- Details of all the authors, including email addresses
- Other details (article title, article category)
- Comments (e.g. suggestions for reviewers)
- Validation report/mmCIF for macromolecular submissions

Types of files for submission

- WORD or OpenOffice file preferably created using **IUCr template**
- LaTeX (using **IUCr template**)
- Figures as PostScript, encapsulated PostScript or TIFF files, but other formats are supported
- Valid CIF/validation report/mmCIF (for structural papers)
- Structure factor/powder data files in CIF format
- Any other supplementary files in format specified in list

Stage 1

- Contact e-mail address
- Article title
- Category
- **Structural paper?**
- Upload main article text

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MSD

(IUCr) new submission

new submission

Stage - 1 - 2 - 3 - 4 - 5 - 6 - 7 - 8
New submission

New submission details

E-mail address*

Repeat e-mail address*

Article title*

Article category

Does your article report a crystal structure?

Upload your article

NB: Do not attempt to upload the same file more than once.
If you experience problems during the file upload please contact support@iucr.org for advice.

File name on your local filesystem

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(IUCr) new submission (IUCr) Notes for authors 2010

Structural Science Online

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Notes for authors 2010

Keywords: Notes for authors.

1. Scientific scope

Section B of Acta Crystallographica publishes papers in which structure is the primary focus of the work reported. The central themes of *Section B* are the acquisition of structural knowledge from novel experimental observations or from existing data, the correlation of structural knowledge with physico-chemical and other properties, and the application of this knowledge to solve problems in the structural domain. *Section B* has broad chemical coverage, encompassing metals and alloys, inorganics and minerals, metal-organics and purely organic compounds. Biological, particularly macromolecular, structural science is covered by *Sections D and F*. A more complete definition of scientific scope is given in an Editorial [*Acta Cryst.* (1994), B50, 1-3].

2. Categories of contributions

Contributions should conform to the general editorial style of the journal.

2.1. Research Papers

Full-length *Research Papers* should not normally exceed 15 journal pages (about 15 000 words).

2.2. Short Communications

Stage 2

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article details

Your file has been received.

Stage - 1 - **2** - 3 - 4 - 5 - 6 - 7

Article details

1. Contact author details

E-mail address*

Repeat e-mail address*

Title

First name(s)*

Surname*

Name qualifier (e.g. Jr, III)

Department

Organization

Street/PO Box*

City*

State/province /country

Post/zip code

Country*

Telephone*

Fax*

2. Details of the article

Article title*

Authors (one per line, in article order; please indicate the contact author)

What does the overall submission and review procedure involve?

The overall procedure involves six stages:

- **Stage 1**
You will be asked to provide your e-mail details and the article title, and to select your article also be asked to upload a **single** file of the text of your article. Details of the file required are
 - **Stage 2**
You will be asked to give further details of your article (see above).
 - **Stage 3**
You will be asked to upload graphics files and supplementary data for your article (see below should only click on the **CONTINUE** button when you have uploaded all relevant files and have **review document**.
 - **Stage 4**
You will be invited to select a Co-editor, from a list of those available, to coordinate the review. Comments concerning your article and details of possible referees should be typed into the sp
 - **Stage 5**
A PDF review document is generated from the file(s) you submit and you will be provided with accessing and viewing this document.
- Once your review document is created, the system will assign a Co-editor to your article. You contact details of this Co-editor and a **Co-editor reference code**. The reference code has two digits (e.g. au0165) and should be quoted in all subsequent communications with the Co-editor Office. **You should keep a record of the web address for viewing your article and the Co-editor article.**
- The Co-editor will arrange for the review of your article and will inform you by e-mail of the ou review. You may be asked to submit revised versions of your article (see below). **Please note should only be submitted at the request of the Co-editor handling your article.**
- **Stage 6**
Your submission is now complete and you will be returned to the home page for your article. submit a covering letter at this stage, it may be uploaded using the **contact co-editor** tab.

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Done

Confirmation of receipt of file

Stage 2, continued

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article details

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Stage - 1 - 2 - 3 - 4 - 5 - 6 - 7

Article details

1. Contact author details

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paper details

forward reply

To: jmc61@cam.ac.uk
From: jb@iucr.org
Subject: Receipt of your submission to Acta Crystallographica Section B
Date: 2011-06-09 16:48:07 +0100
*** RECEIPT OF SUBMISSION TO ACTA CRYSTALLOGRAPHICA SECTION B ***

9 June 2011

Dear Author

Thank you for submitting your article entitled:
Molecular origins of commercial laser dye functionality in azacoumarins and quinolones: LD 425, LD 489 and LD 473

for publication in Acta Crystallographica Section B. It has been assigned the following web address:

http://submission.iucr.org/submit/b/review_address/X1Q8fOifme3Ps44L/t065344

IMPORTANT - Please make a careful note of this web address, as you will need it throughout the review process.

To complete your submission (if you have not already done so), please fill out the additional details and upload any source files including a CIF if this is a structural paper. The files should include

(a) a single file in Word, RTF or LaTeX format of the text, tables and figure captions of your article,

(b) a high-resolution graphics file in TIFF, PostScript or encapsulated PostScript format for each figure and scheme, and

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You will be asked to give further details of your article (see above).
 - **Stage 3**
You will be asked to upload graphics files and supplementary data for your article (see below should only click on the **CONTINUE** button when you have uploaded all relevant files and have **review document**.
 - **Stage 4**
You will be invited to select a Co-editor, from a list of those available, to coordinate the review. Comments concerning your article and details of possible referees should be typed into the sp
 - **Stage 5**
A PDF review document is generated from the file(s) you submit and you will be provided with accessing and viewing this document.
- Once your review document is created, the system will assign a Co-editor to your article. You contact details of this Co-editor and a **Co-editor reference code**. The reference code has two digits (e.g. au0165) and should be quoted in all subsequent communications with the Co-editor Office. **You should keep a record of the web address for viewing your article and the Co-editor article.**
- The Co-editor will arrange for the review of your article and will inform you by e-mail of the ou review. You may be asked to submit revised versions of your article (see below). **Please note should only be submitted at the request of the Co-editor handling your article.**
- **Stage 6**
Your submission is now complete and you will be returned to the home page for your article. submit a covering letter at this stage, it may be uploaded using the **contact co-editor** tab.

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- Confirmation of receipt of file
- E-mail sent to author confirming receipt of file
- Tracking number quoted

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Potential problems

- Title and main article text file are checked against previous submissions in our database
- For journals other than C and E, **an exact** duplication of the title or main article text file with one previously submitted will cause the system to ask the author to contact support rather than continuing with the submission
- Software is used to check all uploaded file types – occasionally this may not identify a file type correctly (e.g. where file starts with comments) resulting in problems uploading files

Stage 2, continued

- Enter article details
- Enter email address for each author
- Enter abstract

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File Edit View History Bookmarks Tools Help

(IUCr) article details

Stage - 1 - **2** - 3 - 4 - 5 - 6 - 7 - Article details

1. Contact author details

E-mail address*

Repeat e-mail address*

Title

First name(s)*

Surname*

Name qualifier

(e.g. Jr, III)

Department

Organization

Street/PO Box*

City*

State/province /county

Post/zip code

Country*

Telephone*

Fax*

2. Details of the article

Article title*

Authors (one per line, in article order; please indicate the contact author)

Contact author*	First name(s)	Surname*	E-mail address
<input checked="" type="radio"/>	Carolyn P.	Brock	<input type="text" value="cpbrock@uky.edu"/>
<input type="radio"/>	Xiaogang	Liu	<input type="text" value="xl316@cam.ac.uk"/>
<input type="radio"/>	Jacqueline	Cole	<input type="text" value="jmc61@cam.ac.uk"/>
<input type="radio"/>	Paul G.	Waddell	<input type="text" value="pgw27@cam.ac.uk"/>
<input type="radio"/>			
<input type="radio"/>			
<input type="radio"/>			
<input type="radio"/>			
<input type="radio"/>			
<input type="radio"/>			

Language

Abstract (please paste your abstract into the form below)

The molecular structures of three compounds, LD 425 (C13H14N2O3), LD 489 (C15H15F3N2O2) and LD 473 (C17H19F3N2O), are determined by single-crystal X-ray diffraction at 100 K. LD 425 and LD 489 possess para-quinoidal bond distance patterns in their benzene rings due to inter-ring charge transfer (IRCT) from these rings to the adjoining ring. In contrast to LD 473, chemical substitution of the coumarin single-bonded O with N, to form a quinolone, results in the suppression of this IRCT effect. Instead, intra-ring charge transfer is shown to become more pronounced. See Figure 1 for details.

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(IUCr) article details (IUCr) Online submission inst...

What should I do if I do not have the e-mail address of a co-author?

During submission you will be asked to provide e-mail addresses for all authors. These addresses will be used to inform your co-authors that the article has been submitted. In some cases, e.g. where a co-author is a student who is no longer at your institution, it may be difficult to provide an e-mail address. If you are unable to find an address for a coauthor, you may substitute your e-mail address when filling out the form at [Stage 2](#) of the submission.

[Back to contents](#)

What should I do if I get stuck?

You will find detailed help links throughout the submission pages, and you can use any of these links without stopping the submission. If you are having more serious problems, you should contact support@iucr.org.

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article details

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Stage - 1 - 2 - 3 - 4 - 5 - 6 - 7 - 8
Article details

1. Contact author details

E-mail address*

Repeat e-mail address*

Title

First name(s)*

Surname*

Name qualifier (e.g. Jr, III)

Department

Organization

Street/PO Box*

City*

State/province /county

Post/zip code

Country*

Telephone*

Fax*

2. Details of the article

Article title*

Authors (one per line, in article order; please indicate the contact author)

Contact author*	First name(s)	Surname*	E-mail address
<input checked="" type="radio"/>	<input type="text" value="Carolyn P."/>	<input type="text" value="Brock"/>	<input type="text" value="cpbrock@uky.edu"/>
<input type="radio"/>	<input type="text" value="Xiaogang"/>	<input type="text" value="Liu"/>	<input type="text" value="xl316@cam.ac.uk"/>
<input type="radio"/>	<input type="text" value="Jacqueline"/>	<input type="text" value="Cole"/>	<input type="text" value="jmc61@cam.ac.uk"/>
<input type="radio"/>	<input type="text" value="Paul G."/>	<input type="text" value="Waddell"/>	<input type="text" value="pgw27@cam.ac.uk"/>

Language

Abstract (please paste your abstract into the form below)

The molecular structures of three compounds, LD 425 (C13H14N2O3), LD 489 (C15H15F3N2O2) and LD 473 (C17H19F3N2O), are determined by single-crystal X-ray diffraction at 180 K. Azacoumarins LD 425 and LD 489 possess para-quinoidal bond distance patterns in their benzene rings due to inter-ring charge transfer (IRCT) from these rings to the adjoining ring. In contrast, chemical substitution of the coumarin single-bonded O with N, to form a quinolone, results in the suppression of this IRCT effect. Instead, intra-ring charge transfer is shown to become more pronounced. Such

• Must complete fields marked with asterisks

Stage 3

- All other files (e.g. figures, schemes, structural and supplementary data) can now be uploaded

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Upload source files

Stage -1-2-**3**-4-5-6-7-8
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Molecular origins of commercial laser dye functionality in azacoumarins and quinolones

Carolyn P. Brock*, Xiaogang Liu, Jacqueline Cole and Paul G. Waddell [Modify these details](#)

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Review document (PDF) Tue Jul 26 10:49:45 2011

Abstract More...

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Name	Component	Size	Upload time
t050607_source.docx	Article body	114744	Tue Jul 26 10:25:41 2011 Delete

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revised Word file
 figure
 scheme
 cif
 supplementary material ⓘ

Figure number Part
Scheme number

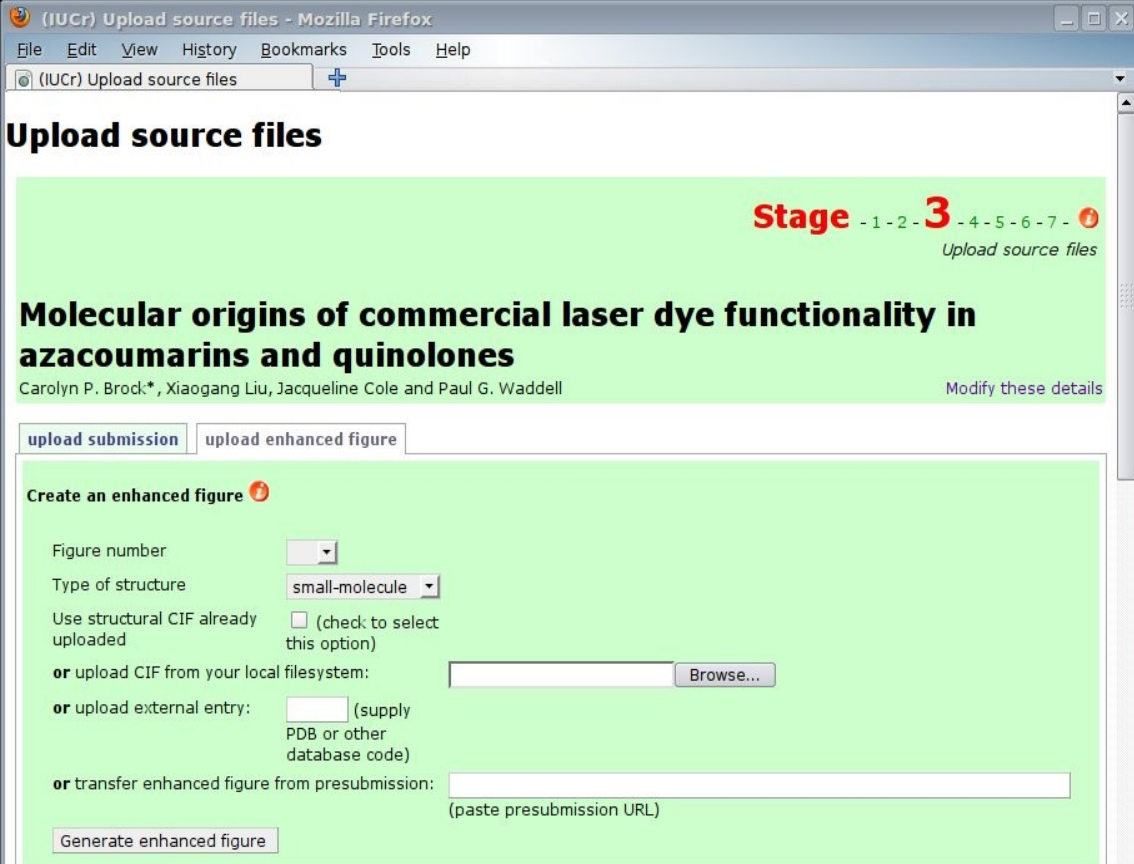
File name on your local filesystem: [Browse...](#)

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FIGURE UPLOAD

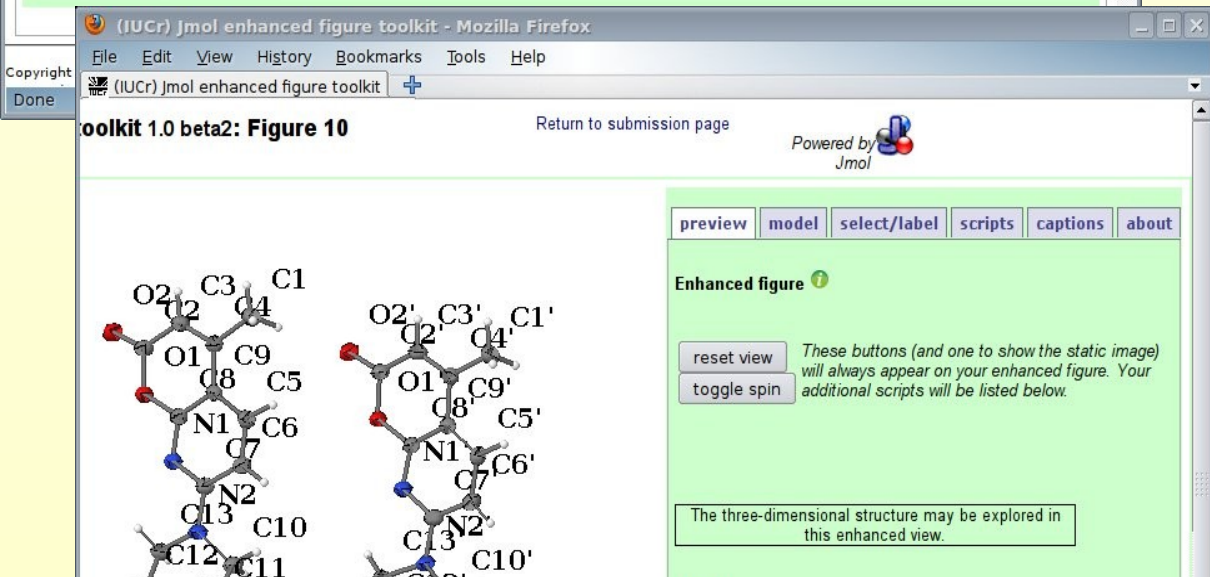
- Click on figure
- Choose figure number and part
- Select file on your system to upload
- Click on upload file



Stage 3, continued

ENHANCED FIGURES

- Toolkit allows easy creation and editing of interactive Jmol figures
- Generate from CIF associated with article
- Upload a new CIF
- Supply a database code
- Import a previously prepared enhanced figure



Stage 3, continued

CORRECTING MISTAKES

- If wrong file uploaded just reupload and file will be overwritten
- Only use delete to remove files no longer required

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Abstract More...

The following files have been deposited for this submission

Name	Component	Size	Upload time
t050607_source.docx	Article body	114744	Tue Jul 26 10:25:41 Delete 2011
t050607fig1.ps	Figure	16448	Tue Jul 26 10:53:04 Delete 2011
t050607fig2.ps	Figure	10807510	Tue Jul 26 10:54:26 Delete 2011
t050607fig3.ps	Figure	12181330	Tue Jul 26 10:55:20 Delete 2011
t050607fig4.ps	Figure	12593502	Tue Jul 26 10:56:35 Delete 2011
t050607fig5.ps	Figure	62880	Tue Jul 26 10:57:50 Delete 2011
t050607fig6.ps	Figure	21167	Tue Jul 26 10:58:21 Delete 2011
t050607fig7.ps	Figure	7985884	Tue Jul 26 10:59:04 Delete 2011
t050607fig8.ps	Figure	33479	Tue Jul 26 11:01:36 Delete 2011
t050607fig9.ps	Figure	25455	Tue Jul 26 11:02:06 Delete 2011

Change ordering of figures

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Stage 3, continued

CORRECTING MISTAKES

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- Only use delete to remove files no longer required
- Figure ordering can be modified

The screenshot displays the IUCr submission interface in Mozilla Firefox. The top window, titled '(IUCr) Upload source files', shows the 'Current version' as '26 July 2011 10:25:41 BST' and a 'Review document (PDF)' link. Below this, there are buttons for 'upload submission' and 'upload enhanced figure'. The main content area lists uploaded files with columns for 'Name', 'Component', 'Image number', 'New Figure number', and 'New Figure part'. The files listed are 't050611fig1.ps', 't050611fig2.ps', and 't050611fig3.ps'. A 'Change ordering of figures' button is visible at the bottom of this list. The bottom window, titled '(IUCr) change figure order - Mozilla Firefox', shows a detailed view of the 'change figure order' process. It lists the available graphical files for the submission, including 't050607fig8.ps' and 't050607fig9.ps'. A 'Change ordering of figures' button is also present in this window, which is circled in red. The interface includes a menu bar with 'File', 'Edit', 'View', 'History', 'Bookmarks', 'Tools', and 'Help'. The browser's address bar shows the URL '(IUCr) change figure order'.

Stage 3, continued

STRUCTURAL PAPER = yes (small molecule structures)

- You will be requested to upload a CIF
- CIF will not upload if file does not pass syntax checks

(IUCr) Upload source files - Mozilla Firefox

File Edit View History Bookmarks Tools Help

(IUCr) Upload source files

	t050607fig4.ps	Figure	12593502	Tue Jul 26 10:56:35 2011	Delete
	t050607fig5.ps	Figure	62880	Tue Jul 26 10:57:50 2011	Delete
	t050607fig6.ps	Figure	21167	Tue Jul 26 10:58:21 2011	Delete
	t050607fig7.ps	Figure	7985884	Tue Jul 26 10:59:04 2011	Delete
	t050607fig8.ps	Figure	33479	Tue Jul 26 11:01:36 2011	Delete
	t050607fig9.ps	Figure	25455	Tue Jul 26 11:02:06 2011	Delete

Change ordering of figures

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revised Word file

figure Figure number Part

scheme Scheme number

cif

supplementary material ⓘ

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Done

(IUCr) Online submission instructions - Mozilla Firefox

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Should I submit supplementary data?

If your article describes a crystal structure study, a CIF (Crystallographic Information File) containing the crystallographic data for all the reported structures will be required for the review process. You will be asked to upload your CIF during the submission procedure. You should ensure that at least a **basic structural check** is run on the final version of your CIF prior to submission. Also, a separate structure factor or Rietveld data file in CIF format should be submitted for each structure reported. Other supplementary materials (e.g. videos) may be submitted; for a full list of allowed file types, click [here](#).

Supplementary material which is for "review only" can be uploaded in the same way as regular supplementary material but it should be made clear on the first page of the material that it is for review only and not for publication.

[Back to contents](#)

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When your article has been successfully uploaded, a Co-editor reference code assigned and a PDF review document

Stage 3, continued

STRUCTURAL PAPER = yes (small molecule structures)







- Structure factor files should be uploaded for each datablock in the CIF
- Datablocks from CIF are listed to allow selection when uploading structure factors or powder data

(IUCr) Upload source files - Mozilla Firefox

File Edit View History Bookmarks Tools Help

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10:55:20 2011

	t050607fig4.ps	Figure	12593502	Tue Jul 26 10:56:35 2011	Delete
	t050607fig5.ps	Figure	62880	Tue Jul 26 10:57:50 2011	Delete
	t050607fig6.ps	Figure	21167	Tue Jul 26 10:58:21 2011	Delete
	t050607fig7.ps	Figure	7985884	Tue Jul 26 10:59:04 2011	Delete
	t050607fig8.ps	Figure	33479	Tue Jul 26 11:01:36 2011	Delete
	t050607fig9.ps	Figure	25455	Tue Jul 26 11:02:06 2011	Delete

Change ordering of figures

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revised Word file

figure

scheme

cif

Figure number Part

Scheme number

Structure factors, powder diffraction data and other supplementary material may also be uploaded.

structure factors

powder diffraction data

other supplementary material

Datablock:

File name on your local filesystem: Browse...

Upload file

I have uploaded all my files - CONTINUE to next stage

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Stage 3, continued

**STRUCTURAL
PAPER = yes (small
molecule structures)**

- CheckCIF report appears in html and PDF format

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Stage - 1 - 2 - 3 - 4 - 5 - 6 - 7 - 8
Upload source files

Molecular origins of commercial laser dye functionality in azacoumarins and quinolones

Carolyn P. Brock*, Xiaogang Liu, Jacqueline Cole and Paul G. Waddell [Modify these details](#)








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- [checkCIF and duplication report \(html\)](#) Tue Jul 26 11:04:24 2011
- [checkCIF and duplication report \(pdf\)](#) Tue Jul 26 11:04:14 2011

Abstract More...

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Name	Component	Size	Upload time	
t050607_source.docx	Article body	114744	Tue Jul 26 10:25:41 2011	Delete
t050607.cif	CIF	53504	Tue Jul 26 11:03:42 2011	
t050607ld425_180k_22apr2011int4sup2.hkl	Structure factors	240021	Tue Jul 26 11:06:08 2011	Delete
 t050607fig1.ps	Figure	16448	Tue Jul 26 10:53:04 2011	Delete
 t050607fig2.ps	Figure	10807510	Tue Jul 26 10:54:26 2011	Delete
 t050607fig3.ps	Figure	12181330	Tue Jul 26 10:55:20 2011	Delete
 t050607fig4.ps	Figure	12593502	Tue Jul 26 10:56:35 2011	Delete
 t050607fig5.ps	Figure	62880	Tue Jul 26 10:57:50 2011	Delete
 t050607fig6.ps	Figure	21167	Tue Jul 26 10:58:21 2011	Delete
 t050607fig7.ps	Figure	7985884	Tue Jul 26 10:59:04 2011	Delete

Stage 3, continued

**STRUCTURAL
PAPER = yes (small
molecule structures)**

- CheckCIF report appears in html and PDF format
- Report shows:
 - checkCIF/PLATON results

The screenshot shows two browser windows. The top window is the IUCr submission interface for 'Stage 3' (Upload source files). It displays the title 'Molecular origins of commercial laser dye functionality in azacoumarins and quinolones' by Carolyn P. Brock*, Xiaogang Liu, Jacqueline Cole and Paul G. Waddell. The current version is from 26 July 2011. A list of reports is shown, including a 'Review document (PDF)' and two 'checkCIF and duplication report' files (html and pdf). The bottom window shows the 'checkCIF/PLATON results' for paper t050611. It lists several alerts (ALERT type 1 to 5) and provides a detailed datablock for 'ld473'.

Datablock: ld473

Bond precision: C-C = 0.0022 Å Wavelength=0.71073
Cell: a=12.1853(5) b=12.2242(4) c=10.6361(3)
alpha=90 beta=93.4529(11) gamma=90
Temperature: 180 K

	Calculated	Reported
Volume	1581.43(9)	1581.43(9)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C17 H19 F3 N2 O	C17 H19 F3 N2 O
Sum formula	C17 H19 F3 N2 O	C17 H19 F3 N2 O
Mr	324.34	324.34
Dx, g cm ⁻³	1.362	1.362
Z	4	4
Mu (mm ⁻¹)	0.110	0.110
F000	680.0	680.0
F000'	680.41	
h,k,lmax	15,15,13	15,15,13
Nref	3617	3601
Tmin,Tmax	0.979,0.987	0.943,0.989
Tmin'	0.965	

Correction method= MULTI-SCAN
Data completeness= 0.996
Theta(max)= 27.460
R(reflections)= 0.0482(2179) wR2(reflections)= 0.1230(3601)
S = 0.996 Npar= 284

Stage 3, continued

**STRUCTURAL
PAPER = yes (small
molecule structures)**

- CheckCIF report appears in html and PDF format
- Report shows:
 - checkCIF/PLATON results
 - Database duplication summary

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Stage - 1 - 2 - 3 - 4 - 5 - 6 - 7 - 8
Upload source files

Molecular origins of commercial laser dye functionality in azacoumarins and quinolones
Carolyn P. Brock*, Xiaogang Liu, Jacqueline Cole and Paul G. Waddell
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Review document (PDF)	Tue Jul 26 10:49:45 2011
checkCIF and duplication report (html)	Tue Jul 26 11:04:24 2011
checkCIF and duplication report (pdf)	Tue Jul 26 11:04:14 2011

Abstract More...

(IUCr) checkCIF/PLATON results for paper t050611 - Mozilla Firefox

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(IUCr) checkCIF/PLATON resu... (IUCr) Online submission inst...

database duplication summary

Datablock: Id425_180k_22apr2011int4

- Chemical name = LD 425
- R factor = 0.061
- Space group = P2(1)/c
- Formula = C13 H14 N2 O3
- a=7.059 b=24.497 c=13.914
- alpha=90 beta=103.559 gamma=90

Datablock: Id473

- Chemical name = LD 473
- R factor = 0.048
- Space group = P2(1)/c
- Formula = C17 H19 F3 N2 O
- a=12.1853 b=12.2242 c=10.6361
- alpha=90 beta=93.4529 gamma=90

Datablock: Id489

- Chemical name = LD 489
- R factor = 0.049
- Space group = P_21/c
- Formula = C15 H15 F3 N2 O2
- a=8.9941 b=11.2954 c=14.3536
- alpha=90 beta=102.537 gamma=90

DATABLOCK: Id473

- Chinnakali, K., Sivakumar, K., Natarajan, S., McGuire, N. K. & Clearfield, A. (1991). *Acta Cryst. C* **47**, 561-563 [details](#)
[Cell: 10.694,12.216,12.356(90,94.24,90) R=4.4 T=Room Temp.(283-303)]

Datablock Id425_180k_22apr2011int4 - ellipsoid plot

76 Y NOMOVE FORCED Prob = 50 Temp = 180

Stage 3, continued

STRUCTURAL PAPER = yes (small molecule structures)

- CheckCIF report appears in html and PDF format
- Report shows:
 - checkCIF/PLATON results
 - Database duplication summary
 - Ellipsoid plots

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Stage - 1 - 2 - **3** - 4 - 5 - 6 - 7 -

Upload source files

Molecular origins of commercial laser dye functionality in azacoumarins and quinolones

Carolyn P. Brock*, Xiaogang Liu, Jacqueline Cole and Paul G. Waddell [Modify these details](#)

upload submission upload enhanced figure

Current version 26 July 2011 10:25:41 BST [Upload source files](#)

Review document (PDF)	Tue Jul 26 10:49:45 2011
checkCIF and duplication report (html)	Tue Jul 26 11:04:24 2011
checkCIF and duplication report (pdf)	Tue Jul 26 11:04:14 2011

Abstract More...

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(IUCr) checkCIF/PLATON resu... (IUCr) Online submission inst... [Delete](#)

Datablock Id473 - ellipsoid plot

PLATON-Aug 2 09:30:40 2011 - (180711)

Z -52 Id473 P2(1)/c R = 0.05 RES= 0 -176 X

Stage 3, continued

STRUCTURAL PAPER = yes (macromolecular structures)

- mmCIF is requested
- Validation report is required

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http://submissionstest.iucr.org:8600/submit/d/new_upload/11Gsu5iBFY25

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(IUCr) Upload source files

Structural features of peroxisomal catalase from the yeast *Hansenula polymorpha*

Chris Williams* and Esther Pena-Soler [Modify these details](#)

[upload submission](#) [upload enhanced figure](#)

Current version

2 August 2011 13:30:27 BST [Upload source files](#)

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Abstract [More...](#)

The following files have been deposited for this submission

Name	Component	Size	Upload time	
t050612_source.doc	Article body	205824	Tue Aug 2 13:30:27 2011	Delete
t0506122xq1.mcf	mmCIF	7075665	Tue Aug 2 13:34:56 2011	Delete

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revised Word file

figure

scheme

PDB validation report ⓘ

mmcif ⓘ

Structure factors, powder diffraction data and other supplementary material may also be uploaded.

structure factors

powder diffraction data

other supplementary material ⓘ

File name on your local filesystem: [Browse...](#)

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What is a PDB validation report?

When coordinates and structure factors are deposited with one of the Worldwide Protein Data Bank (PDB) validation report is created and made available to the depositor. The report is usually a plain text file and is sent to the depositor or can be downloaded from the web (click on the following links to see sample reports).

[Back to contents](#)

What is an mmCIF?

mmCIF stands for macromolecular Crystallographic Information File which is a plain text file format for a macromolecular crystallographic experiment and its results. When the coordinates and structure factors are deposited with the RCSB PDB or PDBj an mmCIF for the structure will be created and made available to the depositor. Alternatively, if authors use the IUCr pubBio tool to prepare their paper they will be able to upload their data as an mmCIF. An example of an mmCIF can be obtained by clicking here.

[Back to contents](#)

What do I need to do about copyright?

When your article has been successfully uploaded, a Co-editor reference code assigned and a PDB entry created, you will be sent an e-mail to confirm that your article has entered the review stage. You will also receive a Transfer of Copyright agreement. You should complete and sign this agreement and return it to the Co-editor by e-mail (copyright@iucr.org). The e-mail should include the Co-editor reference code in the Subject line.

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Stage 3, continued

STRUCTURAL PAPER = yes (macromolecular structures)

- Error message appears if authors try to continue without uploading validation report

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Upload source files

Error: Please upload a structural validation report file for this submission.

Stage - 1 - 2 - **3** - 4 - 5 - 6 - 7 -

Upload source files

Structural features of peroxisomal catalase from the yeast *Hansenula polymorpha*

Chris Williams* and Esther Pena-Soler [Modify these details](#)

[upload submission](#) [upload enhanced figure](#)

Current version 2 August 2011 13:30:27 BST [Upload source files](#)

[Review document \(PDF\)](#) Tue Aug 2 13:35:08 2011

Abstract [More...](#)

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Name	Component	Size	Upload time	
t050612_source.doc	Article body	205824	Tue Aug 2 13:30:27 2011	Delete
t0506122xq1.mcf	mmCIF	7075665	Tue Aug 2 13:34:56 2011	Delete

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3. Click on the 'Upload file' button

revised Word file

figure Figure number Part

scheme Scheme number

PDB validation report PDB code

mmCIF

Structure factors, powder diffraction data and other supplementary material may also be uploaded.

structure factors PDB code

powder diffraction data

other supplementary material

Done

Stage 3, continued

STRUCTURAL PAPER = yes (macromolecular structures)

- If validation report not available can continue if explanation is given

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Resolution	
Resolution from map-calculations (low)	19.99Å
Resolution from map-calculations (high)	2.90Å
Resolution from PDB header	2.90Å
R-factors	
R-factor for map	0.188
R-factor from PDB header	0.191
Free R-factor from PDB header	0.223
Structure quality	
Average Real space R-factor (Deviation)	0.163 (0.061)
Average Real-space correlation coefficient (Deviation)	0.947 (0.041)
Average Occupancy-weighted avg temperature factor (Deviation)	43.0Å ² (15.3Å ²)
Padilla-Yeates statistics	
Padilla-Yeates < L >	0.457
Padilla-Yeates <L ² >	0.283
Wilson statistics	

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Molecular origins of commercial laser dye functionality in azacoumarins and quinolones

Carolyn P. Brock*, Xiaogang Liu, Jacqueline Cole and Paul G. Waddell [Modify these details](#)








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t050607.cif	CIF	53504	Tue Jul 26 11:03:42 2011	
t050607ld425_180k_22apr2011int4sup2.hkl	Structure factors	240021	Tue Jul 26 11:06:08 2011	Delete
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 t050607fig1.ps	Figure	16448	Tue Jul 26 10:53:04 2011	Delete
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 t050607fig3.ps	Figure	12181330	Tue Jul 26 10:55:20 2011	Delete
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 t050607fig5.ps	Figure	62880	Tue Jul 26 10:57:50 2011	Delete
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Professor E.V. BOLDYREVA (high pressures; organic solids; hydrogen bonds; crystal engineering; low temperatures; reactivity of solids)

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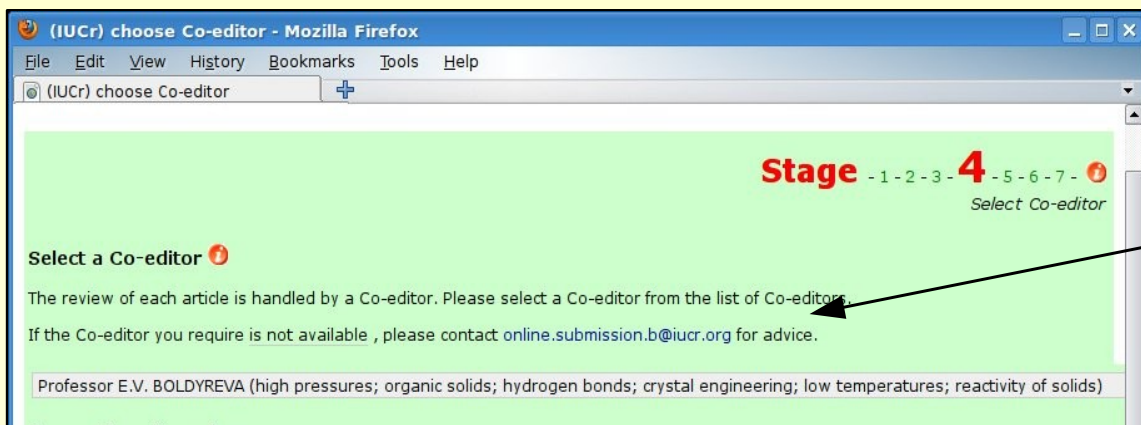
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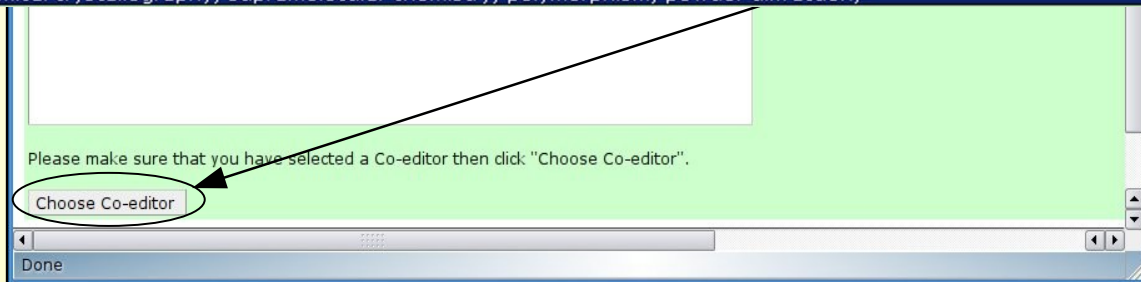
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Professor T.R. WELBERRY (diffuse X-ray scattering; disorder; phase transitions; quasicrystals; computer modelling and simulation)
Dr T.J. WHITE (ceramics; minerals; electron microscopy; powder diffraction)
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Suggestions for referees

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Peter	Strickland	ps@iucr.org

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Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055, USA
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xl316@cam.ac.uk,pgw27@online.submission.b@iucr.org	online.submission.b@iucr.org	Article submission (reference: bk5105)	2011-06-09 17:14:23
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cpbrock@uky.edu (Coedit:jb@iucr.org)	online.submission.b@iucr.org	Article bk5105: new submission bk5105 to Acta Crystallographica	2011-06-09 17:14:23
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This is to inform you as a Co-author that the following article:

Title: Molecular origins of commercial laser dye functionality in azacoumarins and quinolones: LD 425, LD 489 and LD 473
 Author(s): Xiaogang Liu, Jacqueline M Cole* and Paul G Waddell
 Contact author: Professor Jacqueline Cole
 Contact e-mail: jmc61@cam.ac.uk
 Reference: BK5105

Abstract: The molecular structures of three compounds, LD 425 (C₁₃H₁₄N₂O₃), LD 489 (C₁₅H₁₅F₃N₂O₂) and LD 473 (C₁₇H₁₉F₃N₂O), are determined by single-crystal X-ray diffraction at 180 K. Azacoumarins LD 425 and LD 489 possess para-quinoidal bond distance patterns in their benzene rings due to inter-ring charge transfer (IRCT) from these rings to the adjoining ring. In contrast, chemical substitution of the coumarin single-bonded O with N, to form a quinolone, results in the suppression of this IRCT effect. Instead, intra-ring charge transfer is shown to become more pronounced. Such charge transfer trends are present in many quinolones including LD 473. Resonance theory is used to explain these bond pattern changes and assisted spectral blue shifts in relation to their coumarin analogues. The application of this theory offers an effective and intuitive understanding of the structure-property relationship in azacoumarins and quinolones. Such understanding is important for recognising the reaction mechanisms in these compounds such that new laser dyes can be designed with desired spectral shifts.

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Molecular origins of commercial laser dye functionality in azacoumarins and quinolones: LD 425, LD 489 and LD 473

Author(s): Xiaogang Liu, Jacqueline M Cole* and Paul G Waddell
Contact author: Professor Jacqueline Cole
Contact e-mail: jmc61@cam.ac.uk
Paper type: research papers
Received: Thu 9 June 17:14:23 2011

has been submitted to Acta Crystallographica Section B and is now available from the IUCr web server for review.

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Contact author: Professor Jacqueline Cole
Contact e-mail: jmc61@cam.ac.uk

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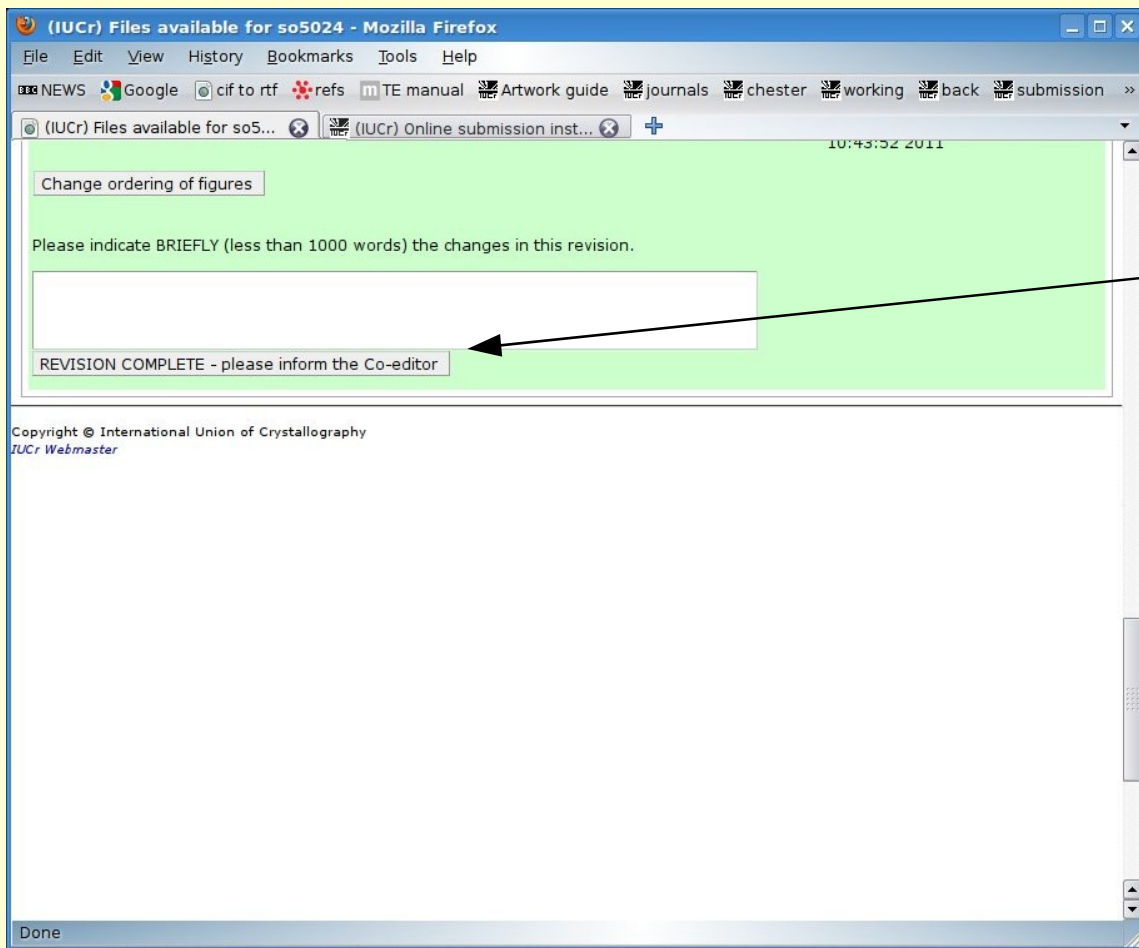
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Repeat e-mail address* cpbrock@uky.edu

Title Professor

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- Can also modify details if any changes to title or authors after submission
- Chester usually take information in the manuscript as being correct (but authors will get proofs)

Some problems

- rev.pdf not created:
 - files may be password protected
 - file may contain macros
 - file may contain character fonts we do not recognise
- Submission not finalized so only tracking number allocated and Co-editor not selected
- Files missing – if author selects `no' at stage 1 in answer to `Does your article report a crystal structure?' then not required to upload CIF
- Missing structure factor/powder data files
- Authors uploading multiple revisions if wrong files uploaded

Some problems, continued

- Authors do not complete submission
 - given two months to complete submission but reminder emails sent as authors often lose details of how to proceed
- Multiple submission using slightly different details and files
- Figures uploaded but not appearing in rev.pdf file
 - problems with figure files, e.g. .tif may contain alpha channels so our figure conversion program stalls

Some problems – LaTeX submissions

- No BibTex file uploaded or not recognised – no citations will appear in rev.pdf
- Figures in wrong format - LaTeX can handle .ps, .jpg or .png but not .tif
- Can normally handle files if all figures are of same format – if mixture of files uploaded can cause problems
- Names of uploaded fig files differ from those referenced in source LaTeX file
- Author used LaTeX macro libraries that are not standard – rev.pdf will not be created at all (solution: adding non-standard library to collection available to submission system but involves a lot of work)
- LaTeX file not in preprint mode

Future development

- Feedback very important
- Integration with contributor ID systems such as ORCID
- Plagiarism checking of all articles (using CrossCheck)
- Integration of electronic copyright/licencing transfer into submission procedure
- Improve documentation for authors and make the process clearer
- Transfer of information collected by tools and templates to submission system
- Improved status information for authors
- Home pages to be extended to authors
- Reference checking of submitted articles