


# Commission on Journals 2011

Crystallography  
**Journals**  
Online



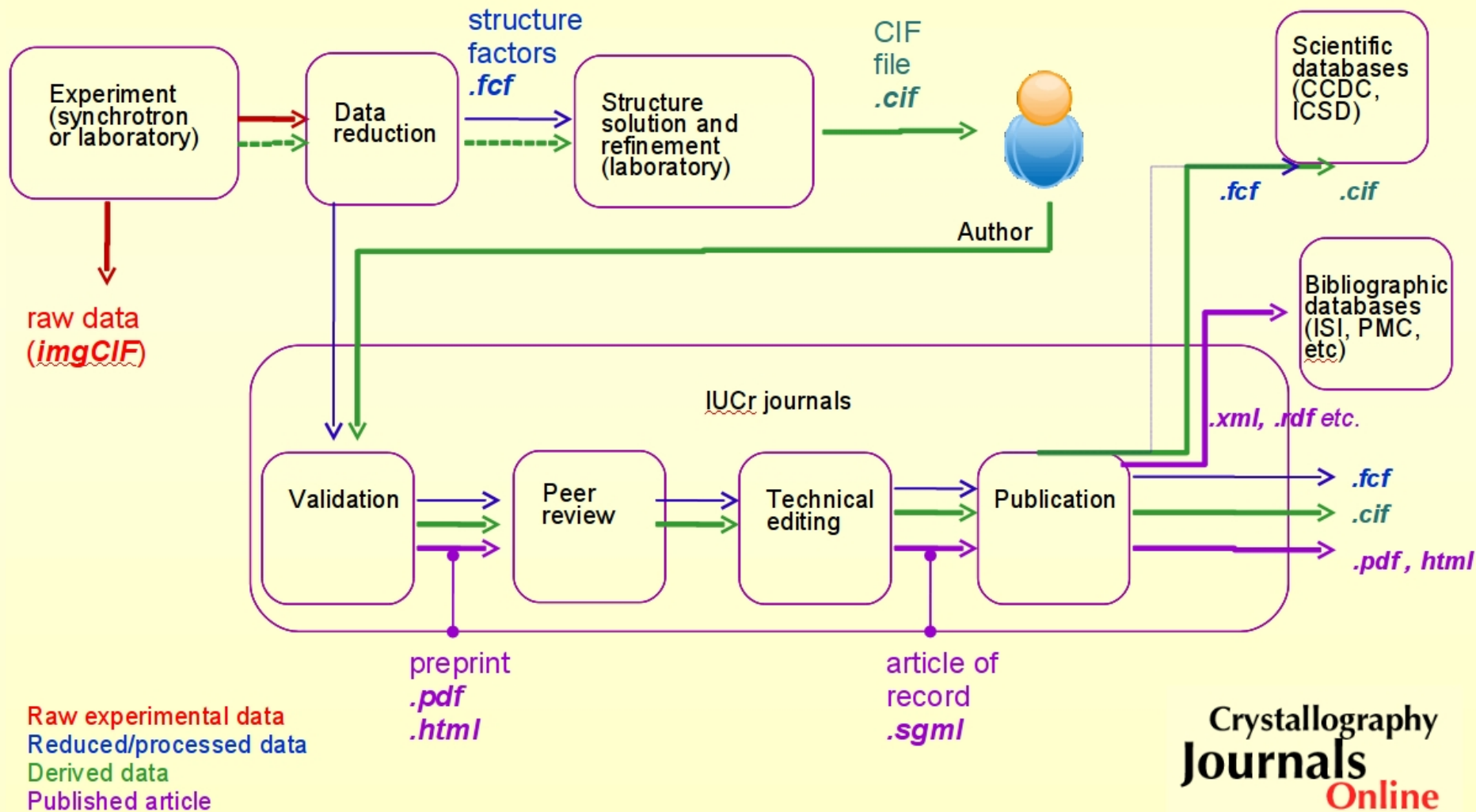
# Submission to publication

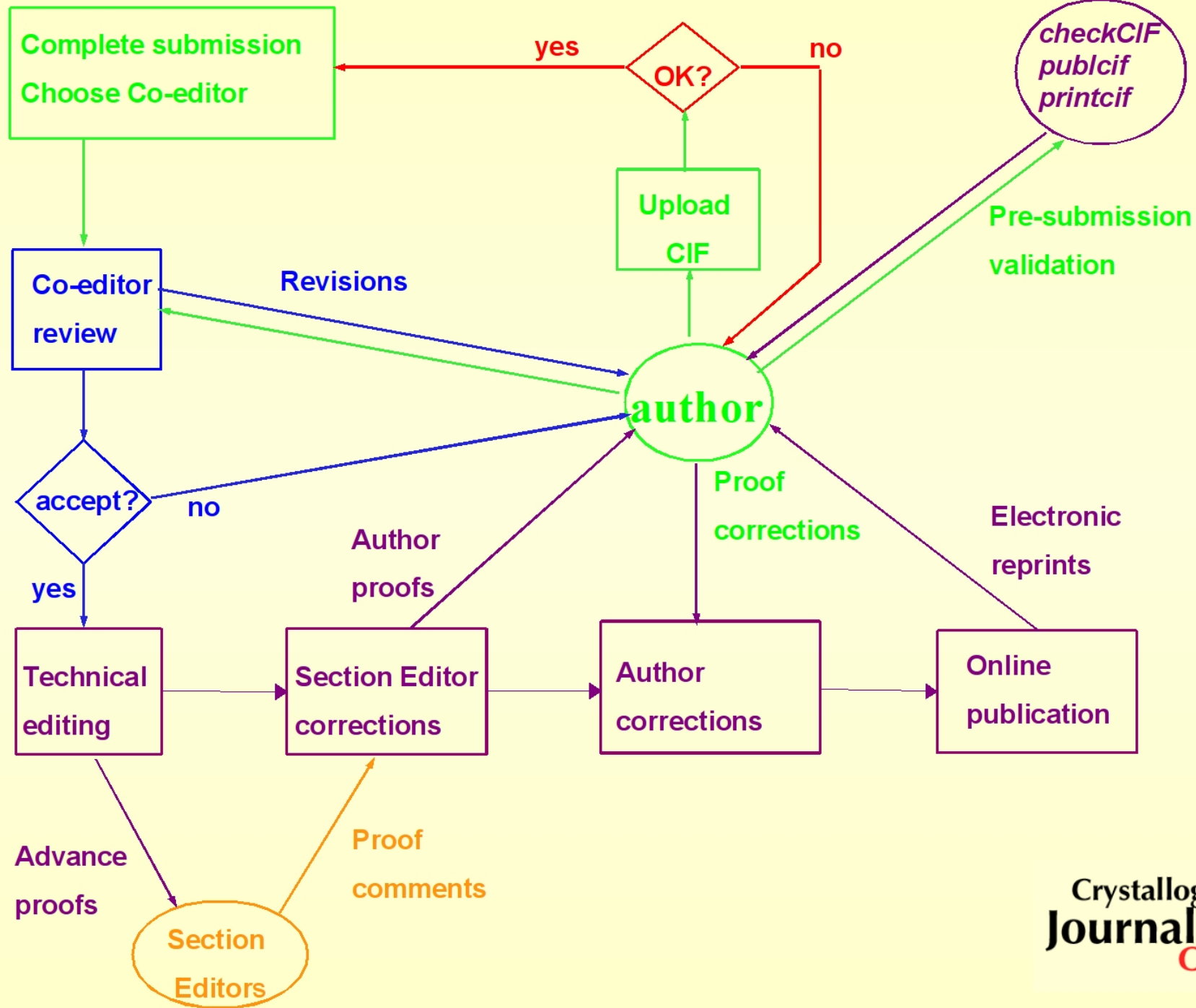
Gillian Holmes

# Dilbert's guide to PowerPoint



# Publication flow in IUCr journals







# Validation

Comparison against a set of test criteria:

Are all the usually expected data and information present?

Are related parameters consistent?

Is the space group correct?

Has the refinement converged?

Are the assigned atom types correct?

**BUT there are limitations e.g.**

Test is not yet implemented or is not practical in these circumstances

Error is not a validation issue

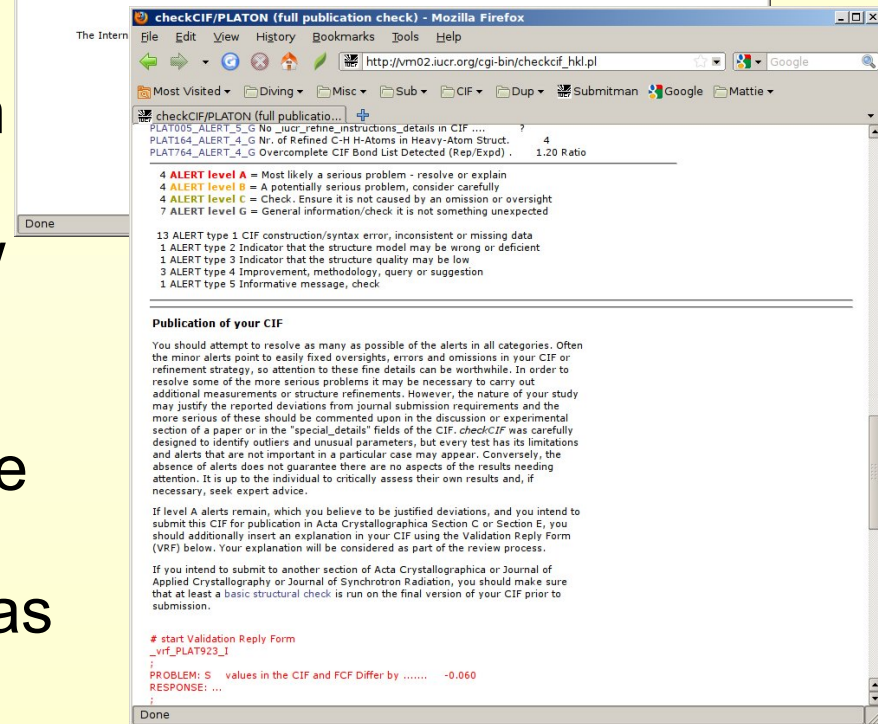
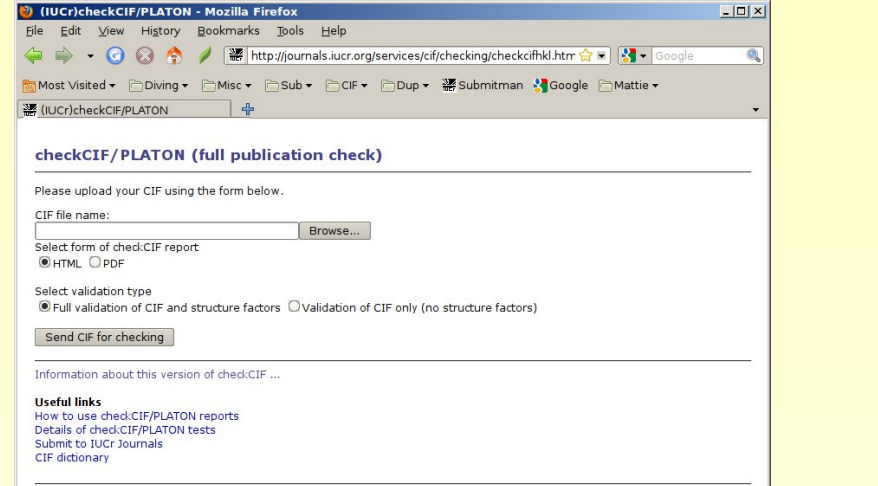
Mistake cannot be detected from data in CIF

Nonsense entries in CIF

# checkCIF

For crystal/molecular structures with a small unit cell

- all structures processed by *checkCIF* upon article submission and the resultant report scrutinised during the peer review process
- structure factor files also now analysed with *checkCIF* during the submission process
- *checkCIF* reports are published as supplementary documents for *Acta Cryst. E* articles



Crystallography  
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Online

<http://journals.iucr.org/services/cif/checking/checkfull.html>

# pubCIF

Desktop CIF publishing editor, validator and formatter for small-molecule, powder, modulated and incommensurate structure CIFs. Available for Linux, Microsoft Windows, MacOS X

CIF and preprint are presented side-by-side and can both be edited. Changes made to one are applied to the other as the user types.

Use *pubCIF* to:

- add required data items using simple wizards that check input and access both dictionary information and data used in previous CIFs
- write paper using a word-processing environment
- prepare standard and customized tables
- check CIF for both syntax and completeness
- print or export preprint of a paper
- check references
- store or retrieve author details from a local database

<http://pubcif.iucr.org>

The image shows a screenshot of a web browser displaying the pubCIF website. The browser title is "(IUCr) Structure Reports Online author services - Mozilla Firefox". The address bar shows the URL <http://journals.iucr.org/services/authorservices.html>. The website header includes navigation links for "Structure Reports Online", "Journals Online", and "supplementary files". The main content area features a blue banner with the text "pubCIF - free software to edit and preview a CIF for publication". Below this, there is a "Download" section with a description of the software and a "Starting with a CIF resulting from a structure refinement, use pubCIF to:" section. The software interface is shown in a window titled "pubCIF - /iucrfs/er/rk2289/rk2289.cif (modified)". The interface includes a menu bar (CIF Edit Preprint Tools Help IUCr), a toolbar, and a main editing area. The editing area is split into two panes: the left pane shows a text editor with CIF data items and a preprint section, and the right pane shows a chemical structure diagram of a benzamide derivative. The preprint section includes text describing the synthesis and refinement of the compound. The chemical structure diagram shows a benzamide derivative with a nitrile group (NC) and a carbonyl group (C=O). Below the structure, there is a "Related literature" section with references to Ambrosi et al. (1994), Brakhage (1998), Sundaresan et al. (2008), Kamala et al. (2008), and Nizam Mohideen et al. (2007). At the bottom of the software window, there is a "pubCIF - log messages" window showing the results of VCIF syntax checking, which reported no errors.

pubCIF takes a crystallographic information file (CIF) and prepares a formatted paper (Preprint) in the style of *Acta Crystallographica* Sections C and E.

The CIF and the Preprint are presented side-by-side and are both editable. Changes made to one are applied to the other as you type.

Starting with a CIF resulting from a structure refinement, use *pubCIF* to:

- Add data items required for publication,

pubCIF - /iucrfs/er/rk2289/rk2289.cif (modified)

```
231 in chloroform and heated for two minutes. The resulting
232 crystals suitable for XRD studies.
233
234
235 _publ_section_exptl_refinement
236
237 The hydrogen atoms were placed in calculated positions
238 0.98\AA, O-H = 0.82\AA and refined in the riding model
239 displacement parameters: <math>U_{11}</math> (H) = 1.2<math>\times 10^{-4}</math>,
240 methylene, methine groups, <math>U_{11}</math> (H) = 1.5<math>\times 10^{-4}</math>,
241 group and <math>U_{11}</math> (H) = 1.5<math>\times 10^{-4}</math> for hydro:
242
243 The 1876 Friedel pairs were merged ('MERG 2' instruction
244 refinement).
245
246
247
248 # $Chemical Data
249
250 data_I
251
252 _audit_creation_method SHELLXL97
253 _chemical_name_systematic
254 2-(Hydroxy[1-(4-methoxyphenyl)-4-oxo-3-phenylazetidin-2-yl
255
256 _chemical_name_common ?
257 _chemical_melting_point ?
258 _chemical_formula_moiety 'C20 H18 N2 O3'
259 _chemical_formula_sum 'C20 H18 N2 O3'
260 _chemical_formula_weight 334.36
261
262 pubCIF - log messages
263
264 loop
265 Results of VCIF syntax checking...
266 VCIF reported no errors
267
268 Starting pubCIF checking...
269
270 Finished pubCIF checking
271
272 For full crystallographic checking, visit http://checkcif.iucr.org.
```

Chemical structure diagram showing a benzamide derivative with a nitrile group (NC) and a carbonyl group (C=O).

Related literature

For the uses of acrylonitrile derivatives, see: Ambrosi *et al.* (1994). For the pharmacological properties of  $\beta$ -lactam derivatives, see: Brakhage (1998). For related structures, see: Sundaresan *et al.* (2008); Kamala *et al.* (2008). For related geometrical parameters, see: Nizam Mohideen *et al.* (2007).

(I)

Crystal data	
$C_{20}H_{18}N_2O_3$	$V = 1749.93(9) \text{ \AA}^3$
$M_r = 334.36$	$Z = 4$
Monoclinic, Cc	Mo K $\alpha$ radiation

Crystallography  
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Online

# pubCIF

pubCIF - /iucr/cif/2107/nk2107.cif

- Online checkCIF
- CIF dictionary
- Check citations
- Abstract
- Standard references
- Get related literature
- pubCIF paper creation wizard
- Data input wizard
- Table wizard
- Edit authors
- Save authors in database...
- Spellcheck CIF
- Preferences...

pubCIF - /iucr/cif/checking/jm/jm614af.cif (modified)

pubCIF - log message

Reference list contains uncited references. Would you like to add them to the related literature section as "For related literature, see: Au <-> et al. <-> (2009); Hochberg & Schulz (1993); Hunter & Simpson (1999); Khalaji & Simpson (2009, 2009); Le Baconn, Chuburu, Toupet, Handel, Sobinet, Dechamps-Olivier, Barbier & Aplincourt (2001); Lair & Stark (1989); Li & Simpson (2009); Rigaku (2005); Sobransingh & Kafer (2006); Song <-> et al. <-> (2008); Spek (2009); Westrip (2009).?"

Yes No

pubCIF - /iucr/cif/nk2107/nk2107.cif (modified)

Acta E preprint (organic compounds)

1-Iodotriptycene

Richard Betz, Cedric McClelland and André Scheffer

Mandela Metropolitan University, Summerstrand Campus, Department of Chemistry, University Way, Summerstrand, PO Box Port Elizabeth, 6031, South Africa

Correspondence e-mail: richard.betz@webmail.co.za

Choose the type of table you would like to edit:

- Bonds
- Contacts
- Angles
- Torsion angles
- Hydrogen bonds
- Custom

Choose the data block:

OK Close

The title compound, C<sub>20</sub>H<sub>13</sub>I, is a halogenated derivative of triptycene. The molecule shows crystallographic as well as non-crystallographic C<sub>3</sub> symmetry. The asymmetric unit comprises one third of the molecule. Dispersive I...I contacts [I...I = 3.6389 (3) Å] connect the molecules into dimers. The shortest centroid-centroid distance between two π-systems is 3.8403 (12) Å.

Acta E preprint (organic compounds)

Donor (D)	H atom	Acceptor (A)	Symmetry D	Symmetry H	Symmetry A
1 geom_h...	1 geom_h...	1 geom_h...	1 geom_h...	1 geom_h...	1 geom_h...
2 ?	?	?	?	?	?

Notes on hydrogen-bond geometry (\_jucr\_geom\_hbonds\_special\_details)

Add to CIF Cancel

connect the molecules into dimers. The shortest centroid-centroid distance between two π-systems is 3.8403 (12) Å.

<http://pubcif.iucr.org>

Crystallography  
Journals  
Online

# printCIF

*printCIF* takes a CIF and prepares a formatted paper (preprint) in the style of Sections C and E.

Use *printCIF* to

- create HTML version of article and supplementary information with live *Jmol* visualization of molecular geometry
- create PDF version of article
- create PDF version of article and supplementary document
- create PDF version of supplementary material
- run online *checkCIF* validation
- visualize structure in *Jmol*

<http://publCIF.iucr.org/services/tools/printcif.php>

printCIF - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://publCIF.iucr.org/services/tools/printcif.php

Most Visited Diving Misc Sub CIF Dup Submitman Google Mattie

printCIF

## 1,3-bis(iodomethyl)benzene a re-determination.

Jim Simpson

Department of Chemistry, University of Otago, P.O. Box 56, Dunedin, NEW ZEALAND

The title compound was prepared by metathesis from a di-bromo analogue. Structure has been reported previously [John McAdam *et al.* (2009) *Acta Cryst.* E63, o1573-o1574] but in that report a compound were recrystallised from acetone whereas here they were obtained from methanol. The four unique C atoms in a molecule lie in the plane. In the crystal structure, weak C—H...I interactions link molecules into stacks.  $\pi$ ... $\pi$  stacking is also observed. A structure is further stabilised by short I...I contacts, forming undulating sheets.

### Related literature

For the preparation, see: Moore *et al.* (1986); Kida *et al.* (2005). For related literature, see: Samakande *et al.*, (2007); Asandei *et al.* (2008). For related crystal structures, see: Basaran *et al.* (1992); Fun *et al.* (2009); Jones & Kus (2007); Zhang *et al.* (2007). For details of halogen...halogen interactions, see: Pedireddi *et al.* (1994) and for bond lengths and angles, see: Allen *et al.* (1987). For other structures of organic compounds published recently by the author, see: Osman *et al.* (2009), Hanton *et al.* (2010); Saeed *et al.*, (2010a,b,c,d,e,f,g), Saeed *et al.*, (2009a,b,c,d); Li *et al.* (2009), Shafiq *et al.* (2009); Haider *et al.* (2010).

### Experimental

Crystal data

$C_8H_8I_2$	$V = 462.16 (11) \text{ \AA}^3$
$M_r = 357.94$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 9.0804 (12) \text{ \AA}$	$\mu = 6.73 \text{ mm}^{-1}$
$b = 4.5960 (6) \text{ \AA}$	$T = 89 \text{ K}$
$c = 11.2384 (17) \text{ \AA}$	$0.19 \times 0.17 \times 0.04 \text{ mm}$
$\beta = 99.808 (8)^\circ$	

Data collection

Done

# Enhanced figures

Create *Jmol* enhanced figures

- prior to submission
- during submission
- from submitted CIF
- from other uploaded CIF
- from published structures
- from structures deposited in PDB
- Inorganic, metal-organic or organic structures
- biological macromolecules
- multiple views specified by author
- supports arbitrary *Jmol* scripts

<http://submission.iucr.org/jtkk>

Figure 4 The Jmol enhanced figure of the title compound. The H-bonding situation can clearly be seen by manipulating the various radiobuttons. [view article](#)  
Jmol script terminated

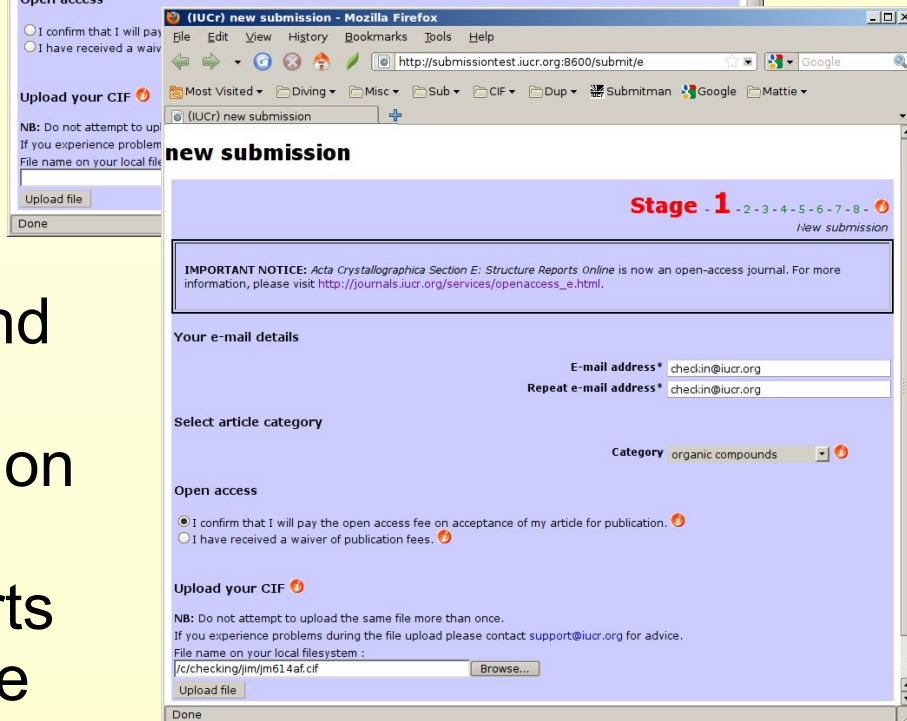
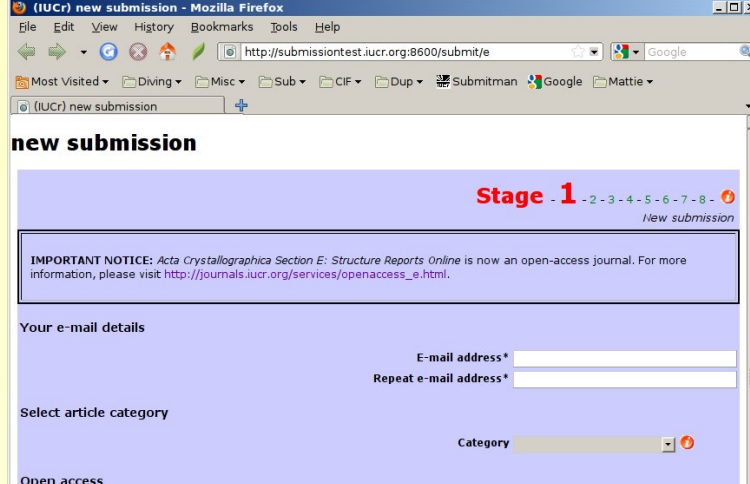
# Submission

Initial upload requires only CIF, e-mail address and category

Authors agree to pay open access fee or enter details of their waiver voucher

CIF is then validated with *vcif* and *checkCIF* and checked for previous submission or publication

If the CIF raises any level A alerts that have not been “justified”, the system displays (and e-mails) a report to help the author correct or justify the relevant alert



# Duplication type: exact

Status	Action
Tracking, review, production, published	Refuse upload and refer to support
Rejected or withdrawn	Refuse upload and refer to support unless submitted to a different journal (in which case pass details of previous Co-editor number and journal to new Co-editor)

# Duplication type: nearly identical

(formulae, authors, cell parameters,  $R$  factors match; files differ)

Status	Action
Tracking, review, production	Ask if a revision and for Co-editor code of the paper; redirect to revision page if answer matches duplication result.
Rejected or withdrawn	If submitted to same journal, tell authors their submission is similar to a previously RJ or WD paper, ask if they wish to continue, ask them to justify publication, redirect to original Co-editor. If submitted to a different journal, pass details to new Co-editor.
Published	Inform authors that their submission is similar to a published paper, ask if they wish to continue, ask them to justify publication. Authors will need to be given a link to the abstract page of previous article.

# Duplication type: rerefinement

Status	Action
Tracking, review, production	Ask if a revision and for Co-editor code of the paper; redirect to revision page if answer matches duplication result.
Rejected or withdrawn	If submitted to same journal, tell authors their submission is similar to a previously RJ or WD paper, ask if they wish to continue, ask them to justify publication, redirect to original Co-editor. If submitted to a different journal, pass details to new Co-editor.
Published	Inform authors that their submission is similar to a published paper, ask if they wish to continue, ask them to justify publication. Authors will need to be given a link to the abstract page of previous article.

# Duplication type: study on same compound

Status	Action
Tracking, review, production	Allow upload, direct to same Co-editor that is handling the matching paper.
Rejected or withdrawn	Divert paper to the Co-editor who handled the original paper.
Published	Inform authors that their submission is similar to a published paper, ask if they wish to continue, ask them to justify publication. Authors will need to be given a link to the abstract page of previous article.

# Duplication type: title match

Status	Action
Tracking, review, production	Refuse upload and refer to support



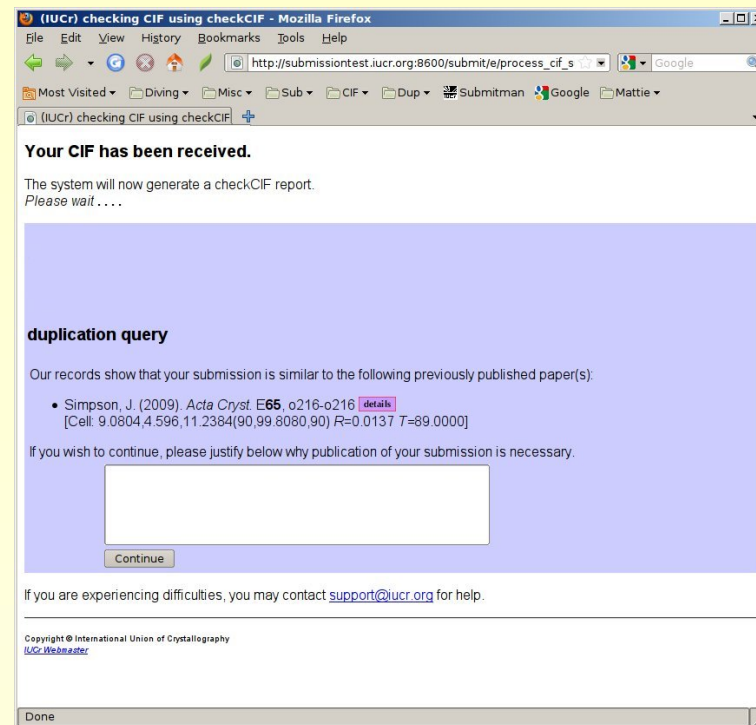
# Duplication detected

The system checks the article against an internal database to determine if the structure has previously been submitted to or published by the IUCr

A reduced cell check is performed

In addition, an automated check is performed against the CSD and ICSD

If a duplication is detected, the author is required to note why their article is worthy of consideration for publication



The screenshot shows a Mozilla Firefox browser window with the address bar displaying [http://submissiontest.iucr.org:8600/submit/e/process\\_cif\\_s](http://submissiontest.iucr.org:8600/submit/e/process_cif_s). The page content includes the following text:

**(IUCr) checking CIF using checkCIF - Mozilla Firefox**

File Edit View History Bookmarks Tools Help

[http://submissiontest.iucr.org:8600/submit/e/process\\_cif\\_s](http://submissiontest.iucr.org:8600/submit/e/process_cif_s) Google

Most Visited Diving Misc Sub CIF Dup Submitman Google Mattie

(IUCr) checking CIF using checkCIF

**Your CIF has been received.**

The system will now generate a checkCIF report.  
Please wait....

**duplication query**

Our records show that your submission is similar to the following previously published paper(s):

- Simpson, J. (2009). *Acta Cryst. E* **65**, o216-o216 [details](#)  
[Cell: 9.0804,4.596,11.2384(90,99.8080,90) R=0.0137 T=89.0000]

If you wish to continue, please justify below why publication of your submission is necessary.

If you are experiencing difficulties, you may contact [support@iucr.org](mailto:support@iucr.org) for help.

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[IUCr Website](http://www.iucr.org)

Done

# File upload

In addition to the CIF, the following files are required:

- structure factors
- at least one figure
- scheme (not inorganics)

Authors are also encouraged to upload a chemical connectivity file

Name	Component	Size	Upload time	
t050615.cif	Article	19103	Mon Aug 8 12:01:31 2011	
t050615sup2.hkl	Structure factors	75978	Mon Aug 8 12:09:29 2011	Delete
t050615fig1.ps	Figure	42143	Mon Aug 8 12:08:00 2011	Delete
t050615fig2.jpg	Figure	370379	Mon Aug 8 12:08:42 2011	Delete
t050615scheme1.tif	Scheme	3942	Mon Aug 8 12:09:16 2011	Delete

# Checking results

(IUCr) checkCIF/PLATON results for paper t050615 - Mozilla Firefox

Alert level G

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the \_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: C4 H4 I1  
Atom count from \_chemical\_formula\_moiety: C8 H8 I2

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the \_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
Atom count from \_chemical\_formula\_sum: C4 H4 I1  
Atom count from the \_atom\_site data: C8 H8 I2

CELL201\_ALERT\_1\_G Difference between formula and atom site contents detected.  
CELL201\_ALERT\_1\_G ALERT: Large difference may be due to a symmetry error - see SYMMG tests  
From the CIF: \_cell\_formula\_units\_Z 2  
From the CIF: \_chemical\_formula\_sum C4 H4 I1  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	of sites	diff
C	8.00	16.00	-8.00
H	8.00	16.00	-8.00
I	2.00	4.00	-2.00

PLAT005\_ALERT\_5\_G No jucc\_refine\_instructions\_details in CIF .... ?  
PLAT164\_ALERT\_4\_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 4  
PLAT764\_ALERT\_4\_G Overcomplete CIF Bond List Detected (Rep/Expd) 1.20 Ratio

4 ALERT level A = Most likely a serious problem - resolve or explain  
4 ALERT level W = A potentially serious problem, consider carefully  
4 ALERT level C = Check. Ensure it is not caused by an omission or oversight  
7 ALERT level G = General information/check it is not something unexpected

13 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

# start Validation Reply Form  
\_vrT\_PLAT923\_I  
? PROBLEM: S values in the CIF and FCF Differ by ..... -0.060  
RESPONSE: ...  
# end Validation Reply Form

Done

(IUCr) checkCIF/PLATON results for paper t050615 - Mozilla Firefox

database duplication summary

- chemical name = \a,\a'-diiodo-p-xylene
- A factor = 0.034
- Space group = P2(1)/c
- Formula = C4 H4 I
- a=9.0804 b=4.596 c=11.2384
- alpha=90 beta=99.808 gamma=90
- Simpson, J. (2009). *Acta Cryst. E65*, o216-o216 [details]  
[Cell: 9.0804 4.596 11.2384(90,99.8080,90) R=0.0137 7=89.0000]

## reference checking results

The following references were not checked in detail as they were not recognized as journal references

Asandei, A. D., Chen, Y., Simpson, C., Gilbert, M. & Moran, I. W. (2008). *Polymer Preprints (ACS, Div. Polym. Chem. J.)*, **49**, 489-490.

Bruker (2006). *APEX2 V2.0-2, SAINT V7.23A and SADABS 2004/1*. Bruker AXS Inc., Madison, Wisconsin, USA. [software reference?]

Hunter, K. A. & Simpson, J. (1999). *TITAN/2000*. University of Otago, New Zealand.

Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan. [software reference?]

Sheldrick, G. M. (1997). University of Göttingen, Germany .

The following references may be incorrectly formatted

Basaran, R., Dou, S.-Q. & Weiss, A. (1992). *Ber. Bunsenges. Phys. Chem.* **96**, 1688-1690. [Unrecognized journal title.]

Samakande, A., Sanderson, R. D. & Hartmann, P. C. (2007). *Synth. Comm.* **37**, 3861--3872. [Unrecognized journal title.]

Westrip, S. P. (2009). pubCIF. In preparation. [Unrecognized journal title.]

## Results of online verification of references to IUCr Journals

Conflicting results for John McAdam, C., Lyall, R. H., Stephen, C. M. & Jim, S. (2009). *Acta Cryst. E65*, o1573--o1574 (searched using volume and page):

McAdam, C. J., Hanton, J. R., Moratti, S. C. & Simpson, J. (2008). *Acta Cryst. E65*, o1573--o1574

Done

Mozilla Firefox

PLATON (Version 180711) FCF-File Validation for: I

For Documentation: <http://www.platonsoft.nl/FCF-VALIDATION.pdf>

Section 1

General Data

Crystal Data From: platon.cif  
Fo/Fc Data From: platon.hkl FCF-TYPE=SHELXL  
Space Group : P21/c  
Wavelength (Ang) : 0.71073  
Unit Cell (CIF) : 9.0804 4.5960 11.2384 90.000 99.808 90.000  
SHELX Wght Pars. : 0.0110 0.3116  
Extinction Par. : 0.0000

Section 2

Reflections with abs(|I(obs) - I(calc)| / SigW(I)) > 3.0

Nr	H	K	L	Theta	I(obs)	I(calc)	Sigma(I)	Ratio	SigW(I)	RatioW
1	1	0	2	4.65	36546.69	42066.27	1136.56	-4.86	1224.79	-4.51
2	-1	1	4	8.59	2674.00	2614.85	42.92	6.04	59.72	4.34
3	-4	6	4	30.00	179.28	337.90	44.63	-3.55	45.72	-3.47
4	-8	1	5	19.85	4404.46	3999.16	103.65	3.91	118.74	3.41
5	-12	2	6	30.45	245.10	392.06	40.23	-3.65	41.71	-3.52
6	5	4	6	25.49	147.68	221.40	21.48	-3.43	22.97	-3.21
7	-6	4	9	27.44	1935.36	2459.95	145.52	-3.60	150.07	-3.50
8	4	4	11	30.96	698.40	1143.22	100.02	-4.45	102.15	-4.35
9	7	0	12	30.79	417.82	639.51	69.65	-3.18	71.18	-3.11
10	-10	1	12	30.65	311.46	487.98	52.92	-3.34	54.37	-3.25
11	-3	1	15	28.82	499.04	647.17	46.95	-3.16	49.33	-3.00

Average = -2.12 -2.20

For I(calc) < 2 Sigma(I) < I(obs) = 10.77 and I(calc) > 14.07

Section 3

Missing Reflections (Asym. Refl. Unit) below sin(theta)/lambda = 0.5

Nr	H	K	L	sin(theta)/lambda	Theta	I(calc)	I(calc)/I(max)
----	---	---	---	-------------------	-------	---------	----------------

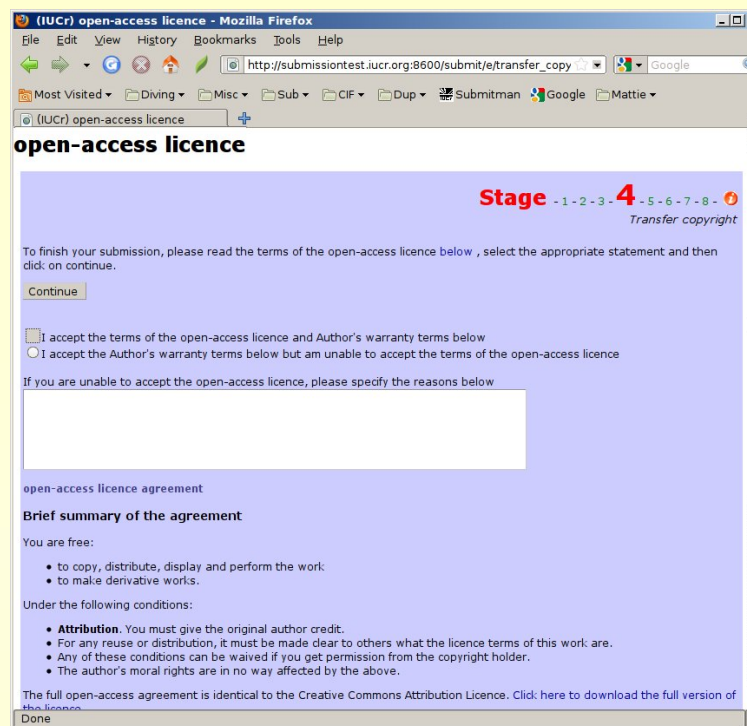
Done

# Open access

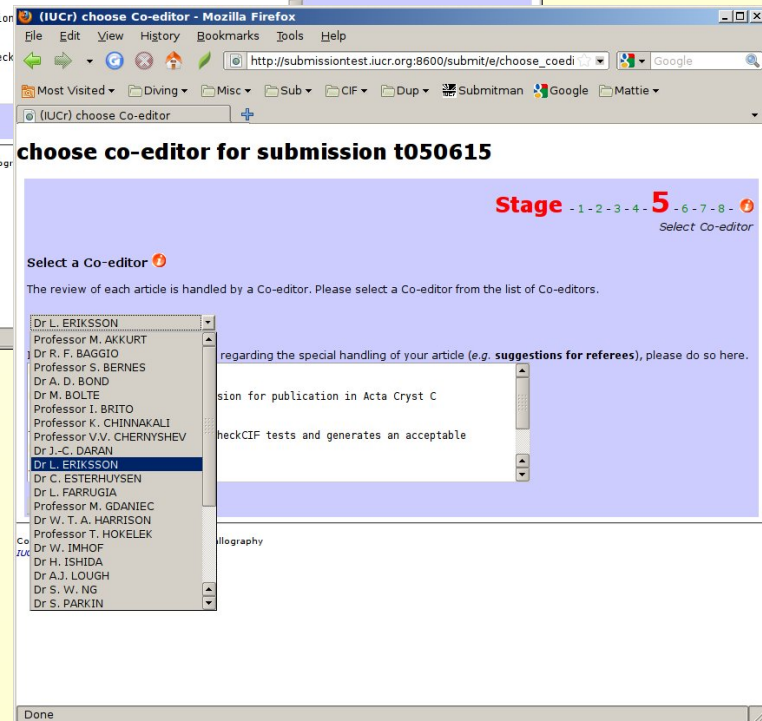
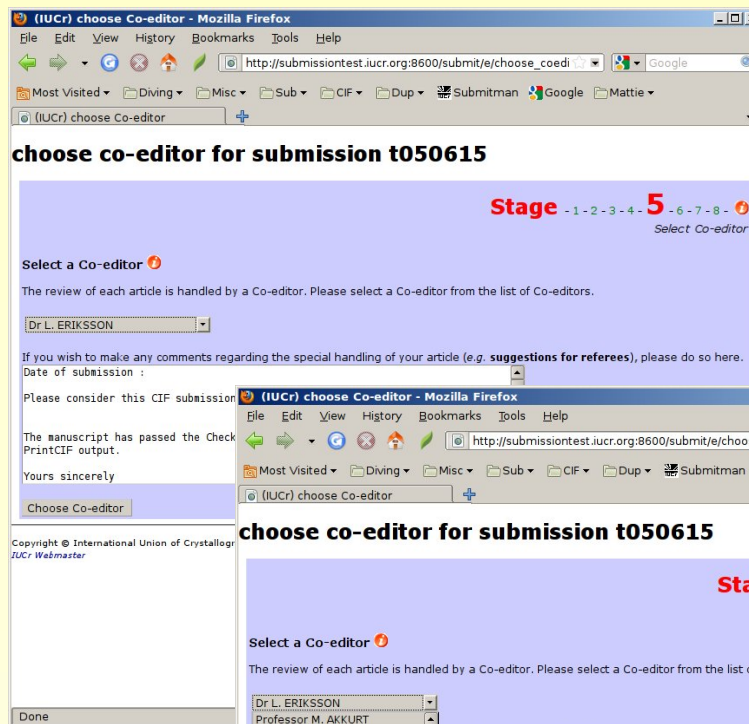
Authors are asked to agree to the terms of the open access licence at this stage

The fee is not paid until the article is accepted

For other journals, the authors are asked to transfer copyright



# Co-editor selection



Duplicate submissions are assigned to the same Co-editor who handled the original submission. Otherwise the author can choose any available Co-editor.

# How Co-editor availability is determined

1. For duplicate structures assign to original Co-editor if active (even if quota = 0), provided category is correct.
2. Select available Co-editors (active, correct journal, article category, language). Determine the quota, number assigned this week and this month and the number of papers in review for each available Co-editor.
3. Select all Co-editors under quota. If none, drop the language test.
4. If still none, factor in the number of articles in review.  
Total review quota = quota \* a journal multiplier  
Discount Co-editors with more in review than number determined.
5. If still none, repeat with doubling of monthly quota.
6. If all else fails, assign to Section Editor

# Review

Over to you!

A complete set of source data and some derived files are available to aid the review process including

- validation reports
- a “difference” file for revised submissions
- **NEW!** check for similar reduced cells in CIF archive

(IUCr) article files - Mozilla Firefox

http://submissionstest.iucr.org:8600/submit/e/review\_addr...

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(IUCr) submission system s... (IUCr) article files

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Review files

IMPORTANT: Please check the Supplementary Materials pages in the review document. These pages cannot be corrected after acceptance.

## 1,3-bis(iodomethyl)benzene a re-determination.

Jim Simpson\* [Modify these details](#)

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<a href="#">Check for similar reduced cells</a>	

Abstract [More...](#)

The following files are available for this submission

Name	Component	Size	Upload time	
hb6323.cif	Article	19103	Mon Aug 8 12:01:31 2011	
hb63231sup2.hkl	Structure factors	75978	Mon Aug 8 12:09:29 2011	<a href="#">Delete</a>
hb6323fin1.nc	Figure	42143	Mon Aug 8 12:08:00 2011	<a href="#">Delete</a>

Done

# Reduced cell check

check for structures with matching reduced cells for the submission hb6325

The following table shows structures with similar reduced cells to those in the submitted CIF. Please note that this comparison is only against structures in the IUCr CIF archive.

Criteria used for search: cell parameters within 2% of largest cell length and all angles within 2°

Datablock: 1						
Co-editor code	Authors	Reference	Sum formula	Space group	Cell parameters	Title
hb6325	Lin, Dong-Dong; Zhang, Li; Xu, Duan-Jun*	THIS ARTICLE	C6 H8 Na2 O10 Zn	P b c a	6.836,9.387,16.552 [90.00,90.00,90.00]	Poly[disodium bis(\m-malonato)zincate(II) dihydrate]
Possible Matches						
is2003	Wang, Yong-Tao*; Tang, Gui-Mei; Qin, Xu-Yang	Acta Cryst. E62 (2006), m582-m584	C6 H8 Mn Na2 O10	P b c a	6.823,9.533,16.493 [90.00,90.00,90.00]	Poly[di-aqua- $\mu$ -malonato-manganese(II)]
qb0022	Barnes, J. C.; Weakley, T. J.	Acta Cryst. C53 (1997), 0--	C6 H8 Cu1 Na2 O10	P b c a	6.814,9.497,16.374 [90.00,90.00,90.00]	Disodium Bis(malonato)cuprate(II) Dihydrate

useful both for finding similar structures....

check for structures with matching reduced cells for the submission sj2551

The following table shows structures with similar reduced cells to those in the submitted CIF. Please note that this comparison is only against structures in the IUCr CIF archive.

Criteria used for search: cell parameters within 2% of largest cell length and all angles within 2°

Datablock: 1						
Co-editor code	Authors	Reference	Sum formula	Space group	Cell parameters	Title
sj2551	Gao, Yu-Xiang*; Wang, Li-Bin; Niu, Yan-Ling; Hao, Lu-Jiang	THIS ARTICLE	C10 H8 Co N4 O5	P 21 21 21	8.012,9.533,15.023 [90.00,90.00,90.00]	catena-Poly[[aqua(pyrazine-2-carboxylato)cobalt(II)]-\m-pyrazine-2-carboxylato]
Possible Matches						
bi2194	Gao, Yu-Xiang*; Wang, Li-Bin; Niu, Yan-Ling; Hao, Lu-Jiang	Acta Cryst. E63 (2007), m1882	C10 H8 Co N4 O5	P 21 21 21	8.012,9.533,15.023 [90.00,90.00,90.00]	catena-Poly[[aqua(pyrazine-2-carboxylato)cobalt(II)]-\m-pyrazine-2-carboxylato]
STRUCTURE FACTOR FILES ARE IDENTICAL						
is2188	Gao, Yu-Xiang*; Wang, Li-Bin; Niu, Yan-Ling; Hao, Lu-Jiang	Acta Cryst. E63 (2007), m2143	C10 H8 N4 O5 Zn	P 21 21 21	7.893,9.762,14.892 [90.00,90.00,90.00]	catena-Poly[[aqua(pyrazine-2-carboxylato- $\kappa^2$ -N <sup>3</sup> ,O)zinc(II)]-\m-pyrazine-2-carboxylato- $\kappa^2$ -N <sup>1</sup> ,O-N <sup>4</sup> ]

and for detecting suspect structures



# Future developments

Structure factor checks to be included in initial validation of submission

*PLATON* tests continually added in response to new problems

Expertise requested for validation of powder data based structures and incommensurate structures

Possible interactive checking of values in the text

Feedback and help on improving tests is always welcome