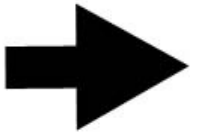
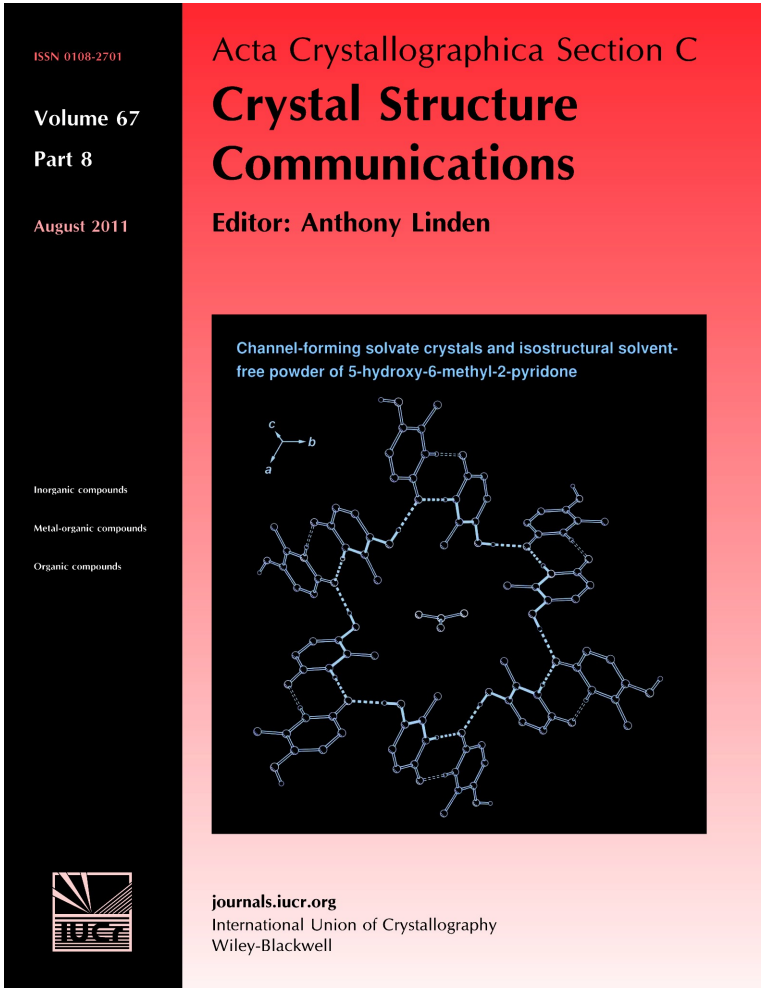
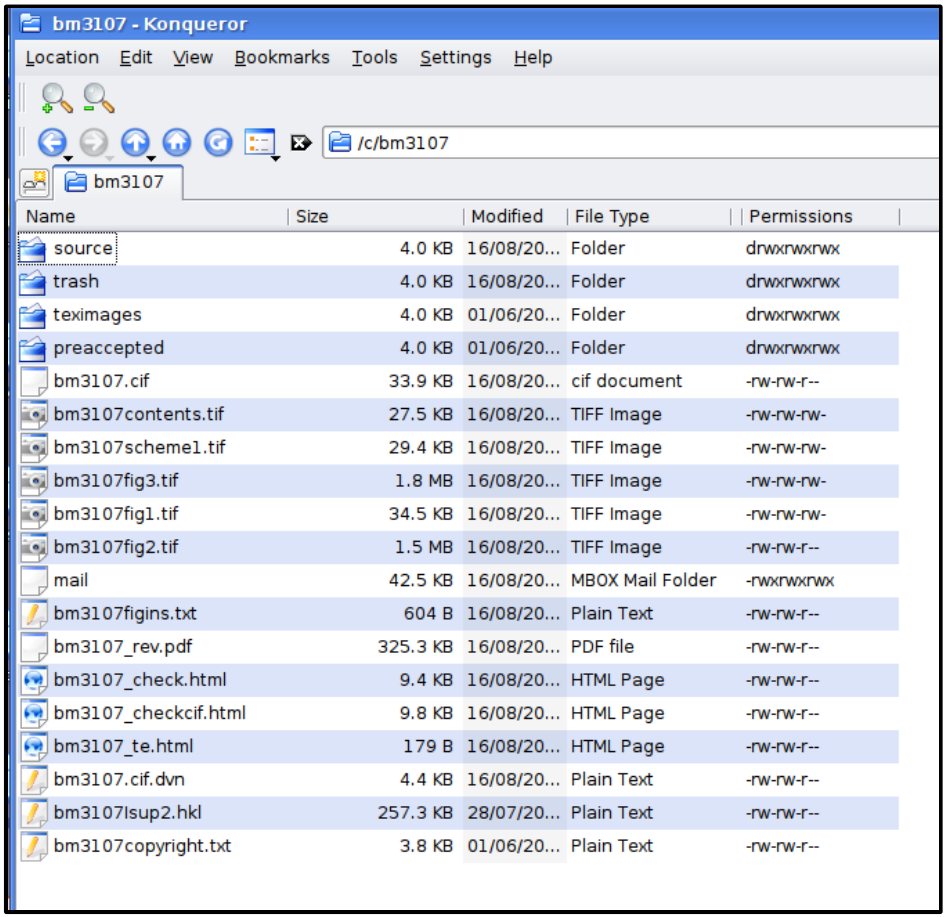
FROM SUBMISSION TO PUBLICATION





On acceptance

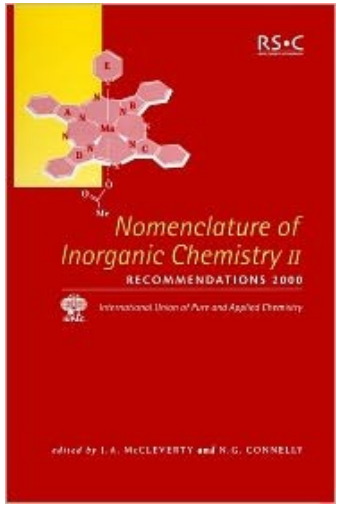
- The final files (CIF, structure factors, artwork *etc*) are moved from the submission system into the production area
- During this process, the artwork is processed automatically to be single column width and have the correct resolution
- *checkCIF* and *PLATON* are run automatically on the final accepted CIF

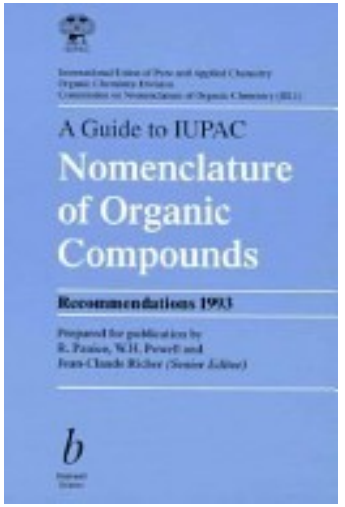


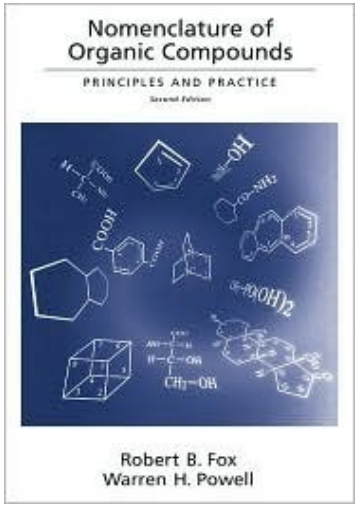
Technical editing stages

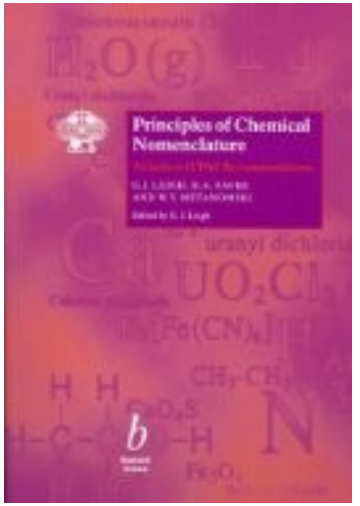
- nomenclature and formula checking
- artwork preparation
- use of *publCIF* to create an SGML file of the paper
- use of typesetting program *3b2* to create a proof from the SGML file
- incorporation of Section Editor and author corrections

Checking and producing chemical names for organic compounds









- Two chemical naming programs are used:
  (a) **Marvin** (ChemAXON; license to check 5000+ names per annum)
  (b) **OPSIN** (freely available as an open-source download; obtained as part of the IUCR's ongoing collaborations with Peter Murray-Rust and the Unilever Cambridge Centre for Molecular Science Information)

- There are two main advantages of using these programs:
  (a) greater accuracy in naming
  (b) the generation of CML (chemical mark-up language) files

- Initial automatic processing for organic papers uses the title and chemical_name_systematic fields to generate schemes

- The chemical-naming software also outputs a systematic name based on the scheme it has created and also outputs a CML file; the CML file is included in the supplementary materials for the paper

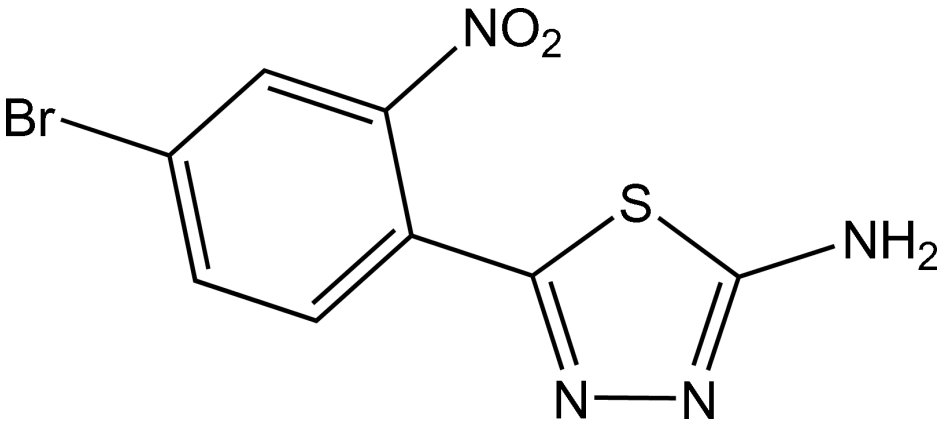
- A comparison is made between the program-generated scheme and the author scheme

Author versus program-produced schemes

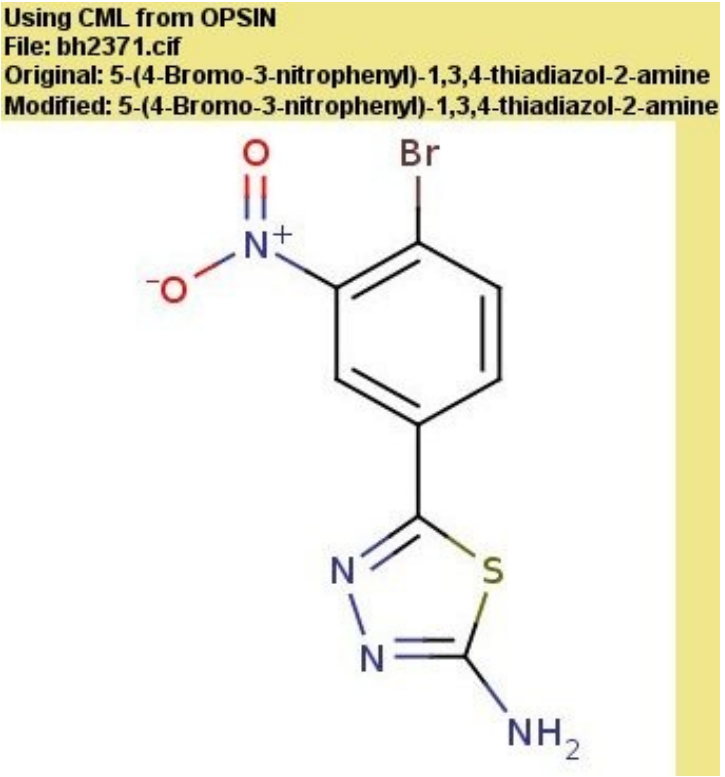
Chemical name from the CIF

2-Amino-5-(4-bromo-3-nitrophenyl)-1,3,4-thiadiazole

Scheme provided by author



Scheme created by program



- If the schemes match, then the chemical name in the CIF is taken as being correct and the systematic name output by the program can be considered to be correct

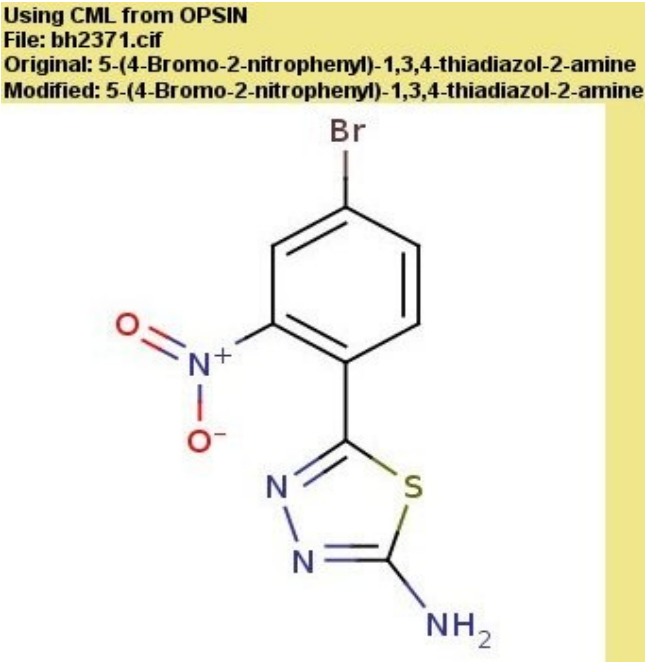
- If the schemes don't match, then either the chemical name in the CIF or the scheme provided is incorrect. The ellipsoid plot can be looked at to determine the correct structure and the scheme or chemical name or both updated

Corrected CIF name and revised scheme

2-Amino-5-(4-bromo-2-nitrophenyl)-1,3,4-thiadiazole

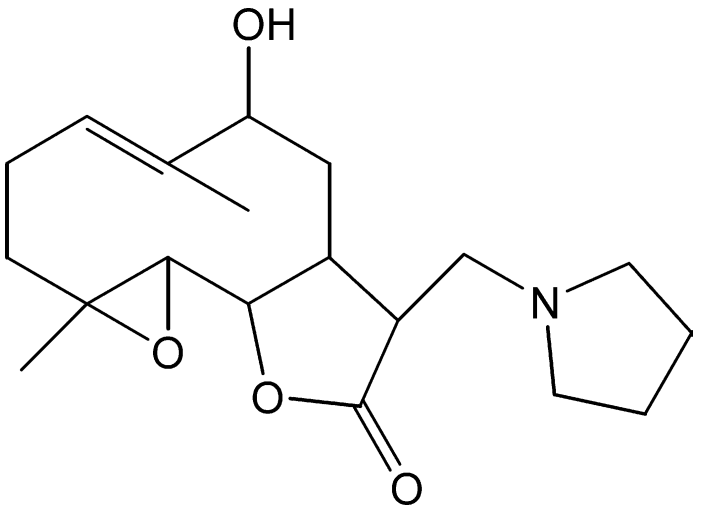
Chemical name created by program

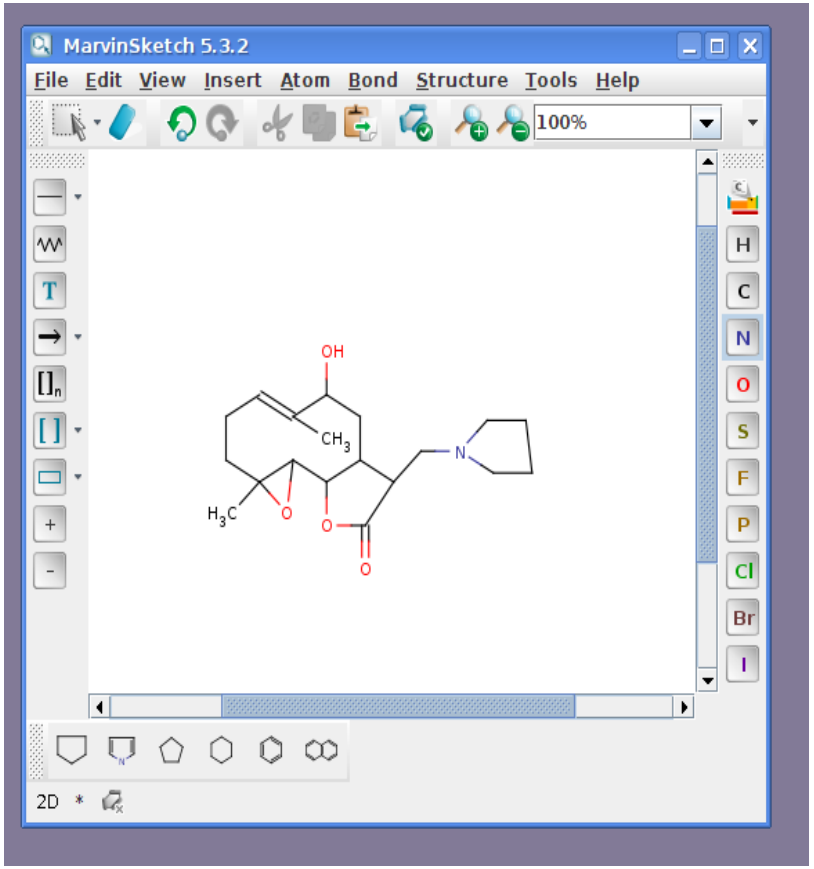
5-(4-Bromo-2-nitrophenyl)-1,3,4-thiadiazol-2-amine

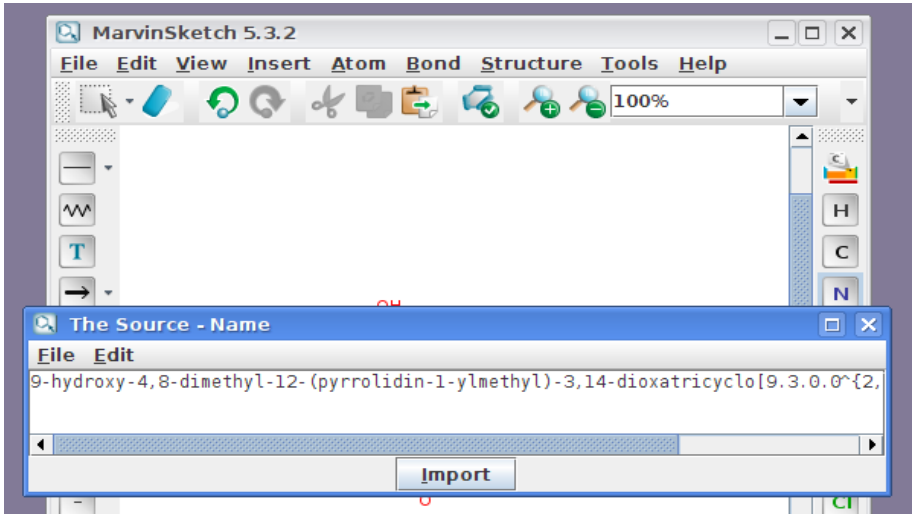


The chemical name in the CIF can now be updated with the final systematic name and the CIF checked once more with the naming program and a final CML file created. The systematic name does not always need to be used, *e.g.* the name provided by an author may be an accepted trivial name.

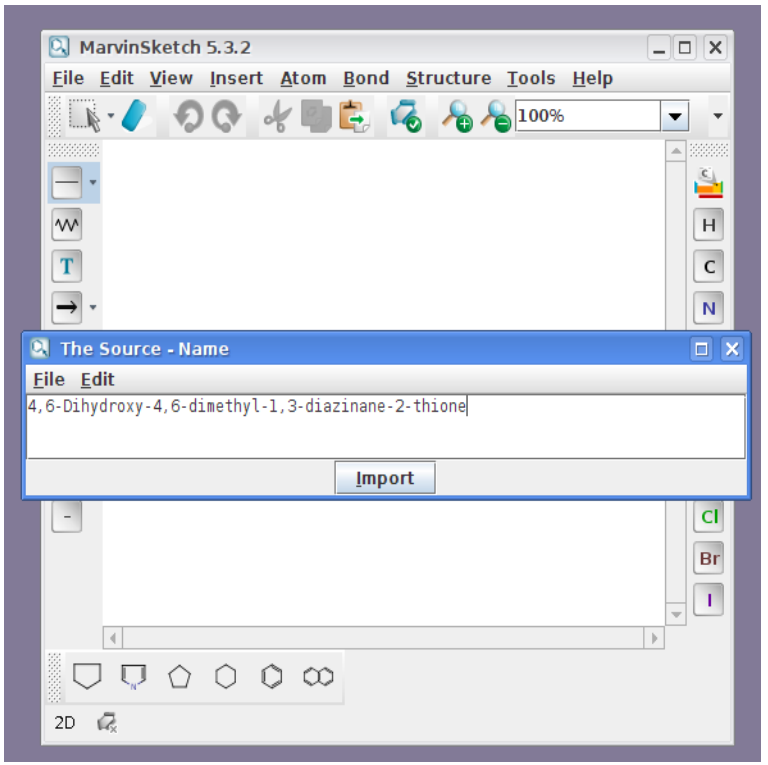
In cases where an author has not provided a useful name and where a structure is somewhat complex, *e.g.* a fused-ring system, then the chemical-naming program can be used to create a systematic name

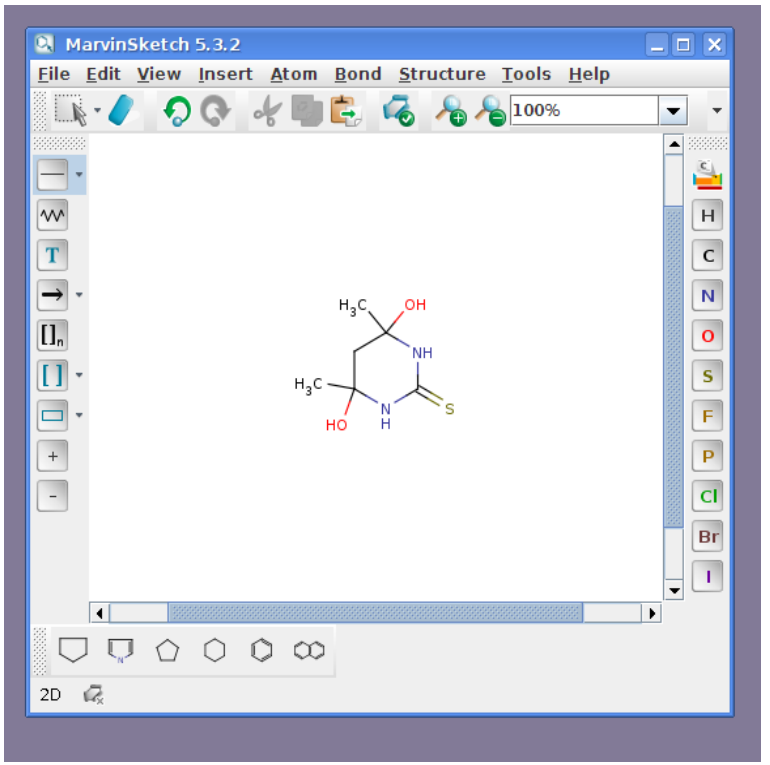






For metal-organic structures, which are not well handled by the chemical-naming programs, organic ligand names can be input manually into *Marvin* for checking against the author scheme





In creating chemical names, the following are some important initial points:-

- identify the main group from the IUPAC table of principal characteristic groups

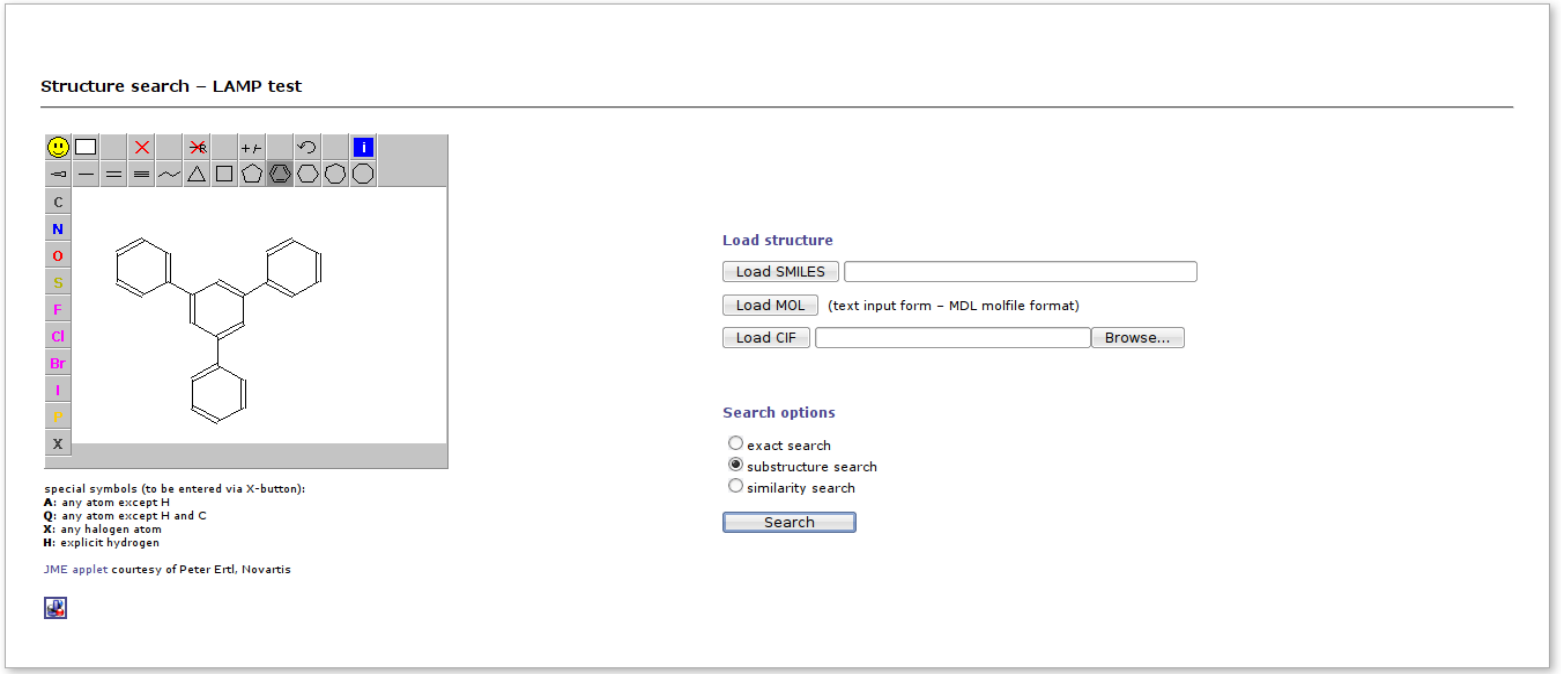
Table 10 General classes of compounds in decreasing order of priority for choosing and naming a principal characteristic group[50]

1	Radicals	13	Aldehydes followed by Thioaldehydes, Selenoaldehydes, and Telluroaldehydes
2	Anions		
3	Cations	14	Ketones followed by Thioketones, Selenoketones, and Telluroketones
4	Zwitterionic compounds		
5	Acids (in the order COOH, $C(O)O_2H$; then their S and Se derivatives followed by sulfonic, sulfinic, selenonic, etc., phosphonic, arsonic, etc., acids)	15	Alcohols and Phenols followed by Thiols, Selenols, and Tellurols
		16	Hydroperoxides followed by Thiohydroperoxides, Selenohydroperoxides, and Tellurohydroperoxides
6	Anhydrides		
7	Esters	17	Amines
8	Acid halides	18	Imines
9	Amides	19	Hydrazines, Phosphanes, etc.
10	Hydrazides	20	Ethers followed by Sulfides, Selenides, and Tellurides
11	Imides		
12	Nitriles	21	Peroxides followed by Disulfides, Diselenides, and Ditellurides

- Alphabetical order of substituents
- Correct nesting of parentheses, *i.e.* [({ [(...)] })], exceptions include fused ring systems, *e.g.* 3-(bicyclo[2.2.0]hexan-2-yl)benzoic acid, and coordination polymers, *e.g. catena*-poly[[(1,10-phenanthroline)zinc]-mu-2,2'-oxydibenzoato]
- Capital letter at the start of the name, ignoring stereochemical designators (*R*/*S*), conformational designators (*cis*/*trans*/*E*/*Z*), positional designators (*ortho*-, *meta*-, *para*-) and terms such as *tert*-
- Usage of kappa (meaning coordination) and mu (meaning bridging) nomenclature for metal-organic structures; omit kappa notation if too complex or if it seems wrong or incomplete

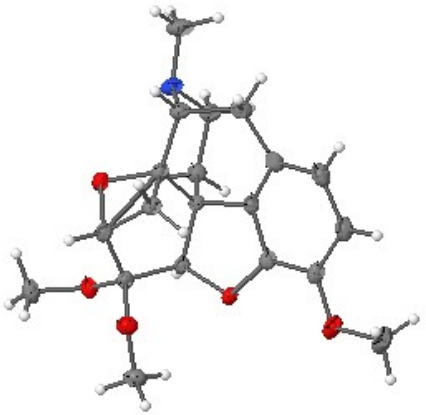
Future developments

- Substructure searching within the IUCr archive



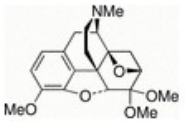
- Replacement for the online 3D page

Structure 4



$C_{20}H_{25}NO_5$

Deschamps, J. R., Coop, A., Parrish, D. A. & Rice, K. C. (2004). *Acta Cryst.* E**60**, o331-o333.



$C_{20}H_{25}NO_5$

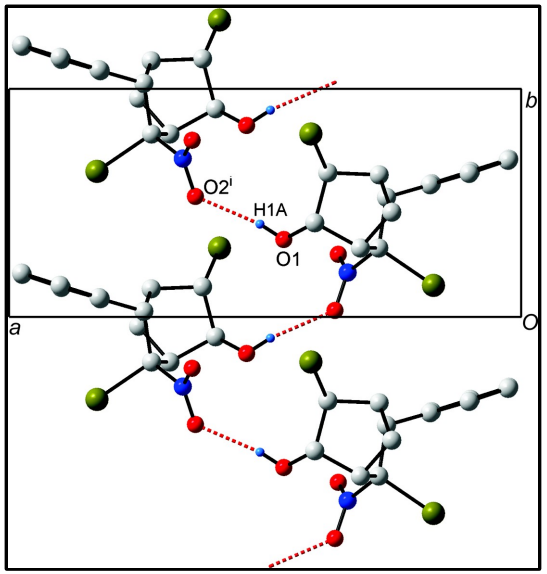
M_r = 359.41	a = 7.509 (2) Å	V = 435.81 (19) Å³
Triclinic	b = 7.777 (2) Å	Z = 1
$P1$	c = 8.430 (2) Å	
	α = 83.776 (6) °	
	β = 68.993 (5) °	
	γ = 71.511 (5) °	

Jmol

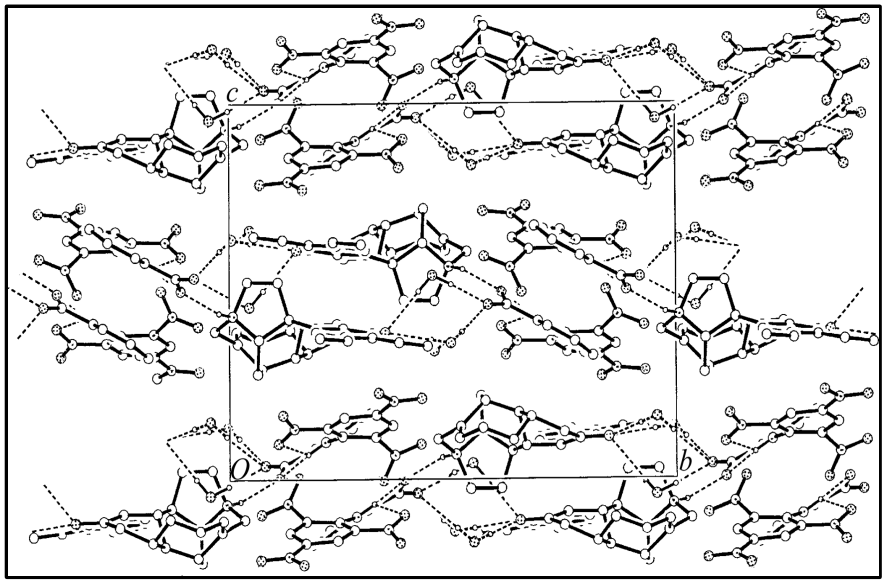
Molecule | Unit cell

Handling of artwork

Colour images should have a resolution of at least 400 dpi (dots per inch) at final size, while monochrome images (black line art on a white background) and greyscale images should have a minimum resolution of 600 dpi.



Colour, 400 dpi



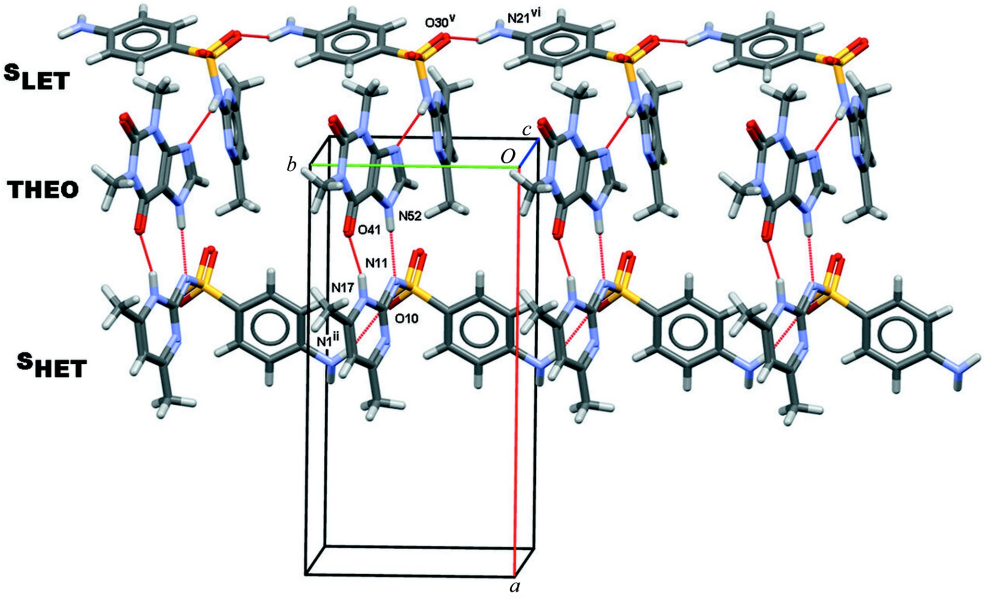
Greyscale, 600 dpi

Handling of artwork

A journal page has a two-column design, and most figures will be sized to fit a single-column width (8.85 cm) when published. In exceptional circumstances, figures will be sized to fit either part-page width (12 cm) or full-page width (18 cm).

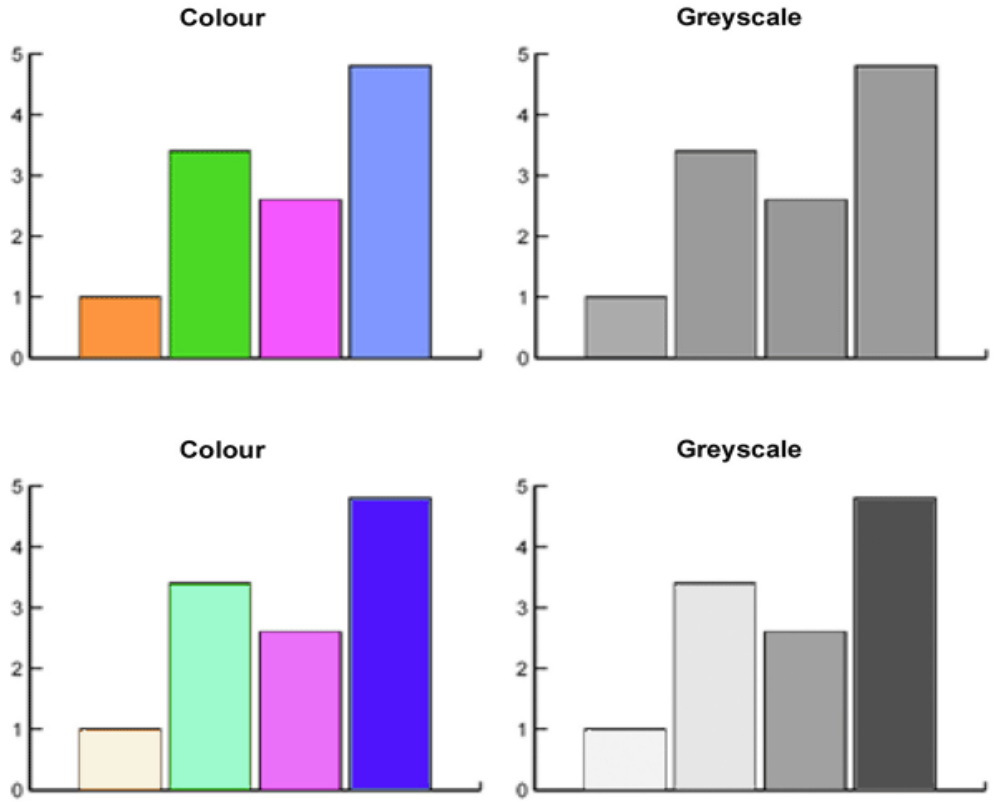
Labelling should generally be roman (upright) and consistent with the text of your article. At the final published size, the labelling on the figure should be approximately 8pt.

Double column figure



Use of colour in figures

Colours should be chosen carefully. In the top half of the figure below, the colours chosen do not appear distinct when the figure is converted to greyscale, so either choose a different set of colours (lower half) or add appropriate labelling.



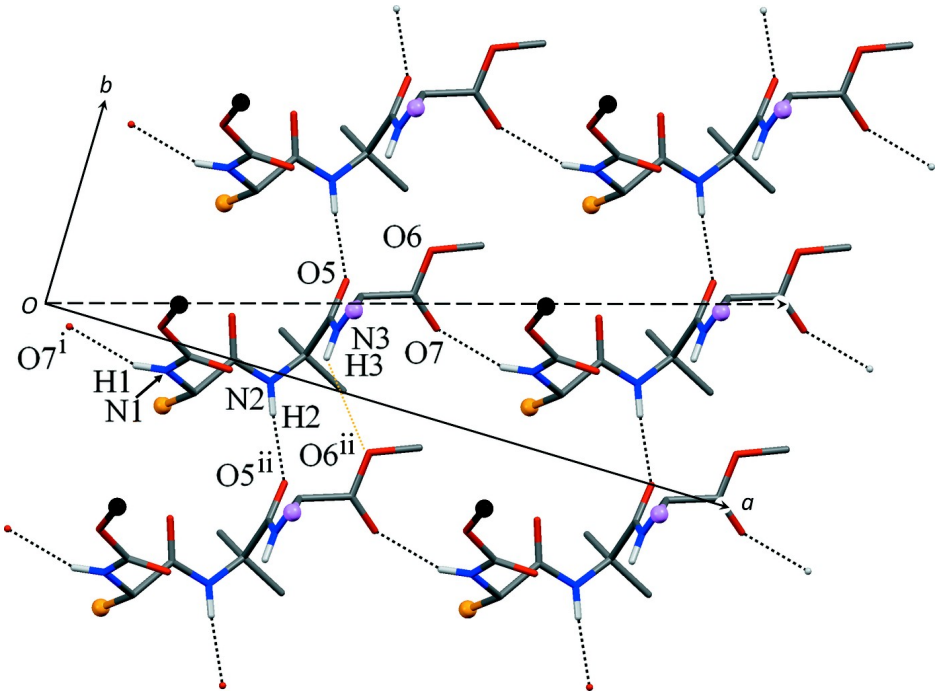
Use of colour in figures

Colour figures are accepted in *Acta C*, but remember that all figures will be printed in black and white.

Figure captions should try not to mention specific colours used for differentiating parts of a figure.

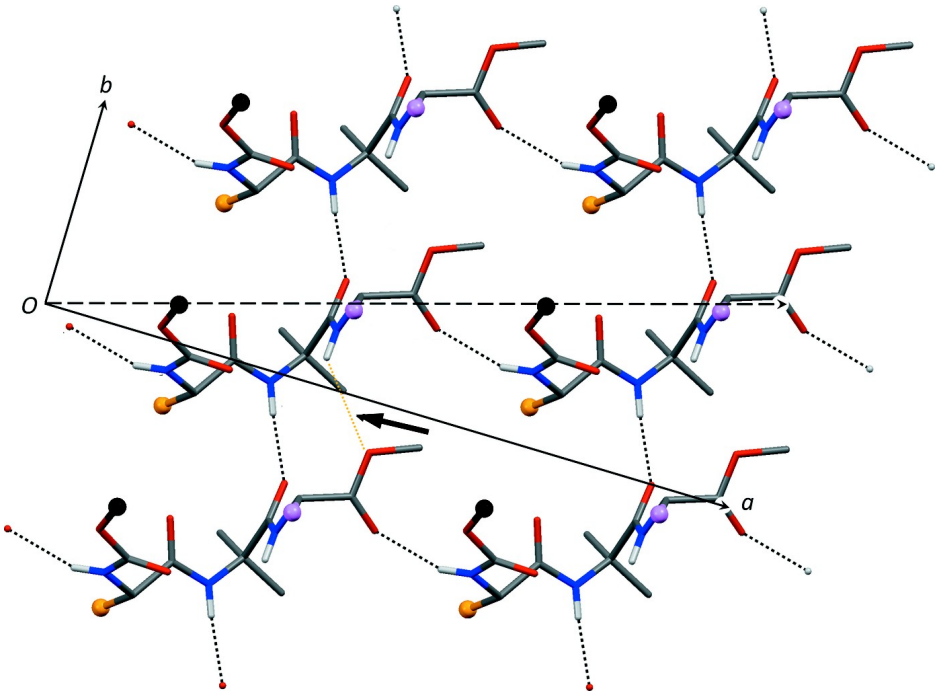
Colour can be mentioned as long as it is not the only way to see the highlighted item,

For example, "A single long N3---H3...O6^{ii} contact (Table 2; orange in the electronic version of the paper)...".



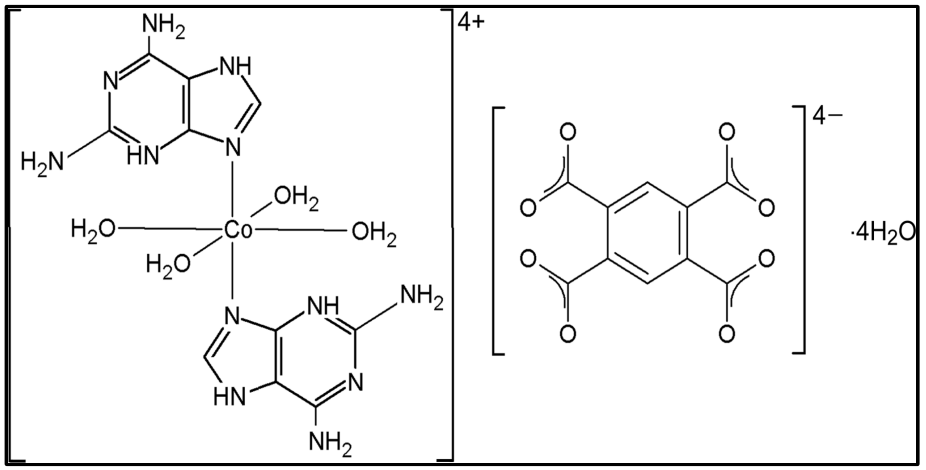
Use of colour in figures

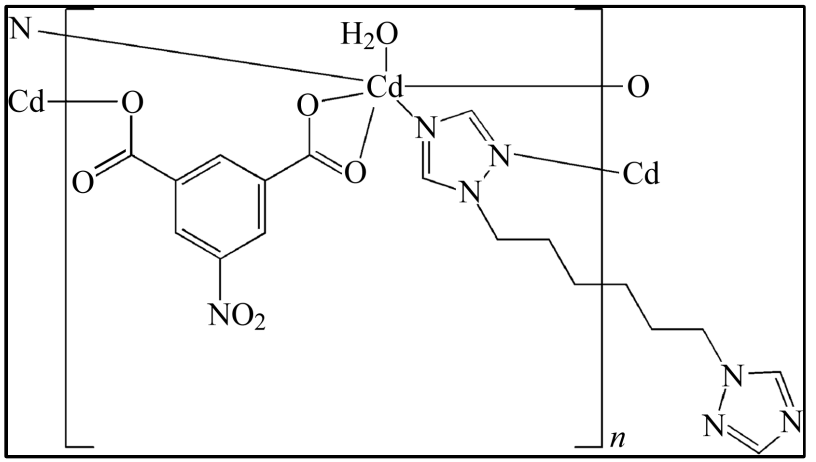
For this example, if labelling is present then the colour description is merely extra information; however, if there was no labelling the figure and caption needs to be adapted, *e.g.* "A single long N---H...O contact (orange in the electronic version of the paper), indicated with an arrow,..."



Chemical schemes

Chemical schemes should be complete, showing all species present in the structure, including counter-ions and solvent molecules in their correct proportions. Charges on ionic species should be included. The relative or absolute stereochemistry should be shown and should be consistent with the ellipsoid plot. Hydrogen bonding should not normally be indicated.





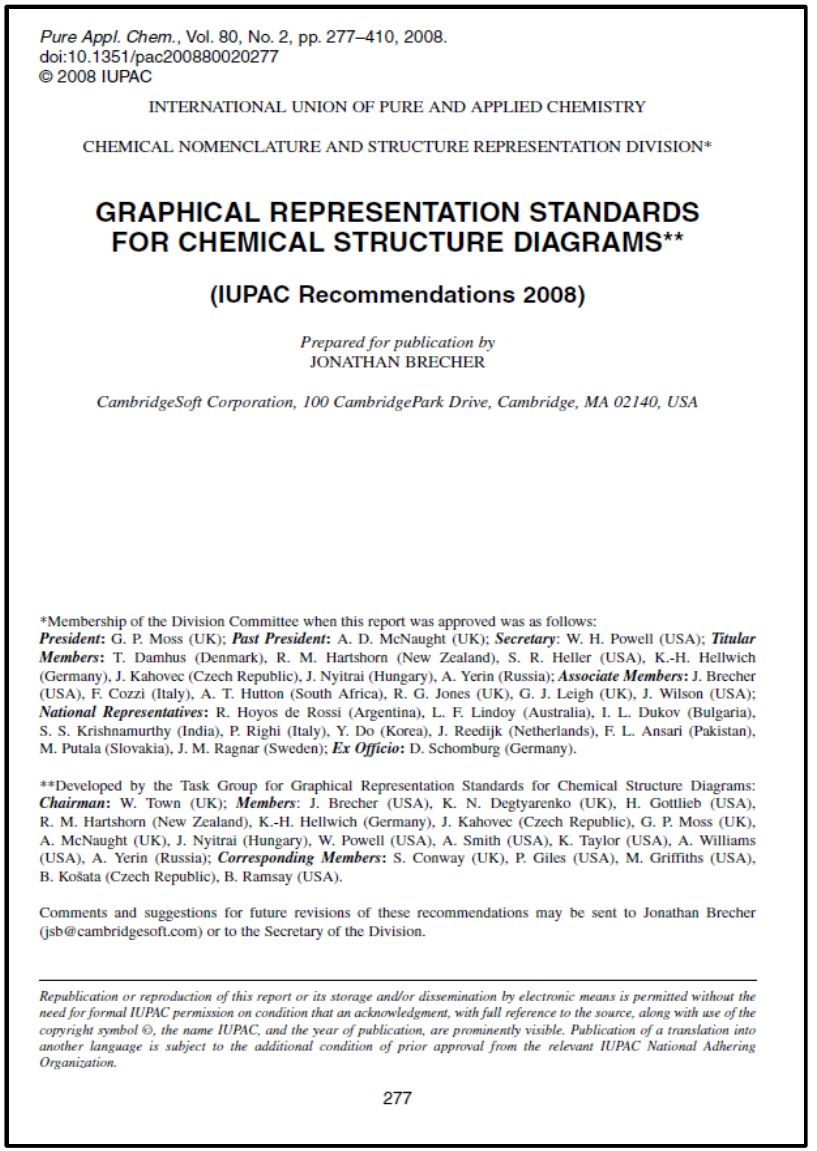
Chemical schemes

- Me for methyl
- Et for ethyl
- Pr for propyl (only in organics as it might mean praseodymium)
- iPr for isopropyl/propan-2-yl
- Bu for butyl,
- iBu for isobutyl
- *s*-Bu for sec-butyl
- *t*-Bu for tert-butyl
- Ac for acetyl (only in organics as it might mean actinium)
- Ph for phenyl
- Cp for cyclopentadienyl (only when coordinated to a metal)

Others allowed but rarely used

- Ms for methylsulfonyl
- Ts for *p*-tolylsulfonyl

Not allowed: py, Bz



Pure Appl. Chem., Vol. 80, No. 2, pp. 277–410, 2008.
doi:10.1351/pac200880020277

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION DIVISION*

GRAPHICAL REPRESENTATION STANDARDS FOR CHEMICAL STRUCTURE DIAGRAMS**

(IUPAC Recommendations 2008)

Prepared for publication by
JONATHAN BRECHER

CambridgeSoft Corporation, 100 CambridgePark Drive, Cambridge, MA 02140, USA

*Membership of the Division Committee when this report was approved was as follows:
President: G. P. Moss (UK); ***Past President***: A. D. McNaught (UK); ***Secretary***: W. H. Powell (USA); ***Titular Members***: T. Damhus (Denmark), R. M. Hartshorn (New Zealand), S. R. Heller (USA), K.-H. Hellwich (Germany), J. Kahovec (Czech Republic), J. Nyitrai (Hungary), A. Yerin (Russia); ***Associate Members***: J. Brecher (USA), F. Cozzi (Italy), A. T. Hutton (South Africa), R. G. Jones (UK), G. J. Leigh (UK), J. Wilson (USA); ***National Representatives***: R. Hoyos de Rossi (Argentina), L. F. Lindoy (Australia), I. L. Dukov (Bulgaria), S. S. Krishnamurthy (India), P. Righi (Italy), Y. Do (Korea), J. Reedijk (Netherlands), F. L. Ansari (Pakistan), M. Putala (Slovakia), J. M. Ragnar (Sweden); ***Ex Officio***: D. Schomburg (Germany).

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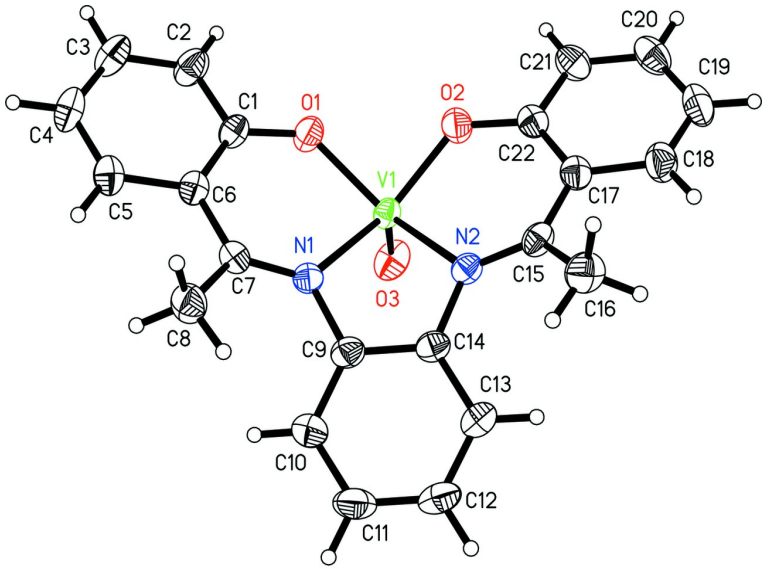
Comments and suggestions for future revisions of these recommendations may be sent to Jonathan Brecher (jsb@cambridgesoft.com) or to the Secretary of the Division.

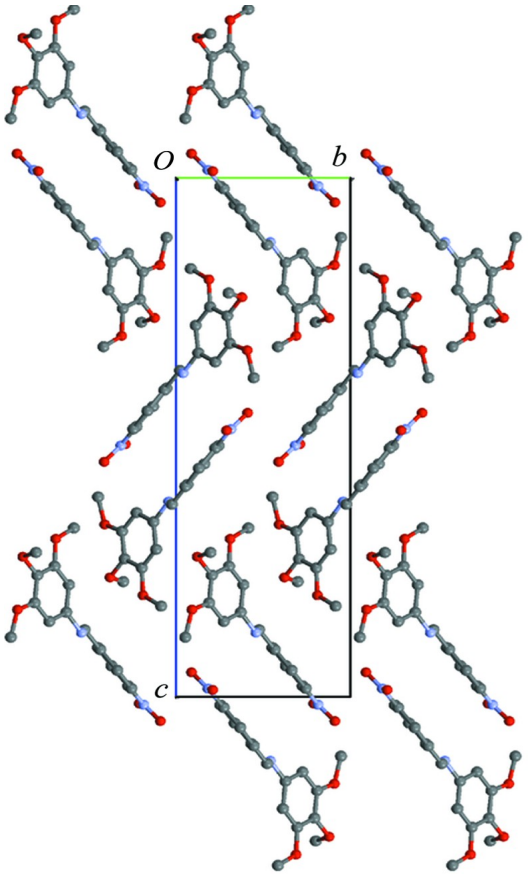
Ellipsoid plots

- On a white background
- Labels should not contain parentheses [e.g. C1 and not C(1)] and should match labels used in the atom-site lists and text
- Labels should not overlap or touch ellipsoids or bonds
- Labelling should be roman and approximately 8pt
- The ellipsoid probability should be stated in the figure caption



Packing diagrams

Packing diagrams should show the cell-axis directions (labelled *a, b*, *c*) and the cell origin (labelled *O*, italic oh), but should normally exclude H-atom sites unless these are involved in hydrogen bonding.



Checklist

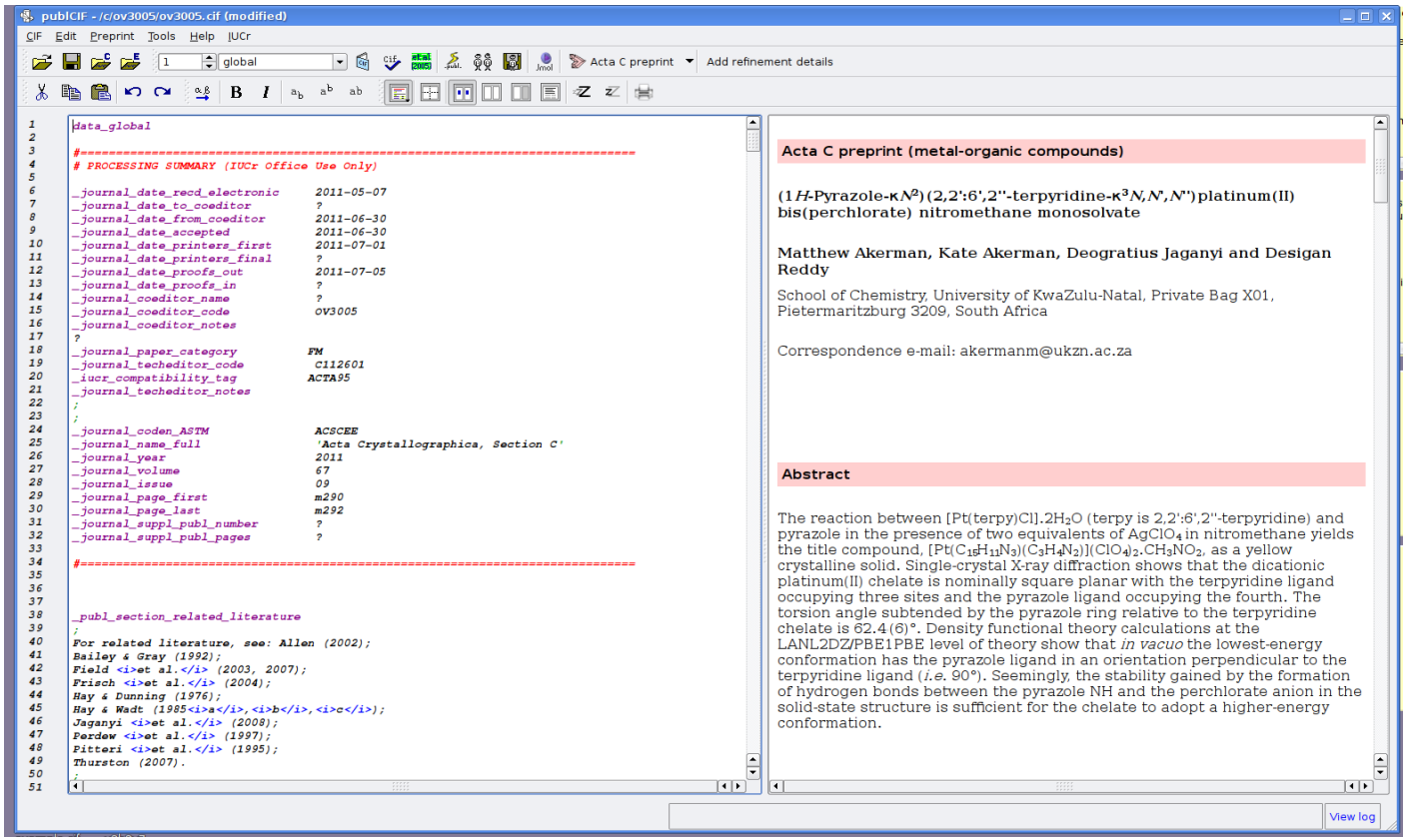
- Images are of sufficiently high resolution (at least 400 dpi for colour images and 600 dpi for monochrome and greyscale images)
- Images are an appropriate size
- Lettering on images is in a standard font and does not vary too much in size
- Colour figures will display satisfactorily when greyscale

The most important items that will help production in Chester are:-

- Chemical schemes contains all components
- Labelling on figures is large enough (8pt) and does not overlap any lines or ellipsoids
- Colour figures display satisfactorily when greyscale

Conversion of CIF to SGML

The technical editor usually edits the CIF as a text file before reading it into *publCIF*. Once in *publCIF*, correct mark-up is applied and reference checking is carried out



Technical editing manual

All editors in the Chester Office use the in-house technical editing or style manual. This outlines editing conventions and ensures consistency across the journals.

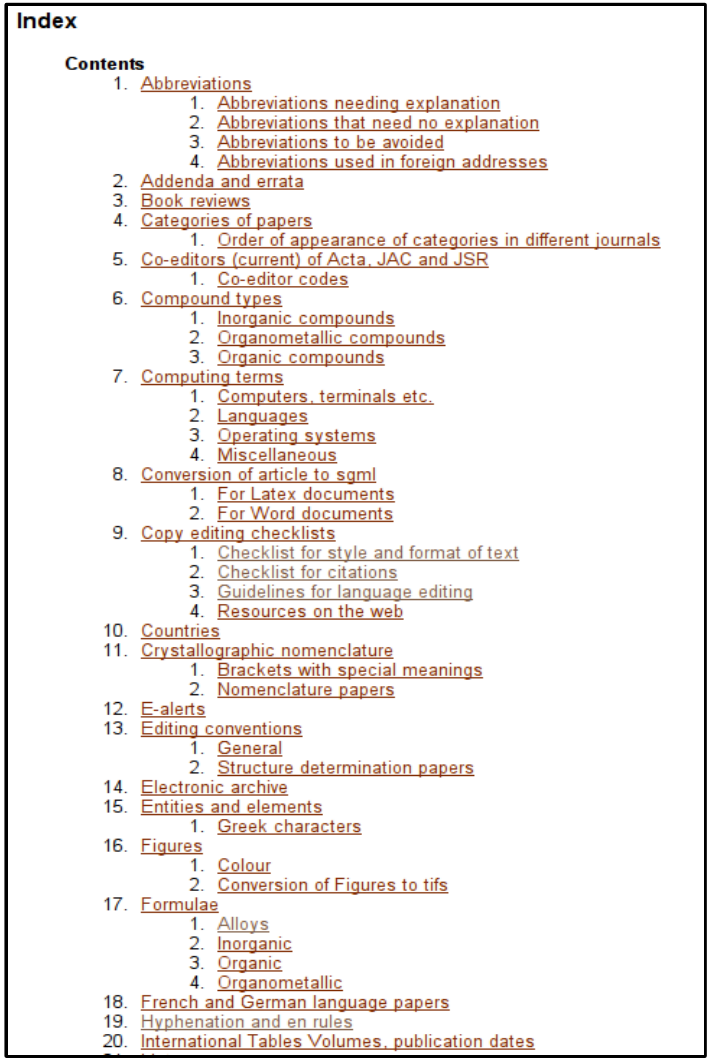
Hyphenation

Hyphenated expressions: non-H atoms, X-ray

Non-hyphenated expressions: cross section; well known method, well centred crystal *etc*.; *R* value

Adjectival phrases should be hyphenated

hydrogen-bond distances
least-squares refinement



Index

Contents

Technical editing manual

Abbreviations

EPR electron paramagnetic resonance

EDX energy-dispersive X-ray diffraction

TEM transmission electron microscopy

General

Centric space group: change to centrosymmetric

C atom, H atom, O atom *etc*. but hydrogen bond

CAD-4 not CAD4

E.s.d. should not be used, s.u. (standard uncertainty) is correct term

Element names: aluminium not aluminum; caesium not cesium; sulfur not sulphur

Hybridization: Csp^2 *etc*.

Technical editing manual

British and American spellings

analyse analyze
behaviour behavior
centre/centring/centred center/centering/centered

Compound types

Inorganic compounds:Those not containing any organic (CxHy) or substituted organic ($C_xH_{y-1}F$, C_xF_y *etc*.) moiety. Examples: Be, Gd_2Pt, C (graphite), SiC, $NaHCO_3$, $K[Co(CN)(CO)_2(NO)]$.

Organometallic compounds: Those containing one or more metal atom and one or more organic moiety (not simply a metal-carbon bond). Al, Ge, As, Sb and Po are defined as metals. Examples: $Ba(CHO_2)_2$, $K_4[Zr(C_2O_4)_4]\cdot 5H_2O$.

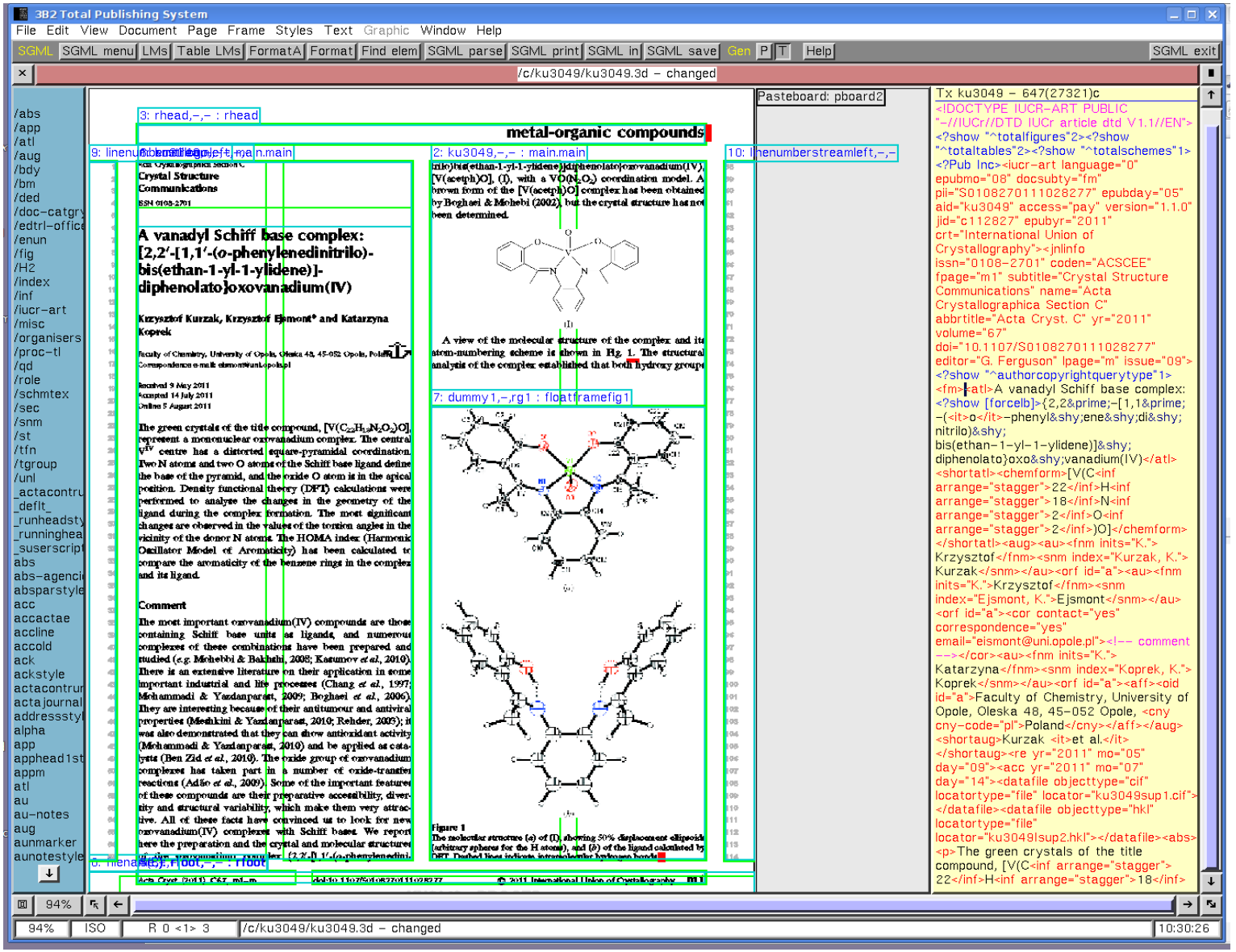
Organic compounds: Those containing carbon and hydrogen (or hydrogen partially or fully substituted by a non-metal) with or without additional non-metals. B, Si, Se, Te and At are defined as non-metals. Example: $C_7H_7N_4$.

Creation of typeset proof from SGML

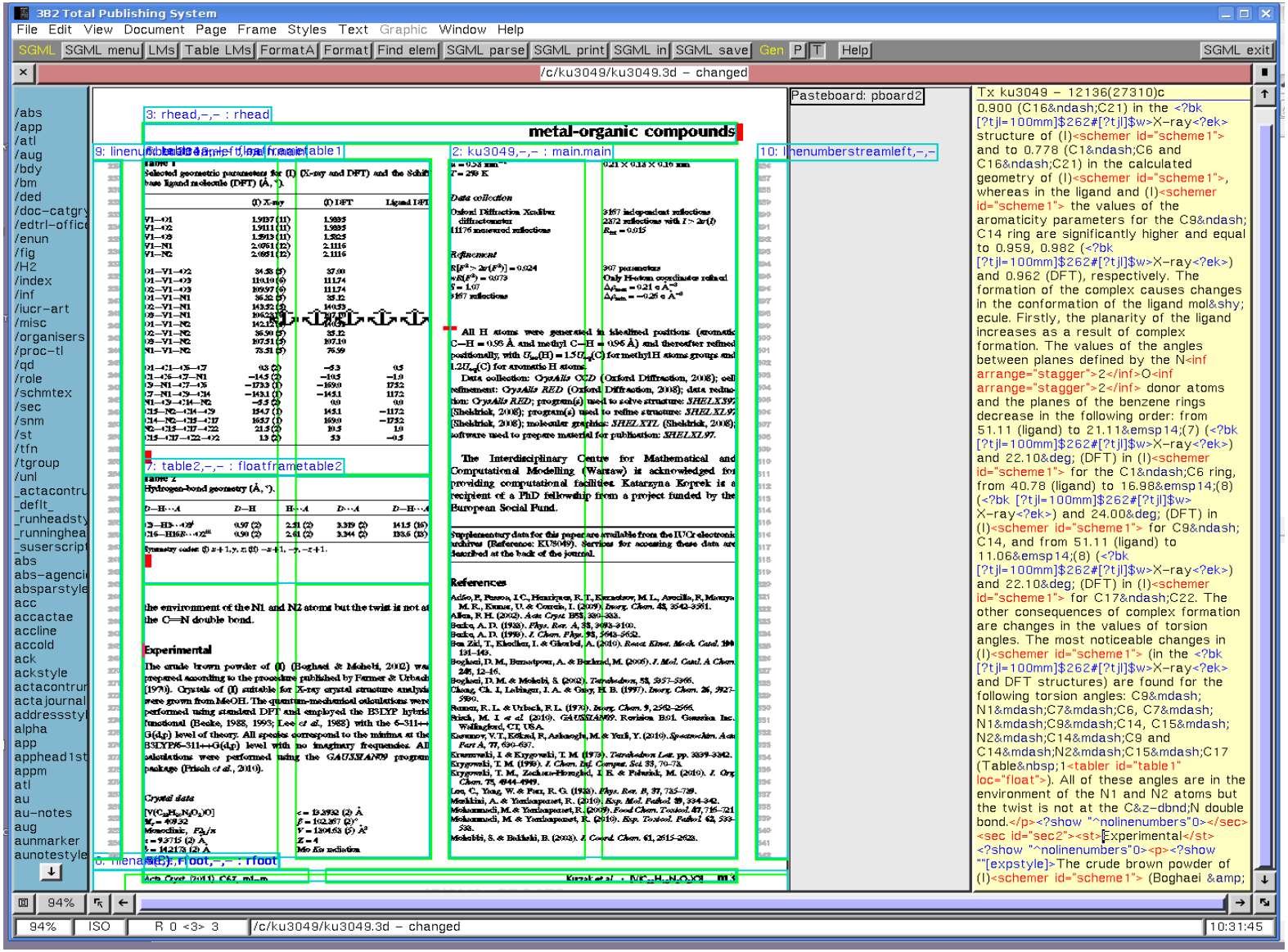
When the technical editor is satisfied with the edited text of the CIF in *publCIF*

- the SGML version of the paper is created
- this is read into the typesetting program *3b2*

- the scheme loads at the end of the first paragraph of the *Comment*

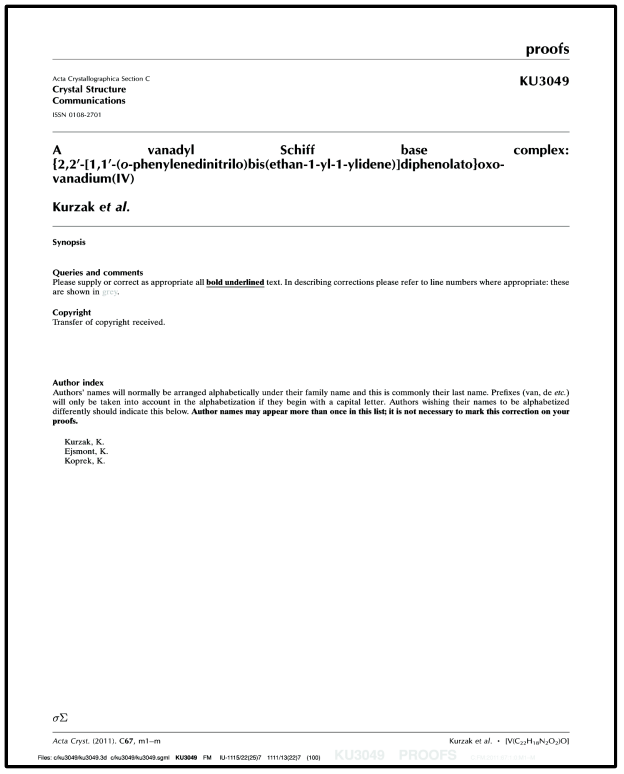


- the artwork and tables are read in as separate moveable frames for ease of placement



Proofing

Once the paper has been formatted in *3b2*, a proof of the paper (the Advance proof) is output and notification is sent to the Section Editor with an attachment containing the proof, structure factors, CIF and html-format checkCIF report.



proofs

Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

KU3049

A vanadyl Schiff base complex: [2,2′-[1,1′-(*o*-phenylenedinitrilo)bis(ethan-1-yl-1-ylidene)]diphenolato]oxo-vanadium(IV)

Kurzak *et al.*

Synopsis

Queries and comments
Please supply or correct as appropriate all **bold underlined** text. In describing corrections please refer to line numbers where appropriate: these are shown in grey.

Copyright
Transfer of copyright received.

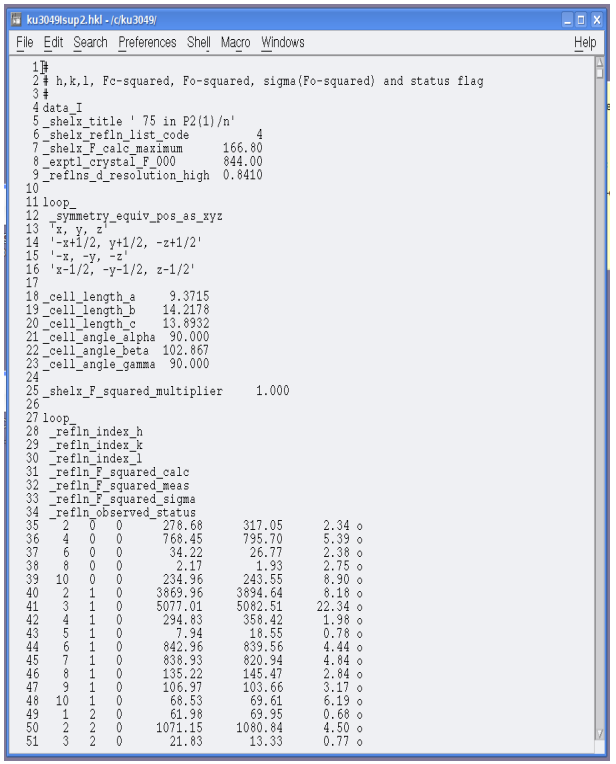
Author index
Authors' names will normally be arranged alphabetically under their family name and this is commonly their last name. Prefixes (van, de etc.) will only be taken into account in the alphabetization if they begin with a capital letter. Authors wishing their names to be alphabetized differently should indicate this below. **Author names may appear more than once in this list; it is not necessary to mark this correction on your proofs.**

Kurzak, K.
Ejsmont, K.
Koprek, K.

$\sigma\Sigma$

Acta Cryst. (2011). C**67**, m1–m Kurzak *et al.* • $[V(C_{22}H_{18}N_2O_2)O]$

Files: c/ku3049/ku3049.3d c/ku3049/ku3049.sgml **KU3049** FM IU-1115/22(25)7 1111/13(227) (100) KU3049 PROOF 7



ku3049lsup2.hkl - /c/ku3049/

File Edit Search Preferences Shell Macro Windows Help

```
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# h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_I
_shelx_title ' 75 in P2(1)/n'
_shelx_refln_list_code          4
_shelx_F_calc_maximum       166.80
_exptl_crystal_F_000        844.00
_reflns_d_resolution_high   0.8410

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 _symmetry_equiv_pos_as_xyz
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 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

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_cell_length_c     13.8932
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_cell_angle_beta  102.867
_cell_angle_gamma  90.000

_shelx_F_squared_multiplier     1.000

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 _refln_index_h
 _refln_index_k
 _refln_index_l
 _refln_F_squared_calc
 _refln_F_squared_meas
 _refln_F_squared_sigma
 _refln_observed_status
   2   0   0      278.68      317.05      2.34 o
   4   0   0      768.45      795.70      5.39 o
   6   0   0       34.22       26.77      2.38 o
   8   0   0        2.17        1.93      2.75 o
  10   0   0      234.96      243.55      8.90 o
   2   1   0     3869.96     3894.64      8.18 o
   3   1   0     5077.01     5082.51     22.34 o
   4   1   0      294.83      358.42      1.98 o
   5   1   0        7.94       18.55      0.78 o
   6   1   0      842.96      839.56      4.44 o
   7   1   0      838.93      820.94      4.84 o
   8   1   0      135.22      145.47      2.84 o
   9   1   0      106.97      103.66      3.17 o
  10   1   0       68.53       69.61      6.19 o
   1   2   0       61.98       69.95      0.68 o
   2   2   0     1071.15     1080.84      4.50 o
   3   2   0       21.83       13.33      0.77 o
```

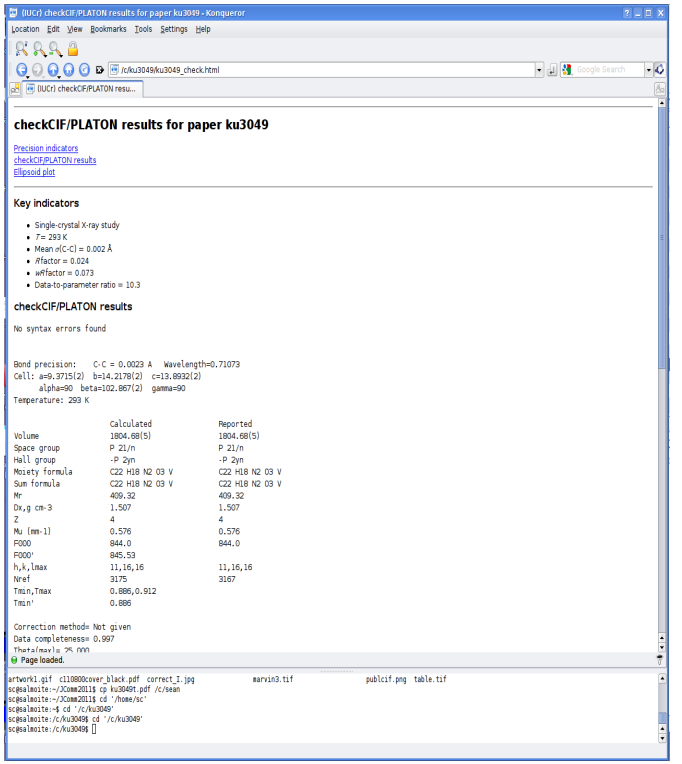

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(IUCr) checkCIF/PLATON resu...

checkCIF/PLATON results for paper ku3049

Precision indicators
checkCIF/PLATON results
Ellipsoid plot

Key indicators

- Single-crystal X-ray study
- *T*= 293 K
- Mean σ(C-C) = 0.002 Å
- *R*factor = 0.024
- *w*Rfactor = 0.073
- Data-to-parameter ratio = 10.3

checkCIF/PLATON results

No syntax errors found

Bond precision: C-C = 0.0023 A Wavelength=0.71073
Cell: a=9.3715(2) b=14.2178(2) c=13.8932(2)
alpha=90 beta=102.867(2) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1804.68(5)	1804.68(5)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H18 N2 O3 V	C22 H18 N2 O3 V
Sum formula	C22 H18 N2 O3 V	C22 H18 N2 O3 V
Mr	409.32	409.32
Dx,g cm-3	1.507	1.507
Z	4	4
Mu (mm-1)	0.576	0.576
F000	844.0	844.0
F000'	845.53	
h,k,lmax	11,16,16	11,16,16
Nref	3175	3167
Tmin,Tmax	0.886,0.912	
Tmin'	0.886	

Correction method= Not given
Data completeness= 0.997
Theta(max)= 25.000

Page loaded.

artwork1.gif cl10800cover_black.pdf correct_I.jpg marvin3.tif publcif.png table.tif
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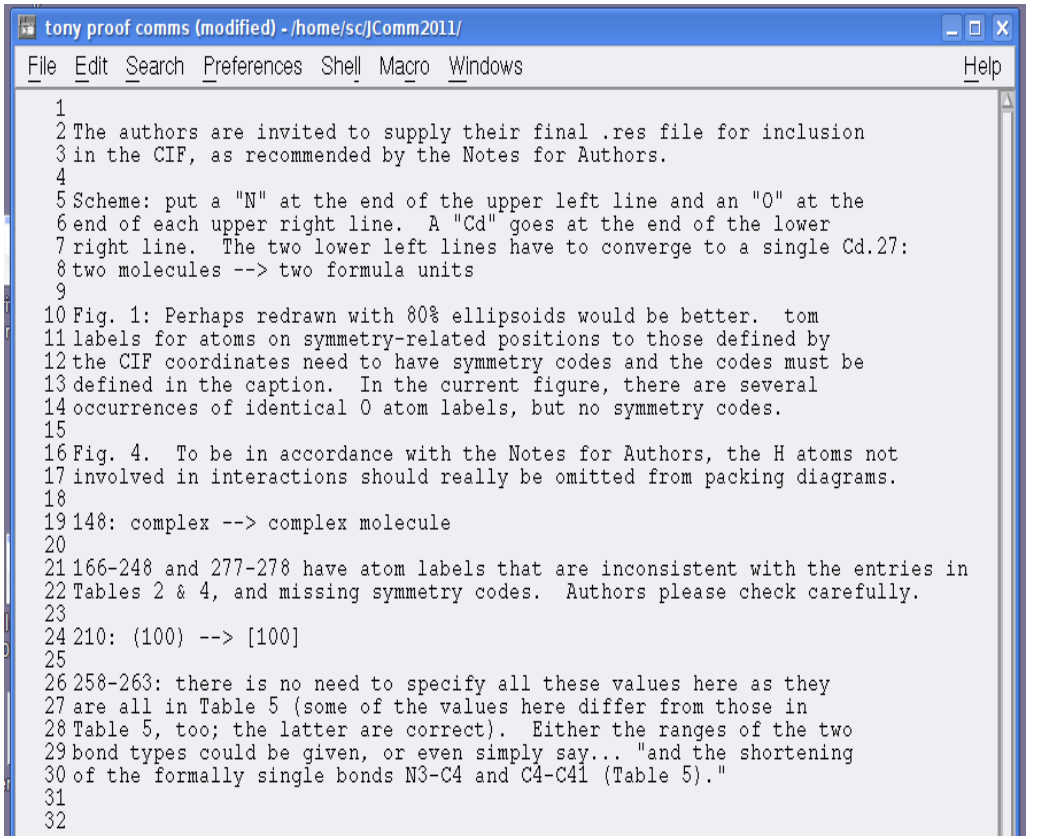
sc@salmoite:~$ cd '/c/ku3049'
sc@salmoite:/c/ku3049$ cd '/c/ku3049'
sc@salmoite:/c/ku3049$

Interaction with the Section Editor

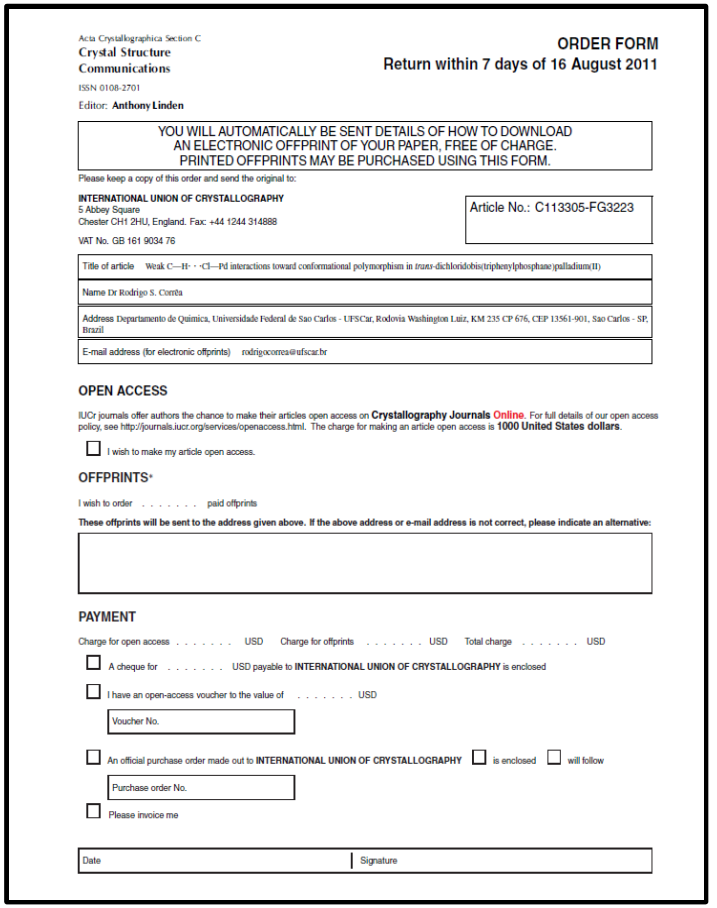
- The Section Editor returns comments and corrections as a text file referring to the line numbering in the proof

- A copy of these comments is sent automatically to the relevant Co-editor, together with a copy of the proof for ease of locating the corrections



Preparation of author proofs

- The Section Editor corrections are made in *3b2*
- Major queries (requests for rerefinements *etc*) are added as Notes at the end of the paper
- The paper is given a final read by a technical editor
- The author proof is generated from *3b2*
- An open access and reprint order form is attached automatically to the proof and a message is sent



Acta Crystallographica Section C
Crystal Structure Communications
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Editor: **Anthony Linden**

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Article No.: C113305-FG3223

Title of article Weak C—H···Cl—Pd interactions toward conformational polymorphism in *trans*-dichloridobis(triphenylphosphane)palladium(II)

Name Dr Rodrigo S. Corrêa

Address Departamento de Química, Universidade Federal de São Carlos - UFSCar, Rodovia Washington Luiz, KM 235 CP 676, CEP 13561-901, São Carlos - SP, Brazil

E-mail address (for electronic offprints) rodrigocorrea@ufscar.br

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Handling of author corrections

- The correspondence author returns proof corrections

- These are analysed and any corrections that relate specifically to questions from the Section Editor are forwarded to the Section Editor for checking

- At this stage the Co-editor might be asked to get involved again

- The paper can also be back-tracked to the pre-accepted stage to allow upload of new files if revisions are significant

- This process continues until the Section Editor is satisfied for the paper to proceed to publication

- For most papers, Section Editor ==> authors ==> publication

Preparing papers for publication

- The paper is given a final read

- All final author and Section Editor corrections are made in *3b2*

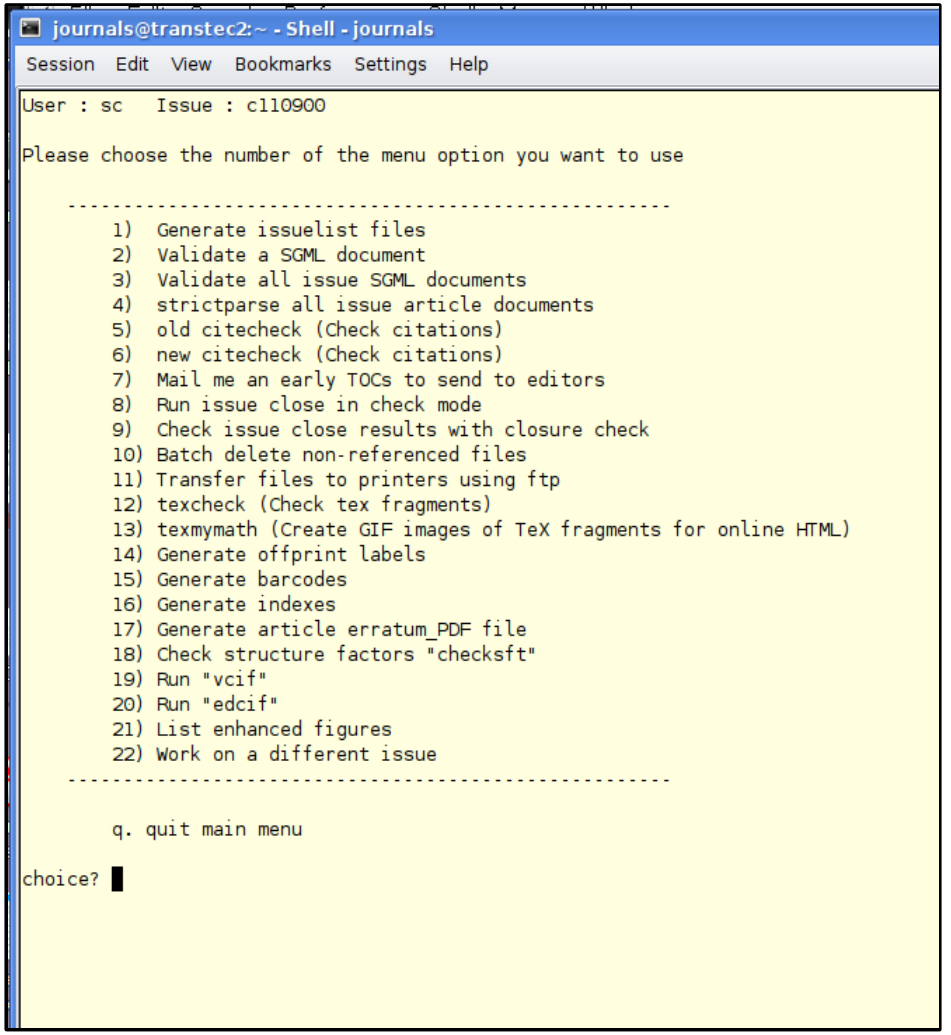
- Columns are balanced and figures and tables are placed in optimum positions

- The paper is added to the current issue in a sequential manner from within *3b2*, an online publication date chosen and page numbers assigned automatically

Online publication tools

Checks are made

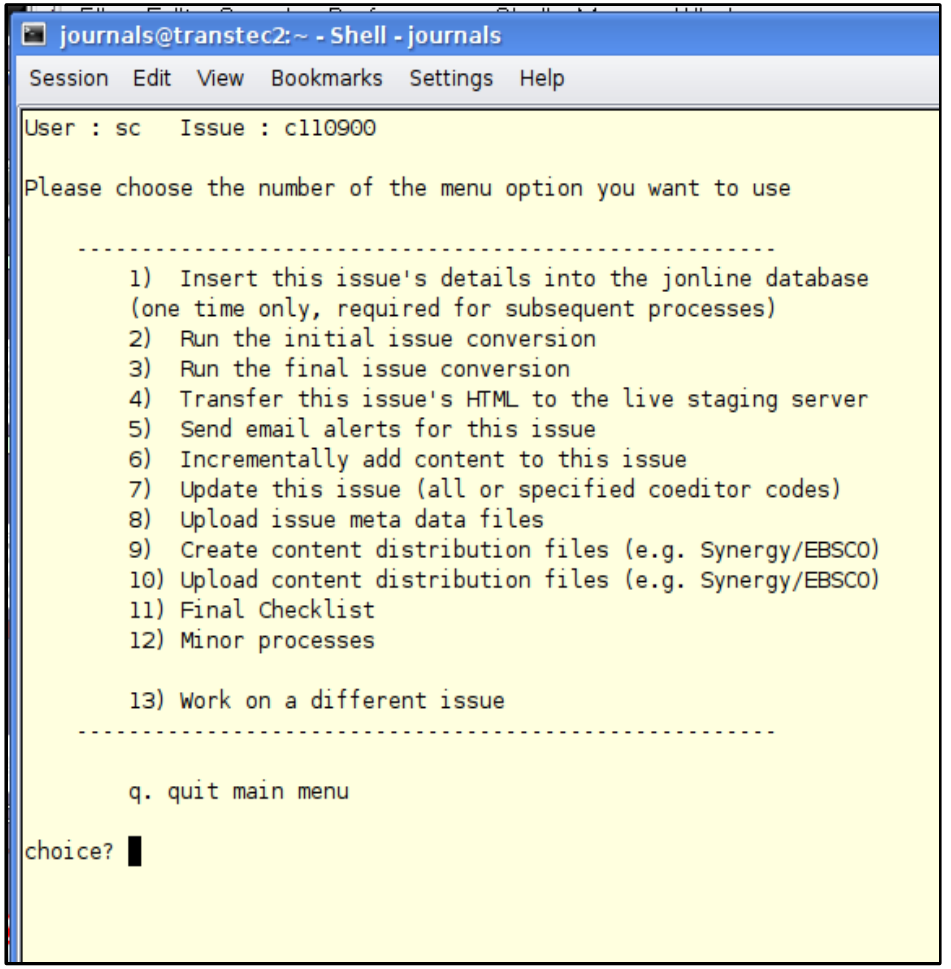
- to make sure that the SGML of each article is compliant
- to ensure that all files associated with a paper are present and correctly named
- to make sure that the CIF for each article has no syntax errors
- to ensure that any Acta citations are correct and that all other references are formatted correctly; non-*Acta* references are also checked against *PubMed*



Online publication tools

Papers are added to the online issue in an incremental manner

- The information for each paper is added to the production database
- The citations are processed
- The artwork is processed
- The online issue contents page is updated



Reprints

- Electronic reprints are sent out once a paper has been published online
- Authors can order printed reprints and these are now produced in the Chester office which ensures a fast turnaround
- If open access is required (*Acta C*) then this is activated as soon as the order is received

electronic reprint

Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701
Editor: **Anthony Linden**

(*E*)-4-[2-(3,4,5-Trimethoxyphenyl)ethenyl]nitrobenzene and its 'bridge-flipped' analogues

Alain Collas and Frank Blockhuys

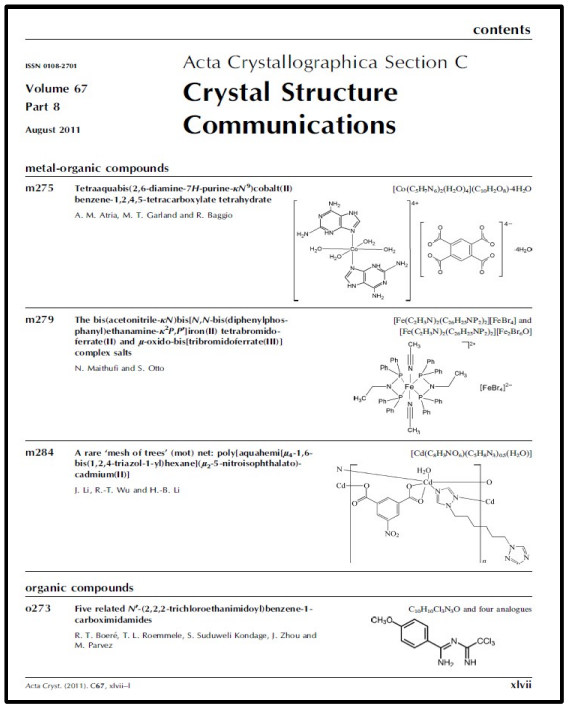
Acta Cryst. (2011). C**67**, o364–o369

Acta Crystallographica Section C: Crystal Structure Communications specializes in the rapid dissemination of high-quality studies of crystal and molecular structures of interest in fields such as chemistry, biochemistry, mineralogy, pharmacology, physics and materials science. The numerical and text descriptions of each structure are submitted to the journal electronically as a Crystallographic Information File (CIF) and are checked and typeset automatically prior to peer review. The journal is well known for its high standards of structural reliability and presentation. *Section C* publishes approximately 1000 structures per year; readers have access to an archive that includes high-quality structural data for over 10000 compounds.

Construction of a printed issue

Once an issue is nearing completion at the end of a month, the number of pages (including the contents pages, adverts, *etc*) that the issue will contain needs to be decided. This must be a multiple of 4 or 8, but will ideally be a multiple of 16 or 32.

The final papers are added to the online issue and the contents pages produced. These parts all exist as PDF files (produced from postscript files) and are concatenated into a single file for printing an issue.



contents

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August 2011

Acta Crystallographica Section C
Crystal Structure Communications

metal-organic compounds

m275 **Tetraaquabis(2,6-diamine-7*H*-purine-κ*N*^{9})cobalt(II) benzene-1,2,4,5-tetracarboxylate tetrahydrate**
A. M. Atria, M. T. Garland and R. Baggio

m279 **The bis(acetonitrile-κ*N*)bis[*N*,*N*-bis(diphenylphosphanyl)ethanamine-κ^2*P*,*P*′]iron(II) tetrabromoferrate(II) and μ-oxido-bis[tribromidoferrate(III)] complex salts**
N. Maithufi and S. Otto

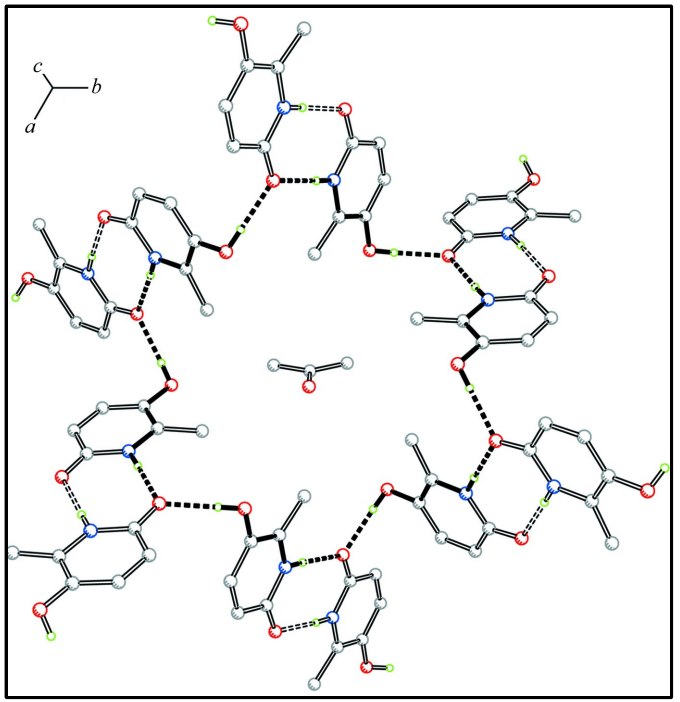
m284 **A rare 'mesh of trees' (mot) net: poly[aquahemi(μ$_4$-1,6-bis(1,2,4-triazol-1-yl)hexane)(μ$_2$-5-nitroisophthalato)-cadmium(II)]**
J. Li, R.-T. Wu and H.-B. Li

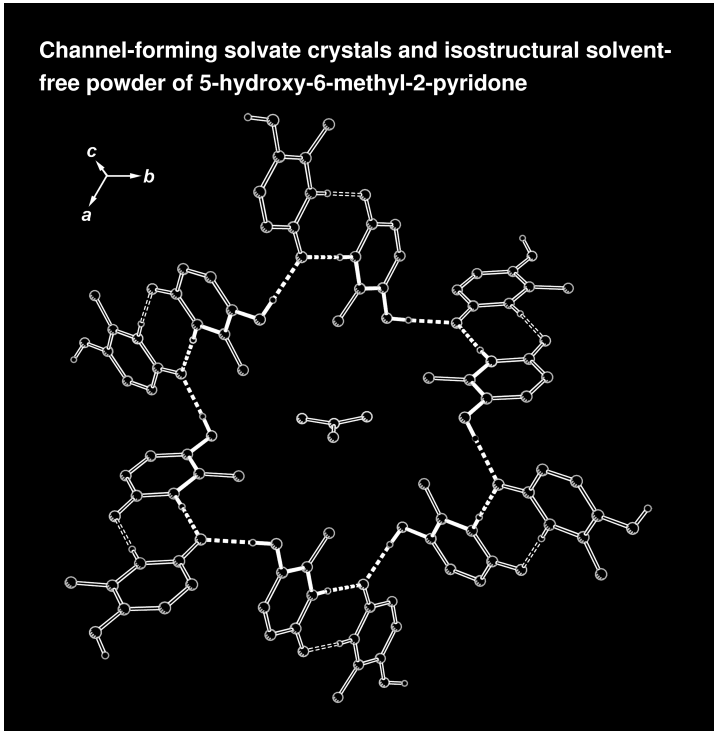
organic compounds

o273 **Five related *N*′-(2,2,2-trichloroethanimidoyl)benzene-1-carboximidamides**
R. T. Boeré, T. L. Roemmele, S. Suduweli Kondage, J. Zhou and M. Parvez

Cover image and cover preparation

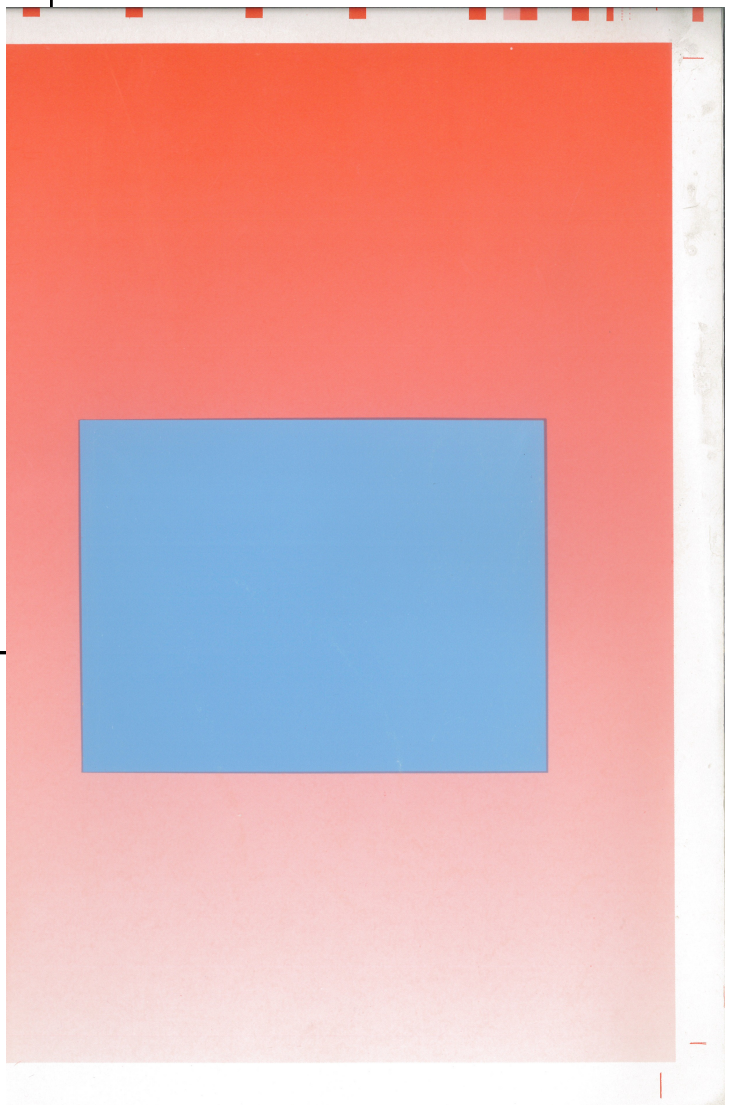
The cover image changes every month and is selected by the Section Editor from the figures that appear in the issue. Ideally the paper chosen will have significant scientific interest.





Cover file sent for printing

Stock cover



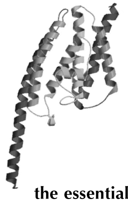
The inside pages

The inside front cover is new every month as it contains the caption for the cover image and the barcode. The inside and outside back covers don't change very often.

Our current printers are Ho Printing in Singapore.

Three files are sent to the printers for each issue

- the outside front and back covers as a single PDF file
- the inside front and back covers as a single PDF file
- all inside pages of the issue as a concatenated PDF file



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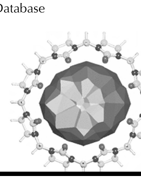

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Volume 67
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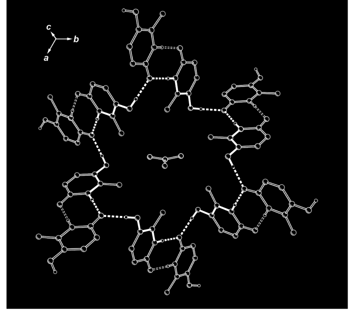
August 2011

Inorganic compounds
Metal-organic compounds
Organic compounds

Acta Crystallographica Section C
Crystal Structure Communications
Editor: Anthony Linden

Channel-forming solvate crystals and isostructural solvent-free powder of 5-hydroxy-6-methyl-2-pyridone



Acta Crystallographica Section C
Crystal Structure Communications
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editor-in-chief
G. Kostorz

section editor
A. Linden

co-editors

contents

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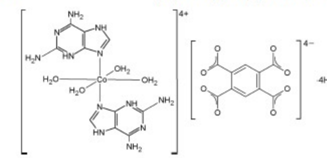
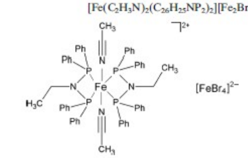
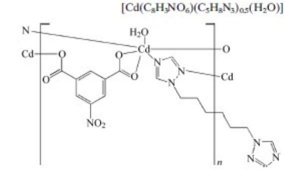
August 2011

Acta Crystallographica Section C
Crystal Structure Communications

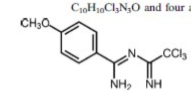
metal-organic compounds







organic compounds



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August issue

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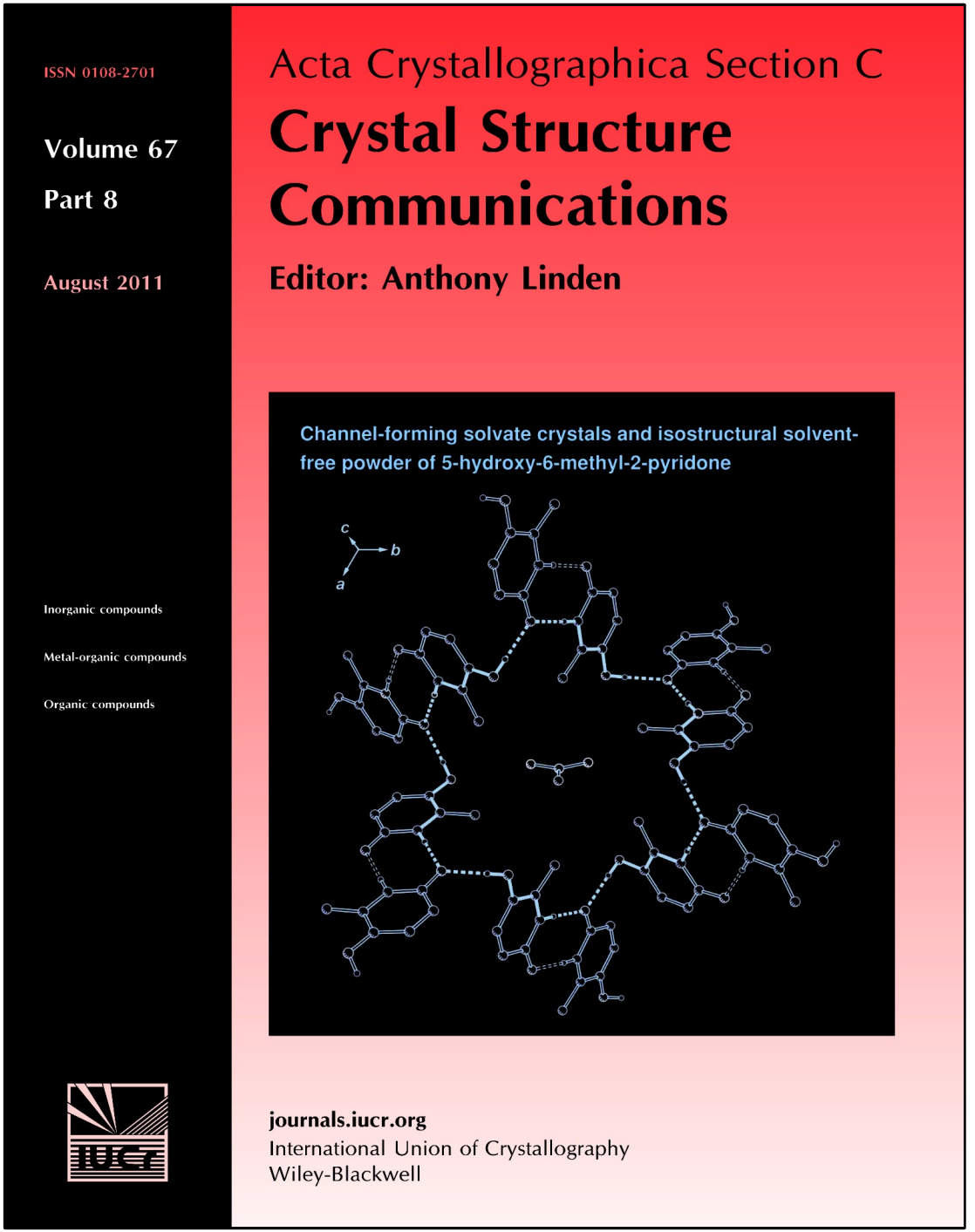

And finally...

Once an issue has been sent for printing, the content (metadata) of the issue is distributed

About ten days later, an unbound version of the issue is received at the Editorial office for final checking and the issue can then be approved for binding and distribution

A copy of the bound and printed issue is sent to the Cambridge Database and a complimentary copy is sent to the author of the paper that appears on the cover

Where the journal content is sent

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