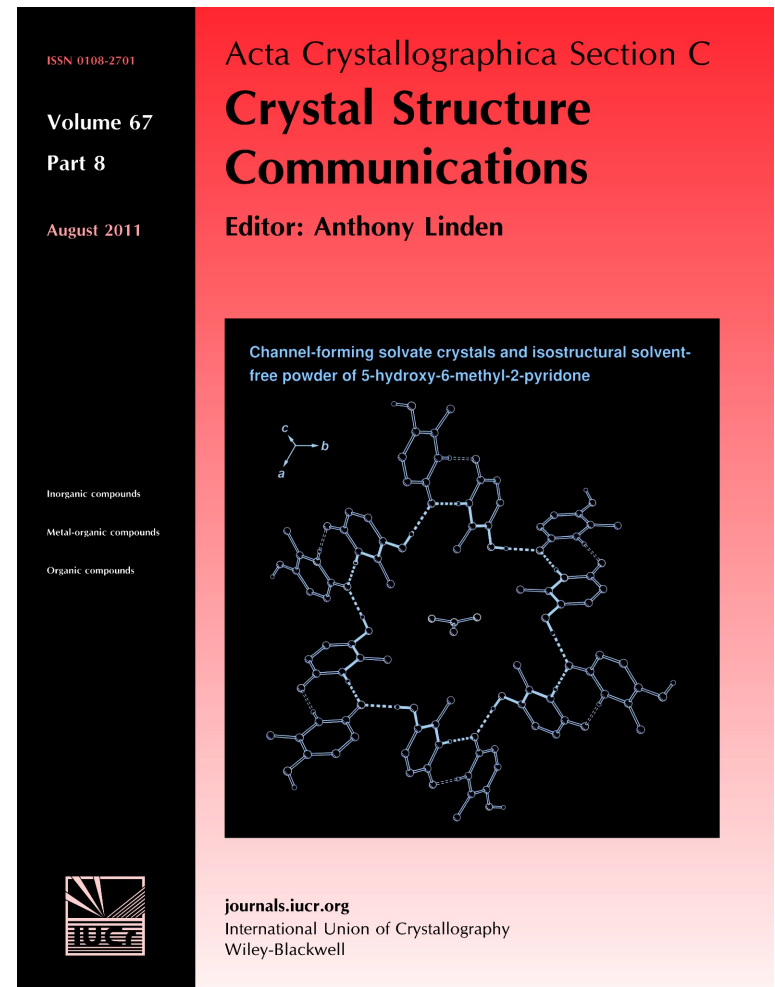
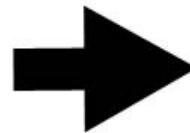
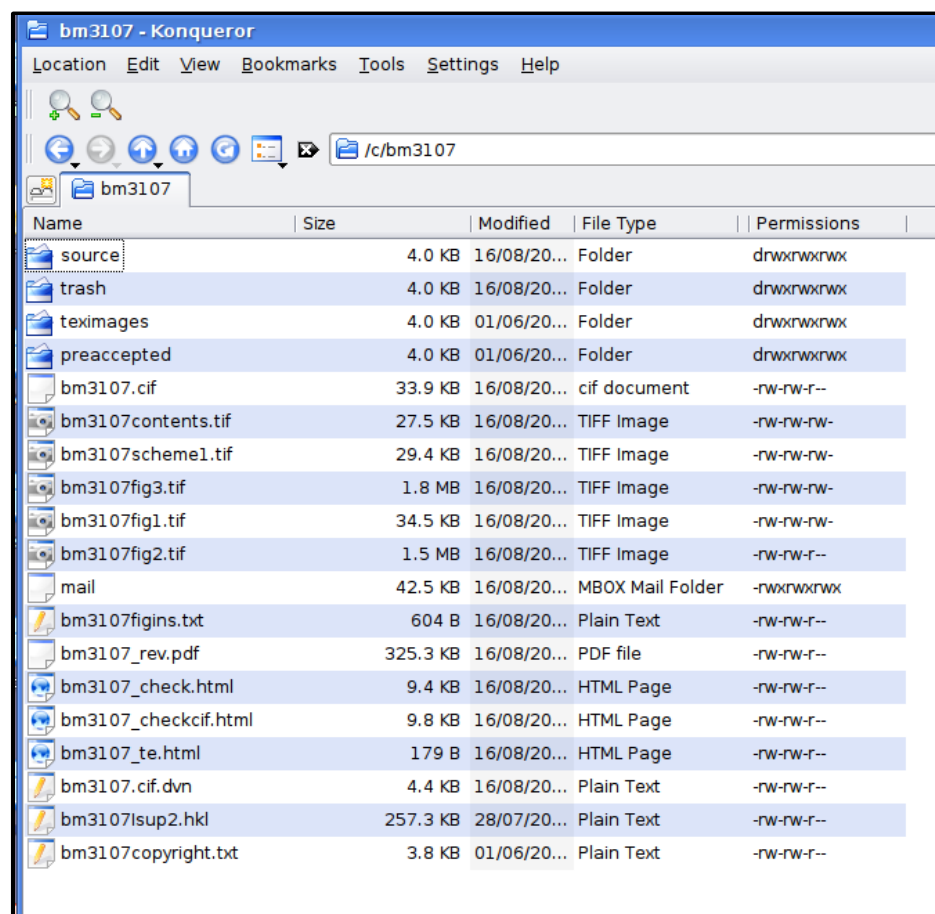


FROM SUBMISSION TO PUBLICATION



On acceptance

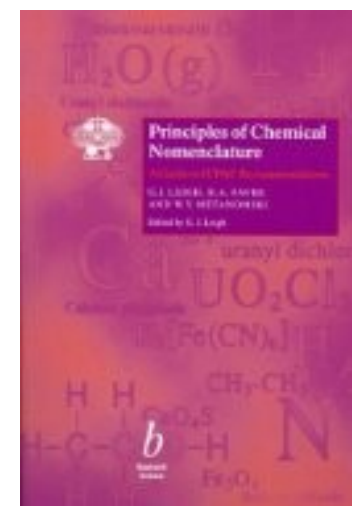
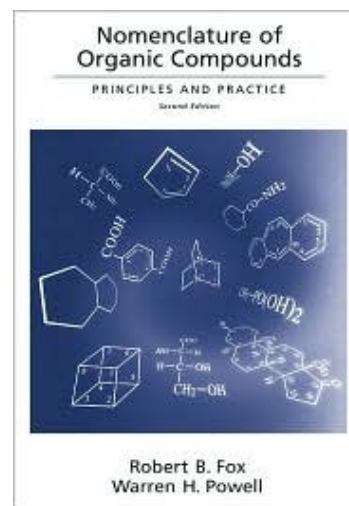
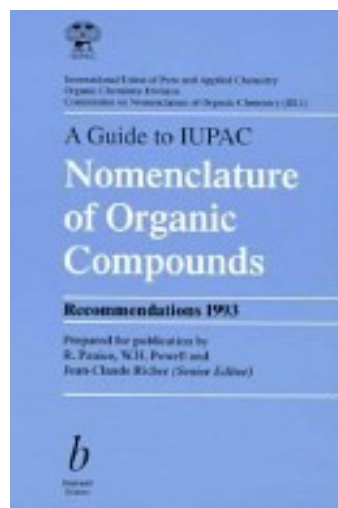
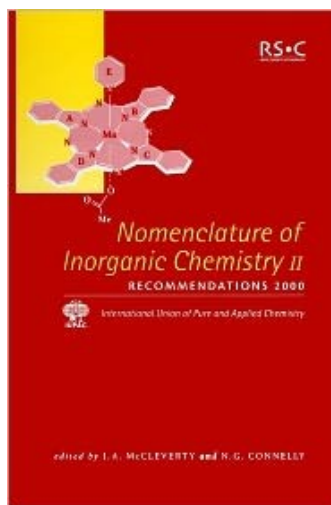
- The final files (CIF, structure factors, artwork *etc*) are moved from the submission system into the production area
- During this process, the artwork is processed automatically to be single column width and have the correct resolution
- *checkCIF* and *PLATON* are run automatically on the final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



Technical editing stages

- nomenclature and formula checking
- artwork preparation
- use of *pubCIF* 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



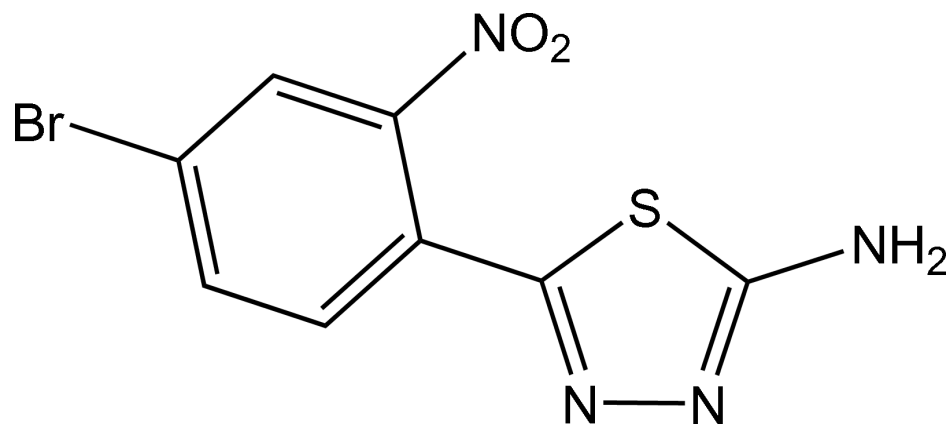
- Two chemical naming programs are used:
 - (a) **Marvin** (ChemAXON; license to check 5000+ names per annum)
 - (b) **OPSIN** (freely available as an open-source download; obtained as part of the IUCR's ongoing collaborations with Peter Murray-Rust and the Unilever Cambridge Centre for Molecular Science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

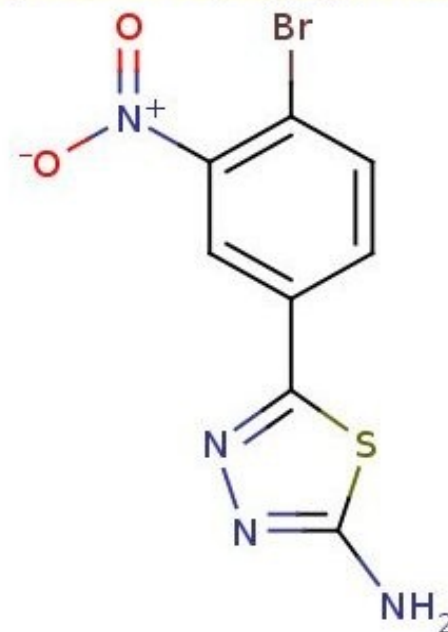
2-Amino-5-(4-bromo-3-nitrophenyl)-1,3,4-thiadiazole

Scheme provided by author



Scheme created by program

Using CML from OPSIN
File: bh2371.cif
Original: 5-(4-Bromo-3-nitrophenyl)-1,3,4-thiadiazol-2-amine
Modified: 5-(4-Bromo-3-nitrophenyl)-1,3,4-thiadiazol-2-amine



- 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

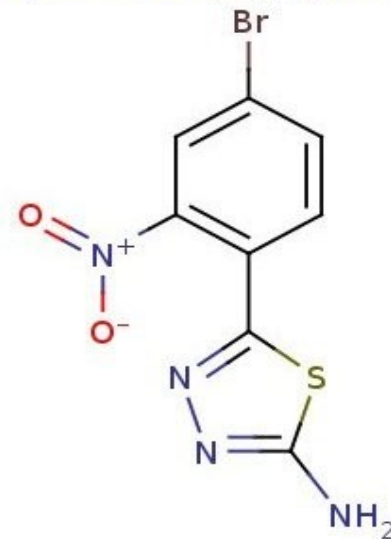
5-(4-Bromo-2-nitrophenyl)-1,3,4-
thiadiazol-2-amine

Using CML from OPSIN

File: bh2371.cif

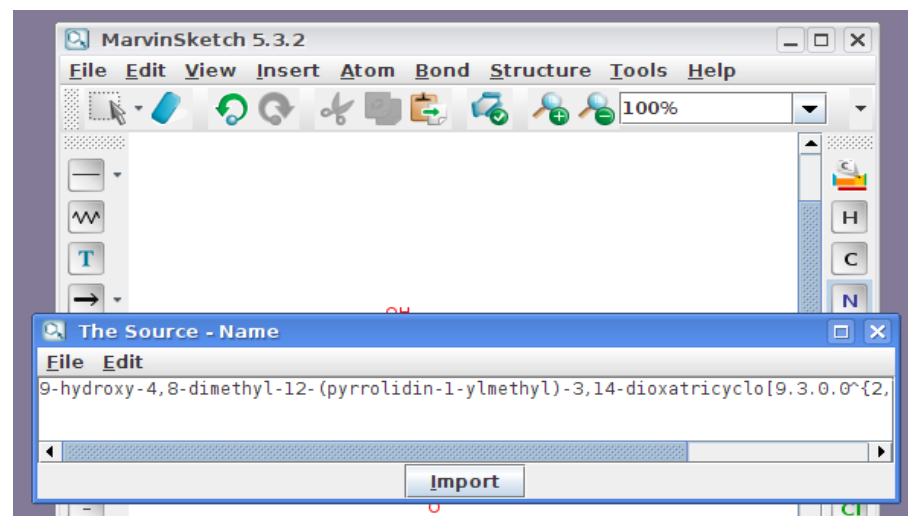
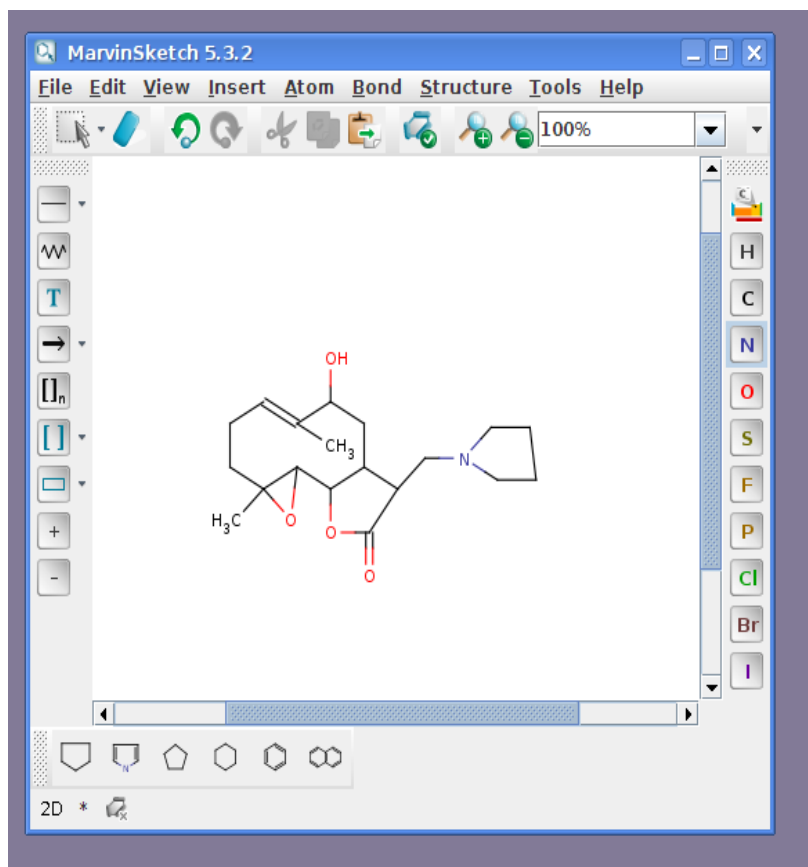
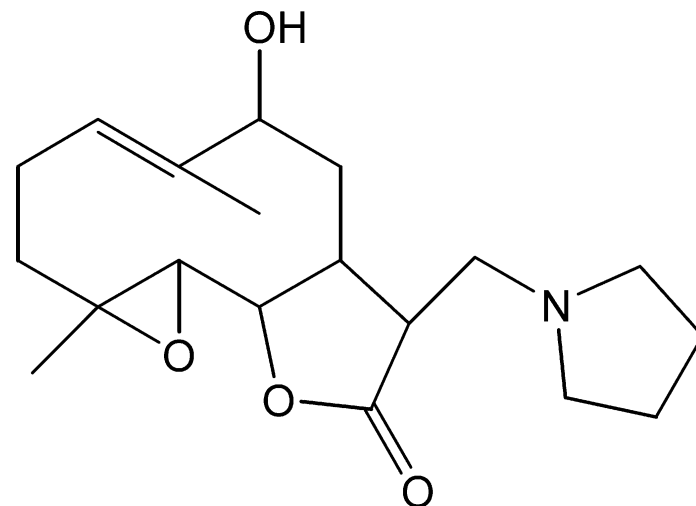
Original: 5-(4-Bromo-2-nitrophenyl)-1,3,4-thiadiazol-2-amine

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

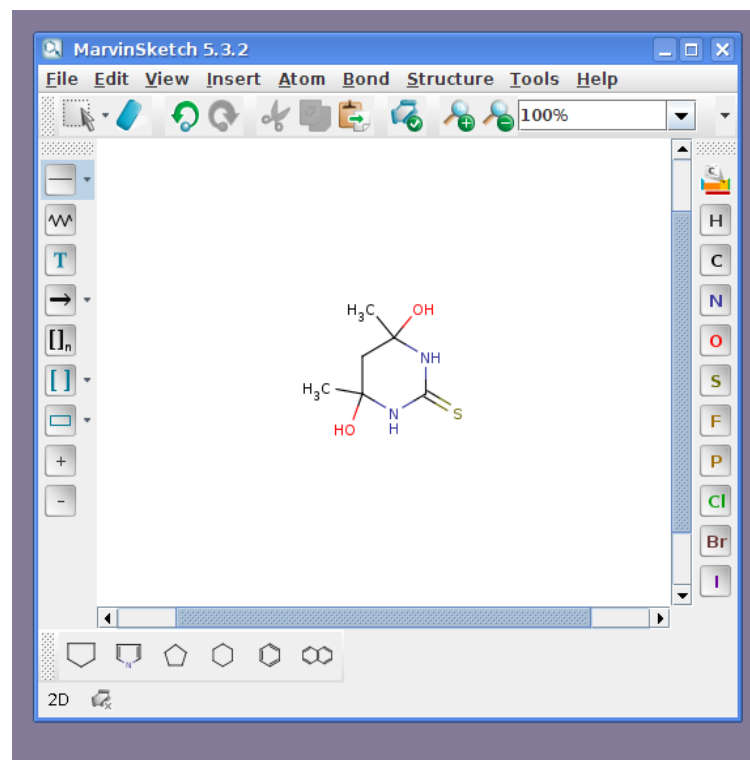
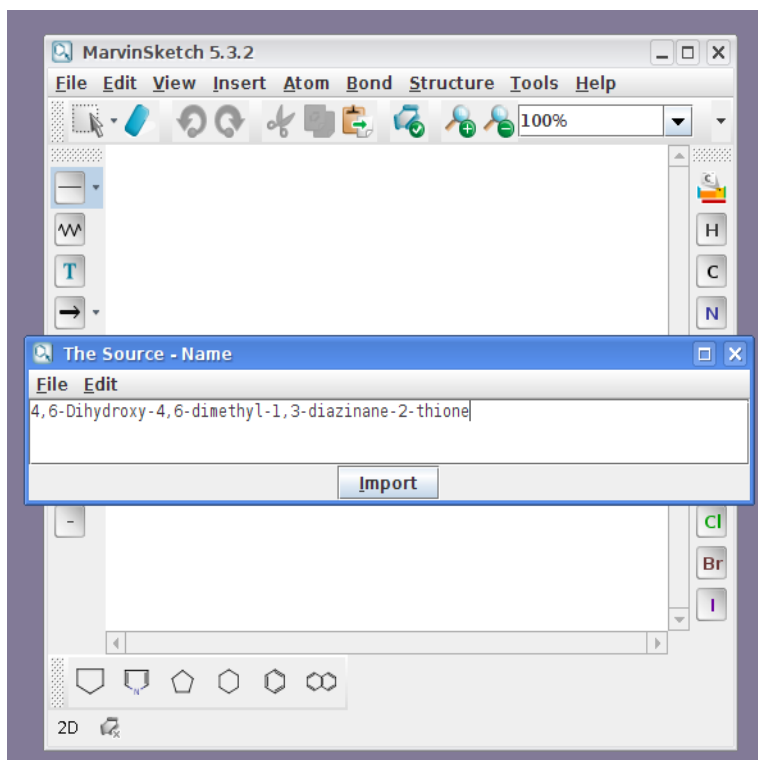


The chemical name in the CIF can now be updated with the final systematic name and the CIF checked once more with the naming program and a final CML file created. The systematic name does not always need to be used, e.g. the name provided by an author may be an accepted trivial name.

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 group⁵⁰

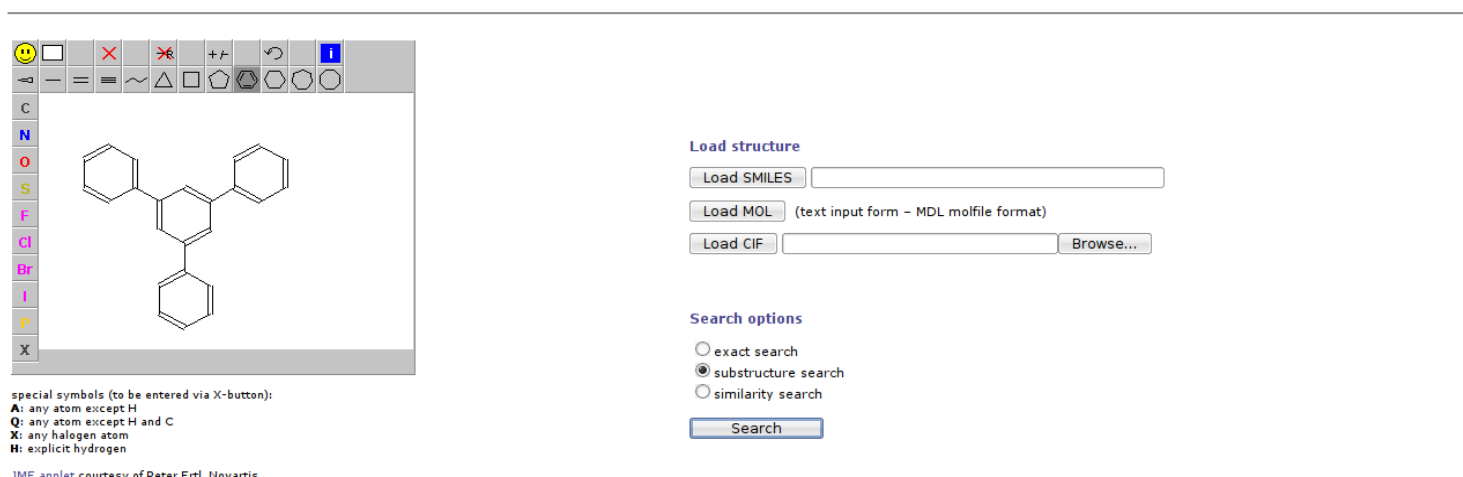
1	Radicals	13	Aldehydes followed by Thioaldehydes, Selenoaldehydes, and Telluroaldehydes
2	Anions	14	Ketones followed by Thioketones, Selenoketones, and Telluroketones
3	Cations	15	Alcohols and Phenols followed by Thiols, Selenols, and Tellurols
4	Zwitterionic compounds	16	Hydroperoxides followed by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

- 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]- μ -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

Structure search – LAMP test



special symbols (to be entered via X-button):
A: any atom except H
Q: any atom except H and C
X: any halogen atom
H: explicit hydrogen

JME applet courtesy of Peter Ertl, Novartis

Search results

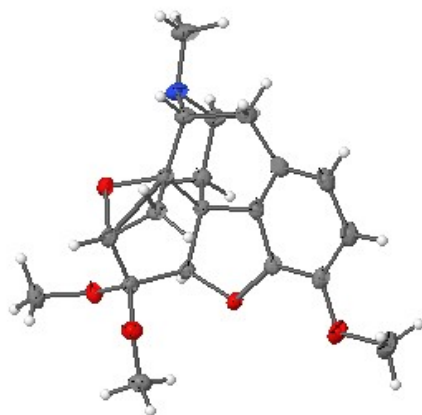
1:13401



1,3,5-Tris(4-methylphenyl)benzene
C₂₇H₂₄
Described in *Acta Cryst.* (2006), E62, o777
[Search for similar structures](#)

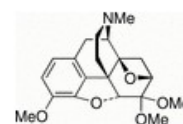
- Replacement for the online 3D page

Structure 4



C₂₀H₂₅NO₅

Deschamps, J. R., Coop, A., Parrish, D. A. & Rice, K. C. (2004). *Acta Cryst.* **E60**, o331-o333.



C₂₀H₂₅NO₅

$M_r =$	$a = 7.509 (2)$	$V = 435.81 (19)$
359.41	Å	Å ³
Triclinic	$b = 7.777 (2)$	$Z = 1$
$P1$	Å	
	$c = 8.430 (2)$	
	Å	
	$\alpha = 83.776$	
	(6) °	
	$\beta = 68.993$	
	(5) °	
	$\gamma = 71.511$	
	(5) °	

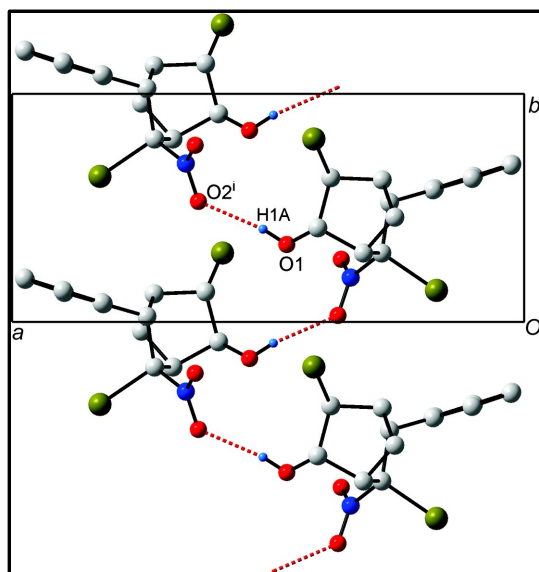
Jmol

Molecule

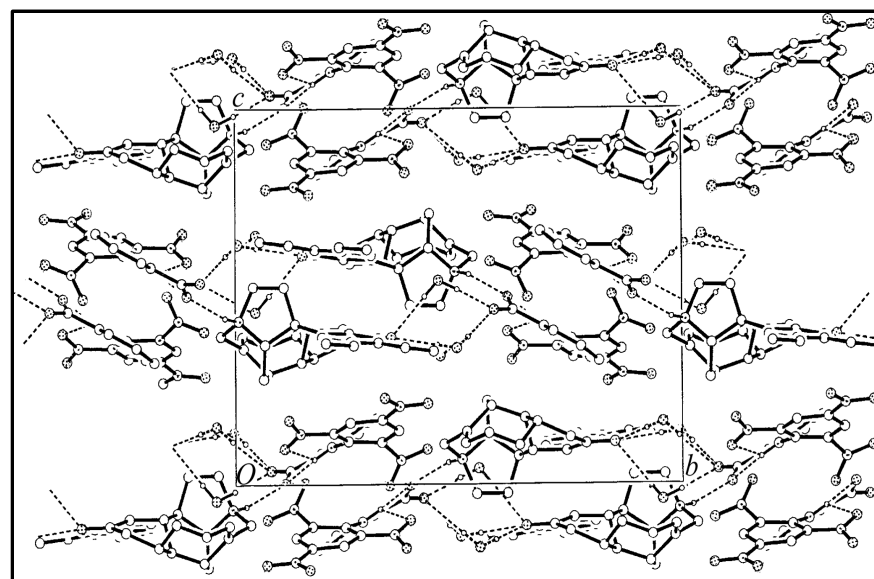
Unit cell

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



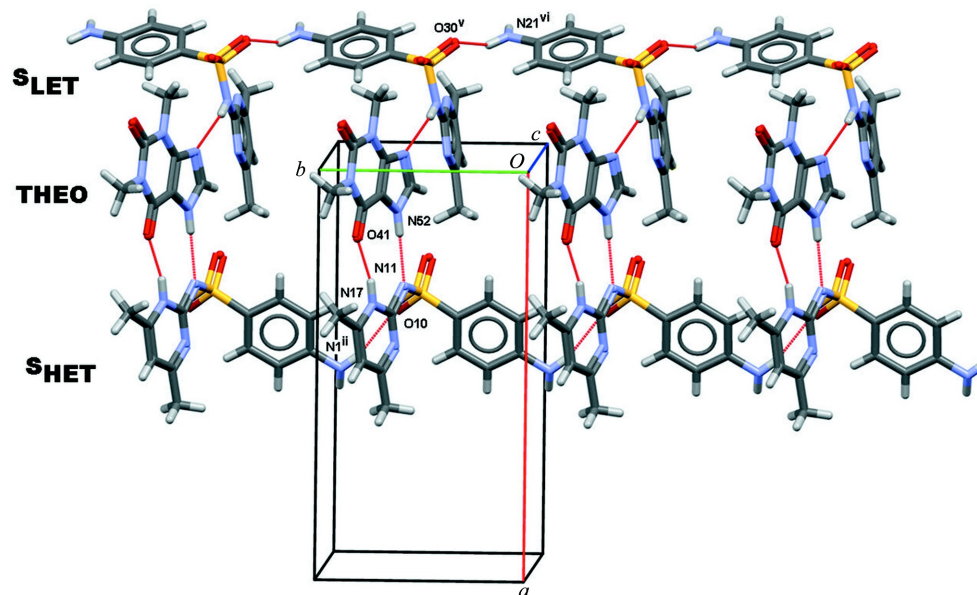
Greyscale, 600 dpi

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).

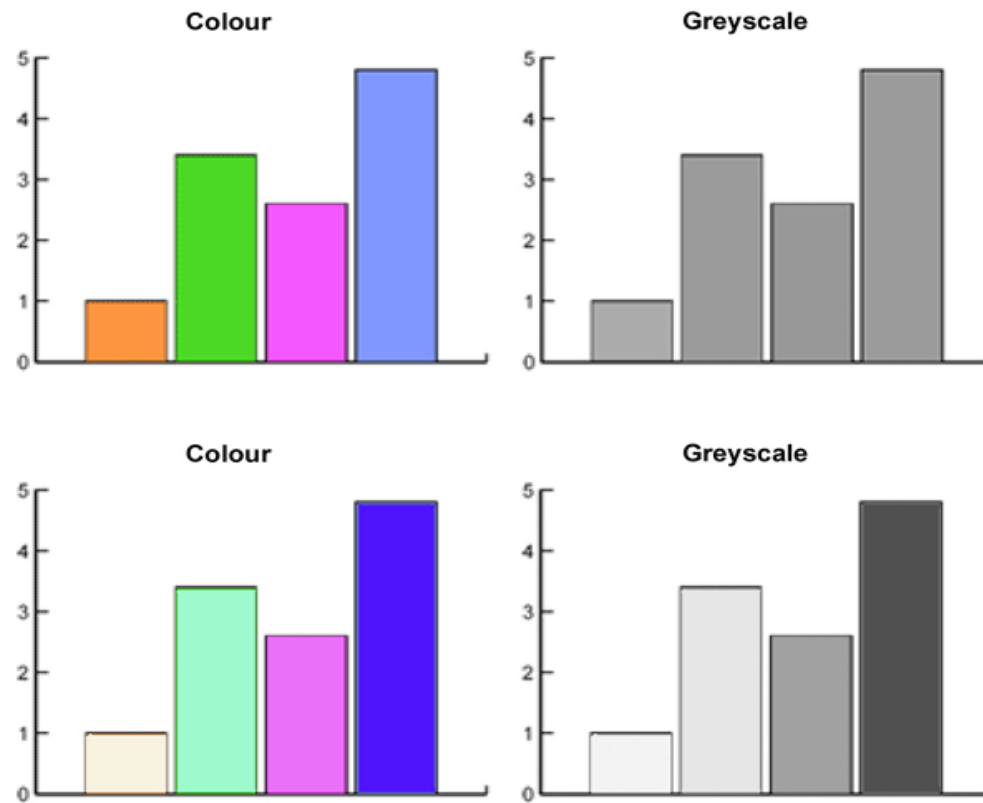
Labelling should generally be roman (upright) and consistent with the text of your article. At the final published size, the labelling on the figure should be approximately 8pt.

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.



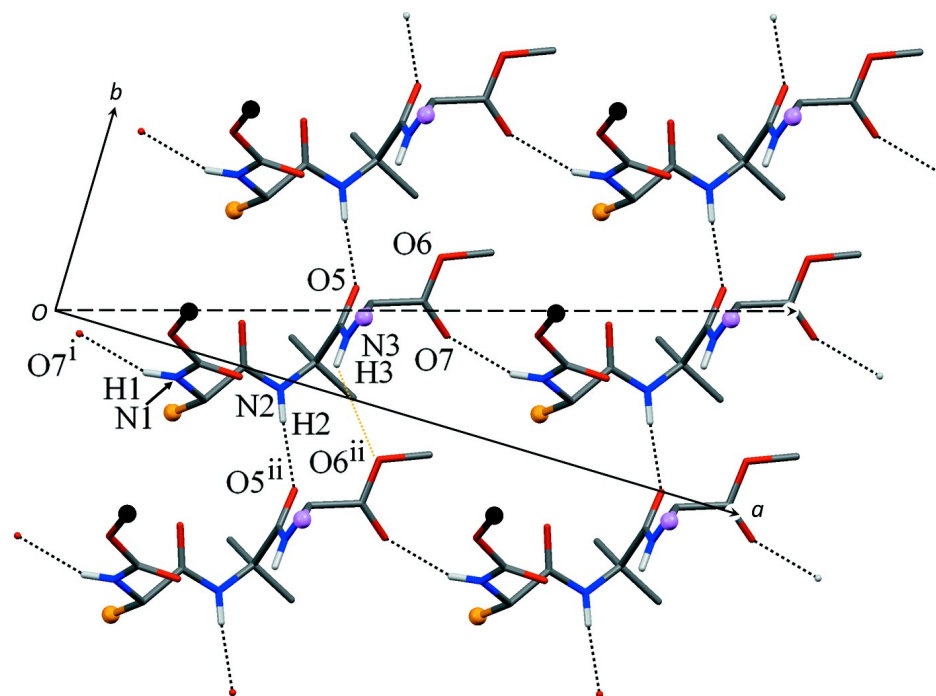
Use of colour in figures

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.

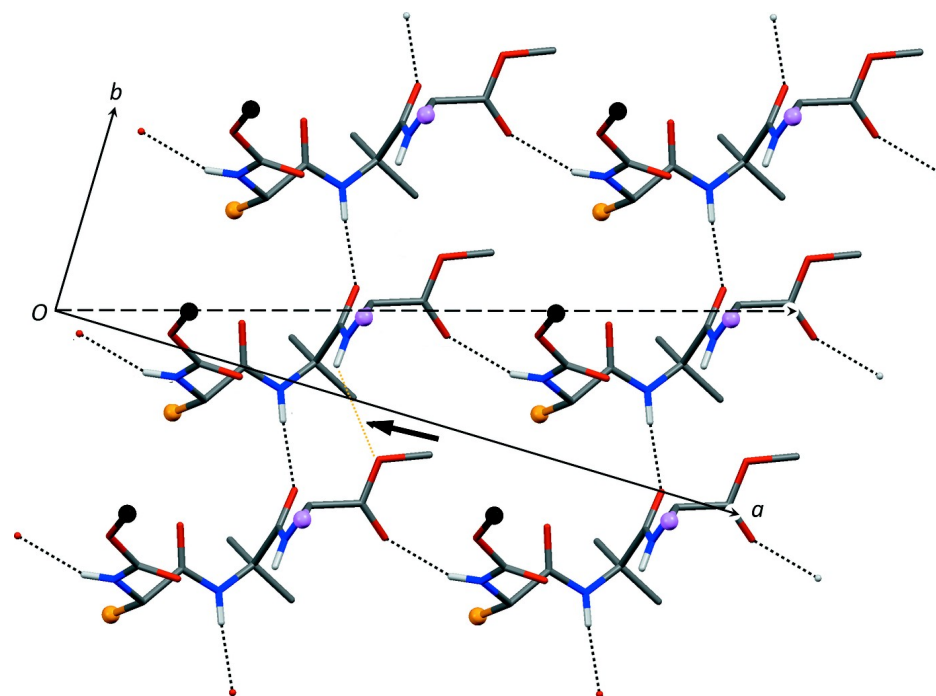
Colour can be mentioned as long as it is not the only way to see the highlighted item,

For example, "A single long N3---H3...O6ⁱⁱ contact (Table 2; orange in the electronic version of the paper)...".



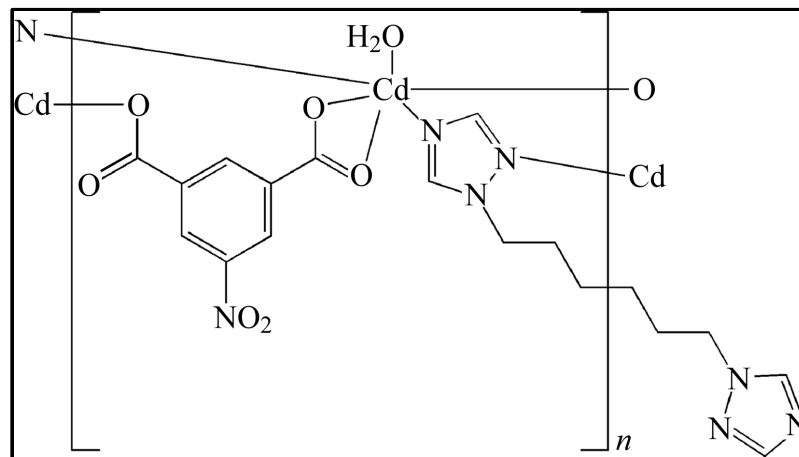
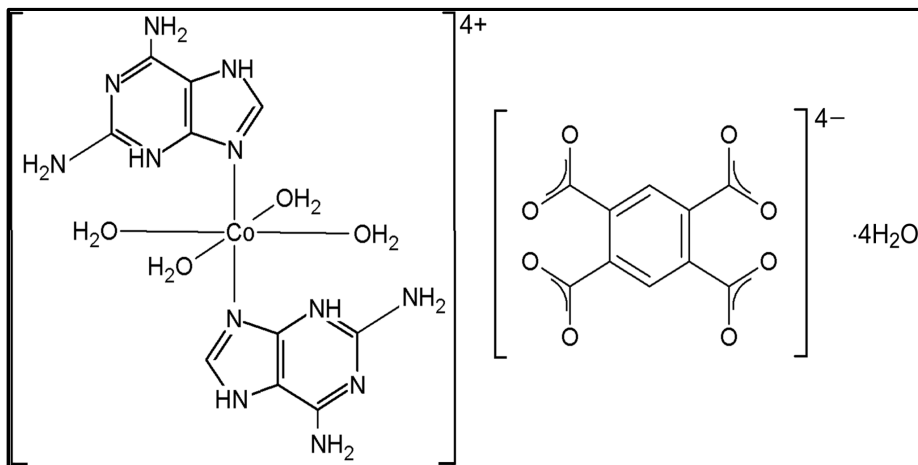
Use of colour in figures

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

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doi:10.1351/pac200880020277
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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:

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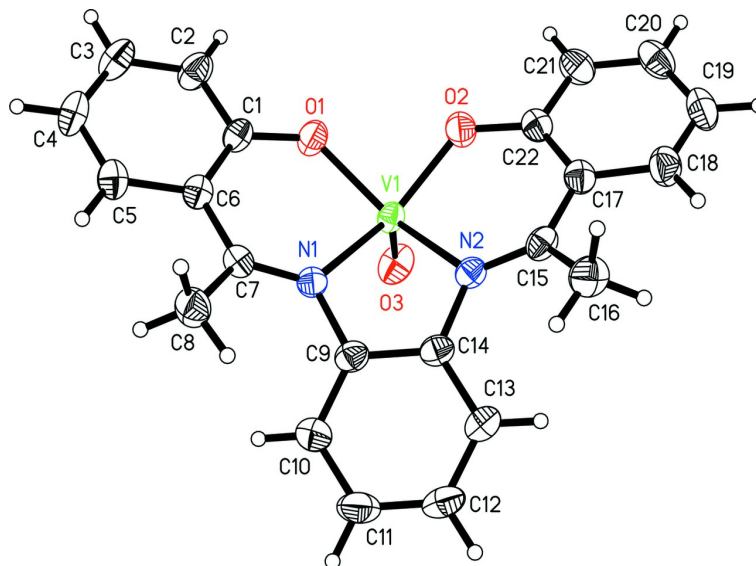
Developed by the Task Group for Graphical Representation Standards for Chemical Structure Diagrams: **Chairman: W. Town (UK); **Members:** J. Brecher (USA), K. N. Degtyarenko (UK), H. Gottlieb (USA), R. M. Hartshorn (New Zealand), K.-H. Hellwich (Germany), J. Kahovec (Czech Republic), G. P. Moss (UK), A. McNaught (UK), J. Nyitrai (Hungary), W. Powell (USA), A. Smith (USA), K. Taylor (USA), A. Williams (USA), A. Yerin (Russia); **Corresponding Members:** S. Conway (UK), P. Giles (USA), M. Griffiths (USA), B. Košata (Czech Republic), B. Ramsay (USA).

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.

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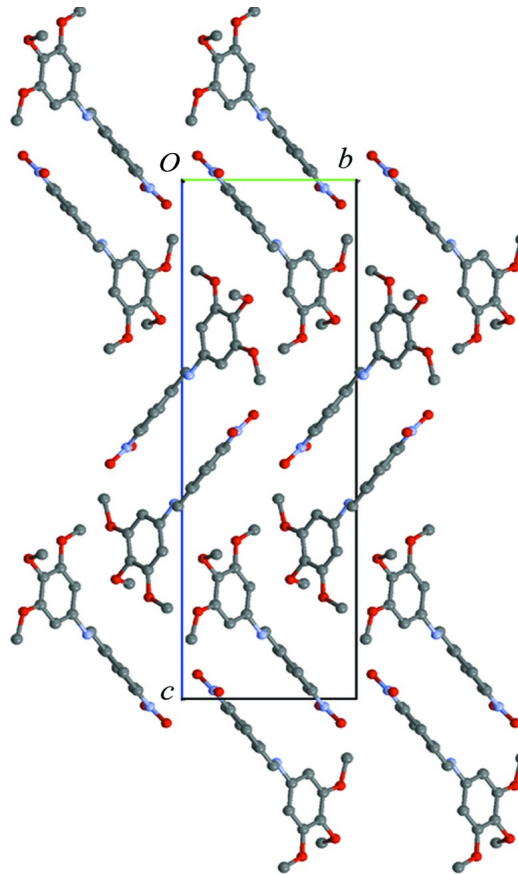
Ellipsoid plots

- 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

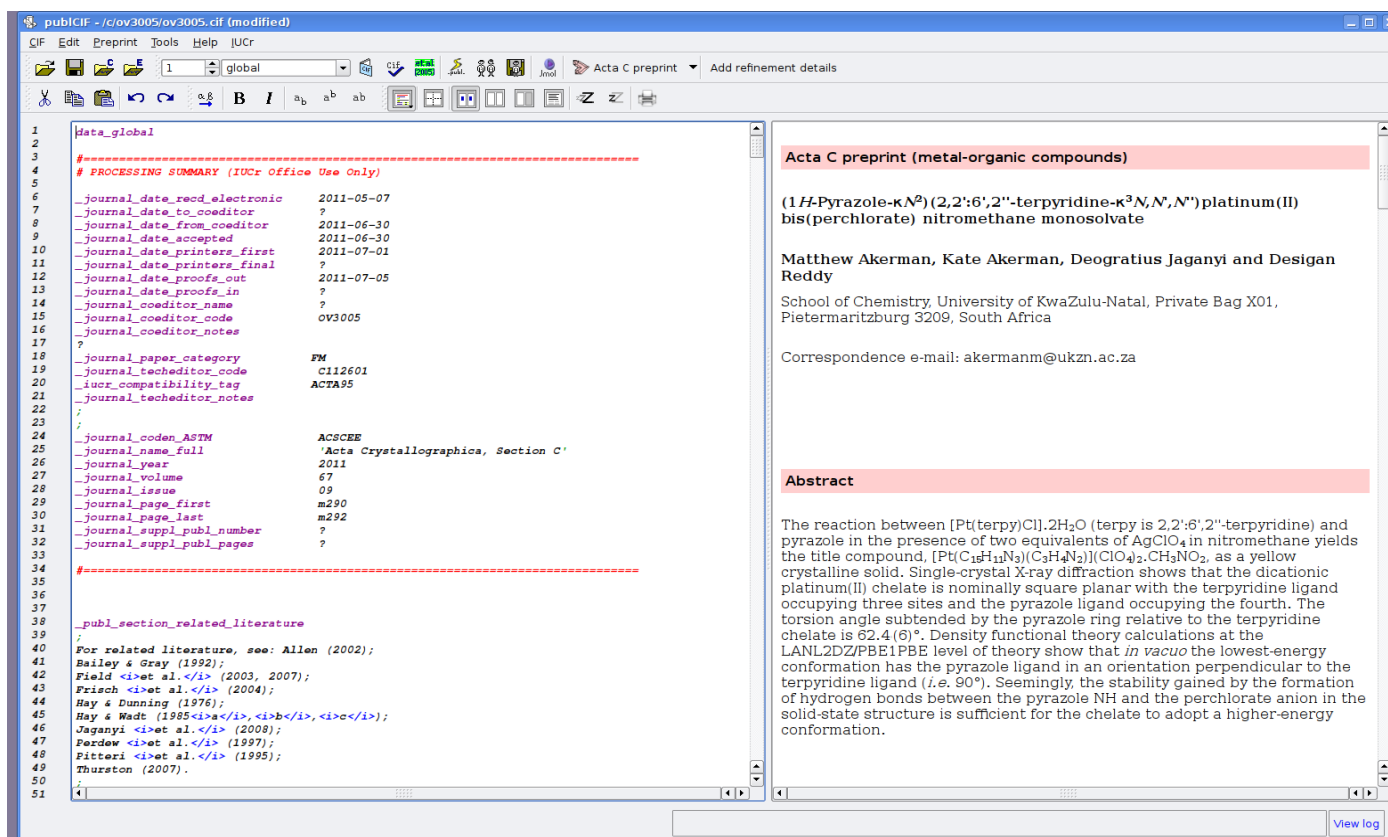
- Images are of sufficiently high resolution (at least 400 dpi for colour images and 600 dpi for monochrome and greyscale images)
- Images are an appropriate size
- Lettering on images is in a standard font and does not vary too much in size
- Colour figures will display satisfactorily when greyscale

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



The screenshot shows the publCIF software interface. The left pane displays the CIF data, and the right pane shows the resulting SGML output.

Acta C preprint (metal-organic compounds)

(1*H*-Pyrazole- $\kappa\Lambda^2$)(2,2':6',2''-terpyridine- κ^3N,N',N'')platinum(II) bis(perchlorate) nitromethane monosolvate

Matthew Akerman, Kate Akerman, Deogratius Jaganyi and Desigan Reddy

School of Chemistry, University of KwaZulu-Natal, Private Bag X01, Pietermaritzburg 3209, South Africa

Correspondence e-mail: akermanm@ukzn.ac.za

Abstract

The reaction between [Pt(terpy)Cl].2H₂O (terpy is 2,2':6',2''-terpyridine) and pyrazole in the presence of two equivalents of AgClO₄ in nitromethane yields the title compound, [Pt(C₁₂H₁₁N₃)(C₃H₄N₂)](ClO₄)₂.CH₃NO₂ as a yellow crystalline solid. Single-crystal X-ray diffraction shows that the dicationic platinum(II) chelate is nominally square planar with the terpyridine ligand occupying three sites and the pyrazole ligand occupying the fourth. The torsion angle subtended by the pyrazole ring relative to the terpyridine chelate is 62.4(6)°. Density functional theory calculations at the LANL2DZ/PBE1PBE level of theory show that *in vacuo* the lowest-energy conformation has the pyrazole ligand in an orientation perpendicular to the terpyridine ligand (*i.e.* 90°). Seemingly, the stability gained by the formation of hydrogen bonds between the pyrazole NH and the perchlorate anion in the solid-state structure is sufficient for the chelate to adopt a higher-energy conformation.

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

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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 (C_xH_y) 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 *pub/CIF*

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

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

3B2 Total Publishing System

File Edit View Document Page Frame Styles Text Graphic Window Help

SGML SGML menu LMs Table LMs FormatA Format Find elem SGML parse SGML print SGML in SGML save Gen P T Help SGML exit

/c/ku3049/ku3049.3d - changed

Pasteboard: pboard2

Tx ku3049 - 12136(27310)c

0.900 (C16–C21) in the <?bk [?tj=100mm]\$262#[?tj]\$w>X-ray<?ek> structure of (I)<schemer id="scheme1"> and to 0.778 (C1–C6 and C16–C21) in the calculated geometry of (I)<schemer id="scheme1">, whereas in the ligand and (I)<schemer id="scheme1"> the values of the aromaticity parameters for the C9–C14 ring are significantly higher and equal to 0.959, 0.982 (<?bk [?tj=100mm]\$262#[?tj]\$w>X-ray<?ek>) and 0.962 (DFT), respectively. The formation of the complex causes changes in the conformation of the ligand mol­ecule. Firstly, the planarity of the ligand increases as a result of complex formation. The values of the angles between planes defined by the N<inf arrange="stagger">2</inf>-O<inf arrange="stagger">2</inf> donor atoms and the planes of the benzene rings decrease in the following order: from 51.11 (ligand) to 21.11&ensp14;(7) (<?bk [?tj=100mm]\$262#[?tj]\$w>X-ray<?ek>) and 22.10° (DFT) in (I)<schemer id="scheme1"> for the C1–C6 ring, from 40.78 (ligand) to 16.98&ensp14;(8) (<?bk [?tj=100mm]\$262#[?tj]\$w>X-ray<?ek>) and 24.00° (DFT) in (I)<schemer id="scheme1"> for C9–C14, and from 51.11 (ligand) to 11.06&ensp14;(8) (<?bk [?tj=100mm]\$262#[?tj]\$w>X-ray<?ek>) and 22.10° (DFT) in (I)<schemer id="scheme1"> for C17–C22. The other consequences of complex formation are changes in the values of torsion angles. The most noticeable changes in (I)<schemer id="scheme1"> (in the <?bk [?tj=100mm]\$262#[?tj]\$w>X-ray<?ek> and DFT structures) are found for the following torsion angles: C9—N1—C7—C6, C7—N1—C9—C14, C15—N2—C14—C9 and C14—N2—C15—C17 (Table 1<tabler id="table1" loc="float">). All of these angles are in the environment of the N1 and N2 atoms but the twist is not at the C—N double bond.

Experimental

The crude brown powder of (I) (Boghél & Méhél, 2012) was prepared according to the procedure published by Farmer & Urbéd (1970). Crystals of (I) suitable for X-ray crystal structure analysis were grown from MeOH. The quantum-mechanical calculations were performed using standard DFT and employed the B3LYP hybrid functional (Becke, 1988, 1993; Lee et al., 1988) with the 6-311+G(d,p) level of theory. All species correspond to the minima at the B3LYP/6-311+G(d,p) level with no imaginary frequencies. All calculations were performed using the GAUSSIAN99 program package (Frisch et al., 2010).

Crystal data

[C₁₆H₁₂N₂O₂]

M_r = 492.52

Monoclinic, *P*2₁/n

a = 9.3715 (2) Å

b = 14.213 (2) Å

c = 2.3932 (2) Å

b = 102.97 (2)°

V = 1204.53 (5) Å³

Z = 4

Mo Kα radiation

Acta Cryst. (2013) C62, m1-m

Kozél et al. - DFT, H₂N, O₂, N1 - B13

metal-organic compounds

3: rhead,-,- : rhead

2: ku3049,-,- : main.main

10: lnumberstreamleft,-,-

TABLE 1

Selected geometric parameters for (I) (C=O and DFT) and the Schétt base ligand molecule (DFT) (Å, °).

	(I) X-ray	(I) DFT	Ligand DFT
V1—O1	1.377 (1)	1.389	
V1—O2	1.511 (1)	1.505	
V1—O3	1.593 (1)	1.582	
V1—N1	2.091 (2)	2.116	
V1—N2	2.091 (2)	2.116	
O1—V1—O2	94.38 (2)	97.00	
O1—V1—O3	110.10 (2)	111.74	
O2—V1—O3	109.97 (2)	111.74	
O1—V1—N1	96.32 (2)	95.32	
O2—V1—N1	163.92 (2)	164.93	
O1—V1—N2	162.12 (2)	163.03	
O2—V1—N2	96.90 (2)	98.12	
O3—V1—N2	107.11 (2)	107.10	
N1—V1—N2	78.31 (2)	78.99	
O1—C1—C2—C7	0.5 (2)	−0.3	0.5
C1—C2—C7—N1	−14.2 (2)	−16.5	−1.0
C2—N1—C7—C8	−17.3 (2)	−16.0	17.2
C7—N1—C2—C1	−14.1 (2)	−14.1	11.2
N1—C2—C1—N2	−0.2 (2)	0.0	0.0
C15—N2—C14—C9	18.4 (2)	14.1	−11.2
C14—N2—C15—C17	16.7 (2)	16.0	−17.2
N2—C15—C17—C12	21.2 (2)	10.5	1.0
C15—C17—C12—C13	1.3 (2)	2.3	−0.5

TABLE 2

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
O2—H2A...O2 ⁱⁱ	0.97 (2)	2.31 (2)	3.319 (2)	141.5 (16)
O3—H3A...O2 ⁱⁱ	0.90 (2)	2.41 (2)	3.344 (2)	138.6 (16)

Symmetry codes: (i) x+1, y, z; (ii) −x+1, −y, −z+1.

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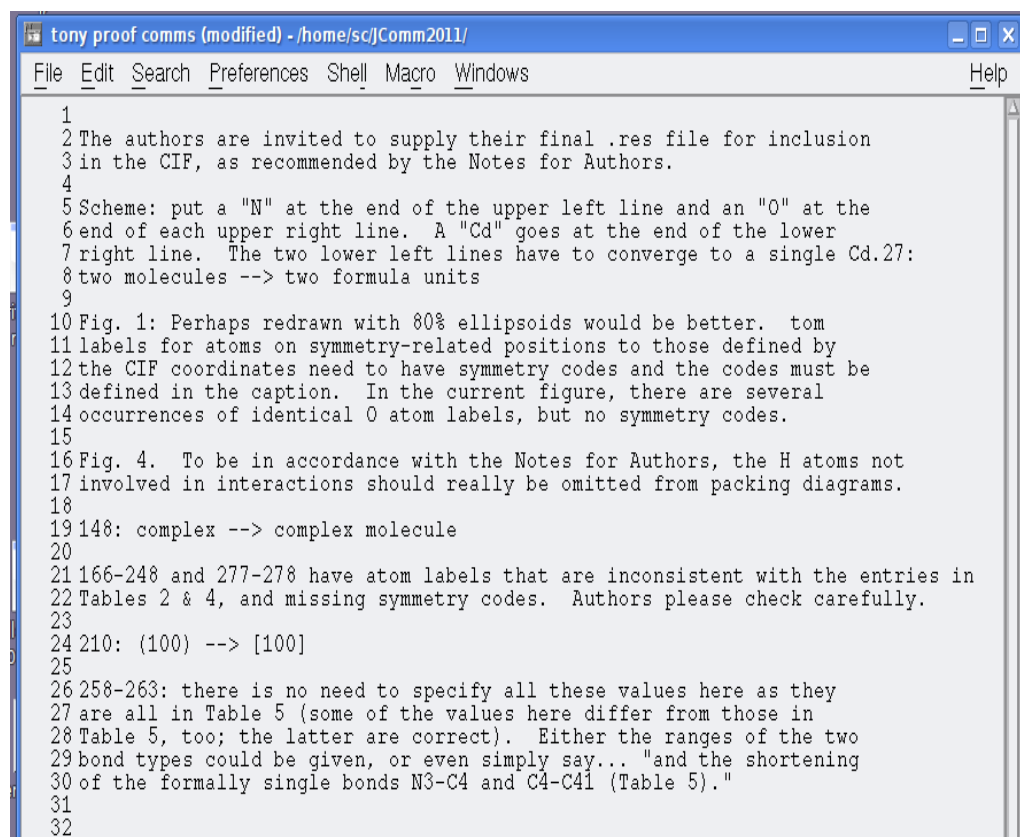
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1
2 The authors are invited to supply their final .res file for inclusion
3 in the CIF, as recommended by the Notes for Authors.
4
5 Scheme: put a "N" at the end of the upper left line and an "O" at the
6 end of each upper right line. A "Cd" goes at the end of the lower
7 right line. The two lower left lines have to converge to a single Cd.27:
8 two molecules --> two formula units
9
10 Fig. 1: Perhaps redrawn with 80% ellipsoids would be better. tom
11 labels for atoms on symmetry-related positions to those defined by
12 the CIF coordinates need to have symmetry codes and the codes must be
13 defined in the caption. In the current figure, there are several
14 occurrences of identical O atom labels, but no symmetry codes.
15
16 Fig. 4. To be in accordance with the Notes for Authors, the H atoms not
17 involved in interactions should really be omitted from packing diagrams.
18
19 148: complex --> complex molecule
20
21 166-248 and 277-278 have atom labels that are inconsistent with the entries in
22 Tables 2 & 4, and missing symmetry codes. Authors please check carefully.
23
24 210: (100) --> [100]
25
26 258-263: there is no need to specify all these values here as they
27 are all in Table 5 (some of the values here differ from those in
28 Table 5, too; the latter are correct). Either the ranges of the two
29 bond types could be given, or even simply say... "and the shortening
30 of the formally single bonds N3-C4 and C4-C41 (Table 5)."
31
32
```

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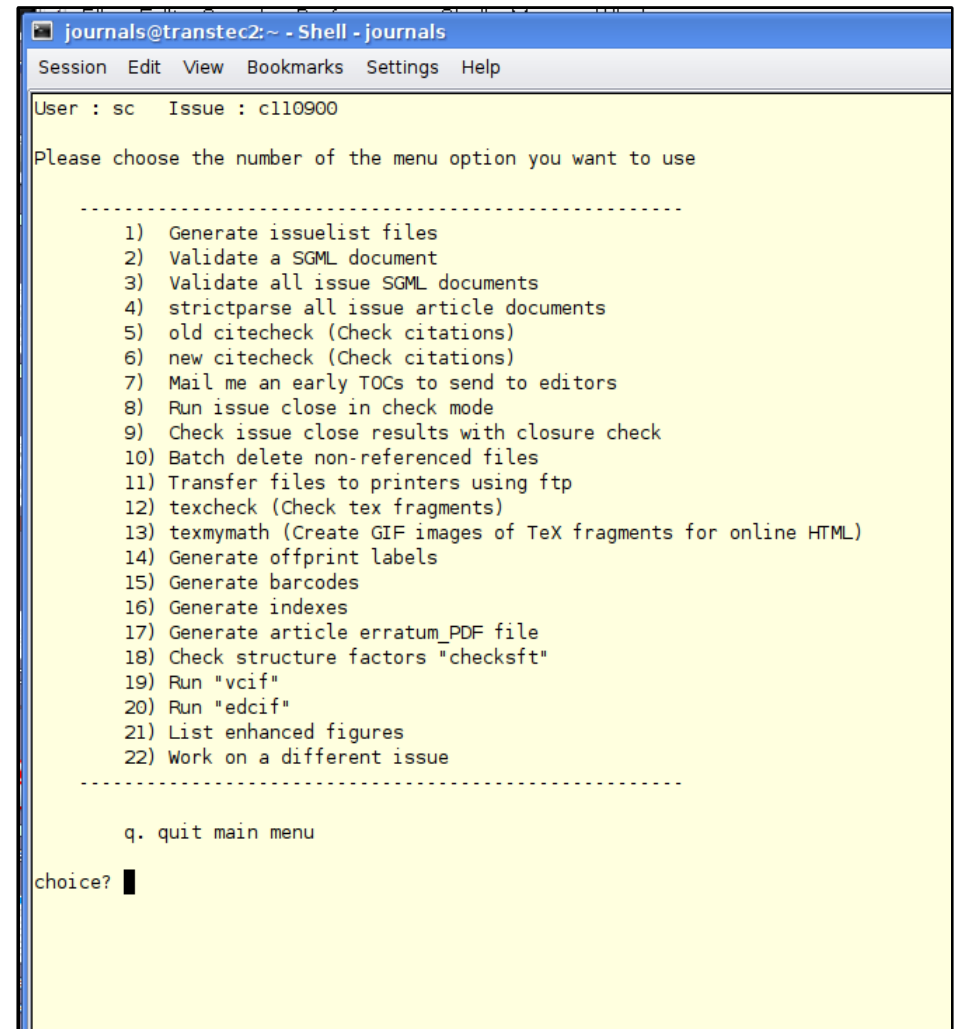
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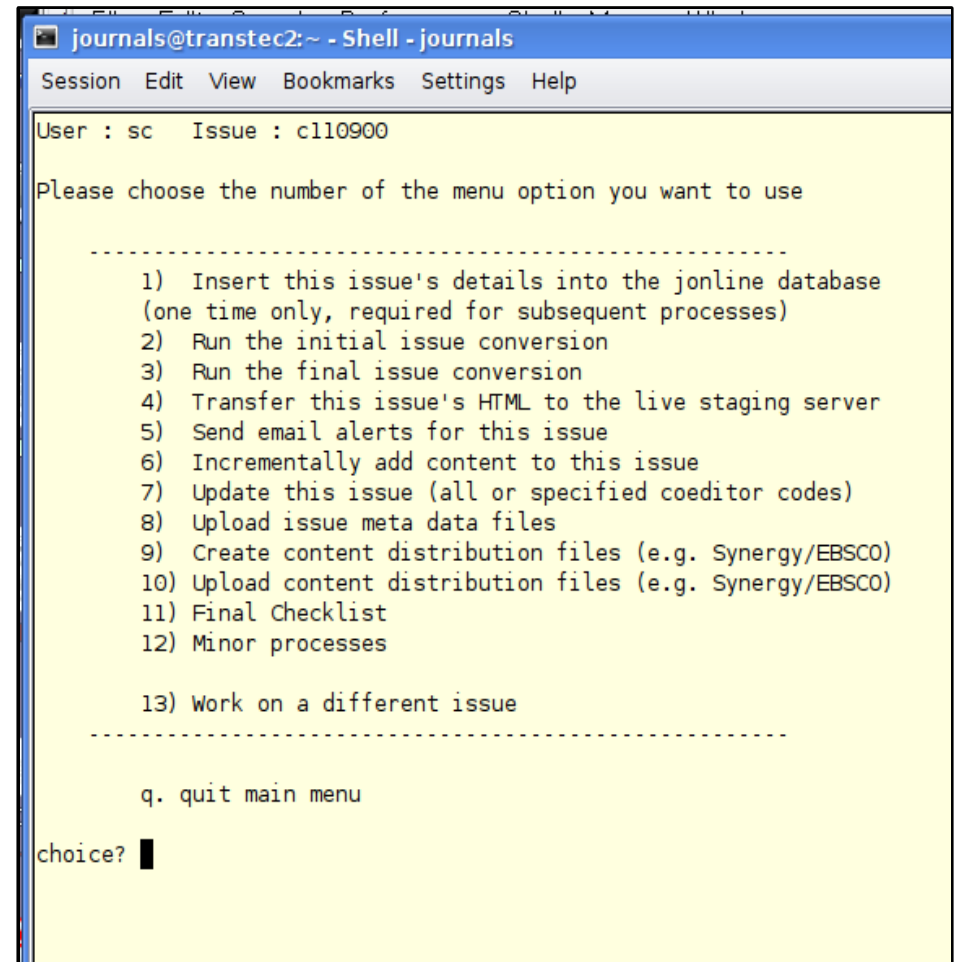


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Editor: Anthony Linden

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

Alain Collas and Frank Blockhuys

Acta Cryst. (2011). C67, o364–o369

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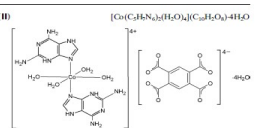
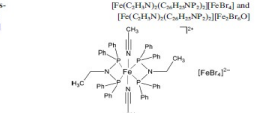
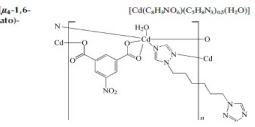
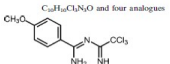
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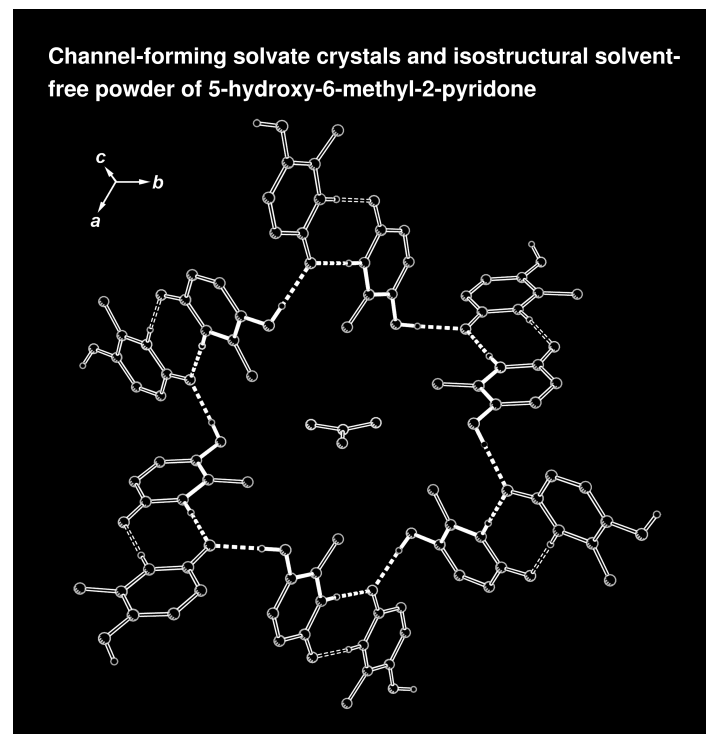
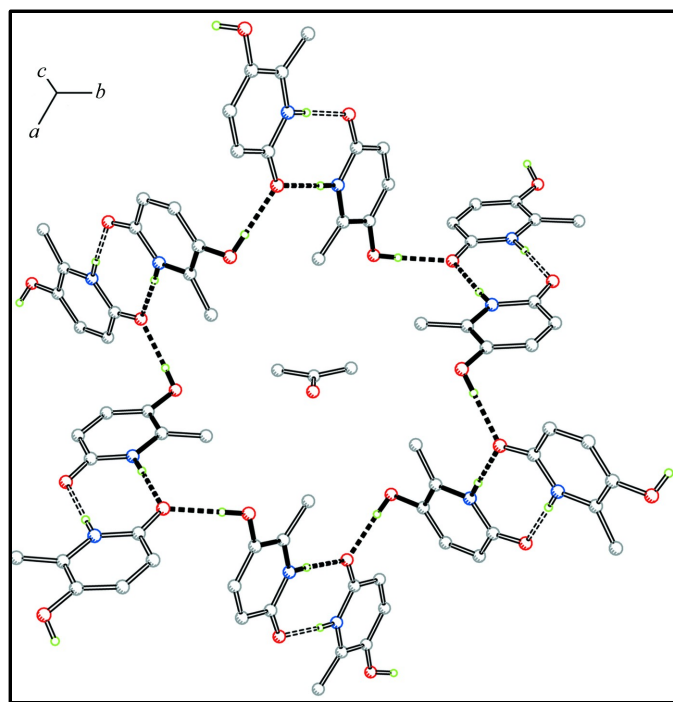
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m279	The bis(acetonitrile- κ^N)bis(<i>N,N</i> -bis(diphenylphosphoryl)ethanamine- κ^N) μ_2 iron(II) tetrabromidoferrate(II) and μ -oxido-bis(tribromidoferrate(III)) complex salts N. Matzuli and S. Otto 
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o273	Five related <i>N'</i> -(2,2,2-trichloroethanimido)benzene-1-carboximidamides R. T. Berez, T. L. Rossmelle, S. Sudawell Kondage, J. Zhou and M. Parez 
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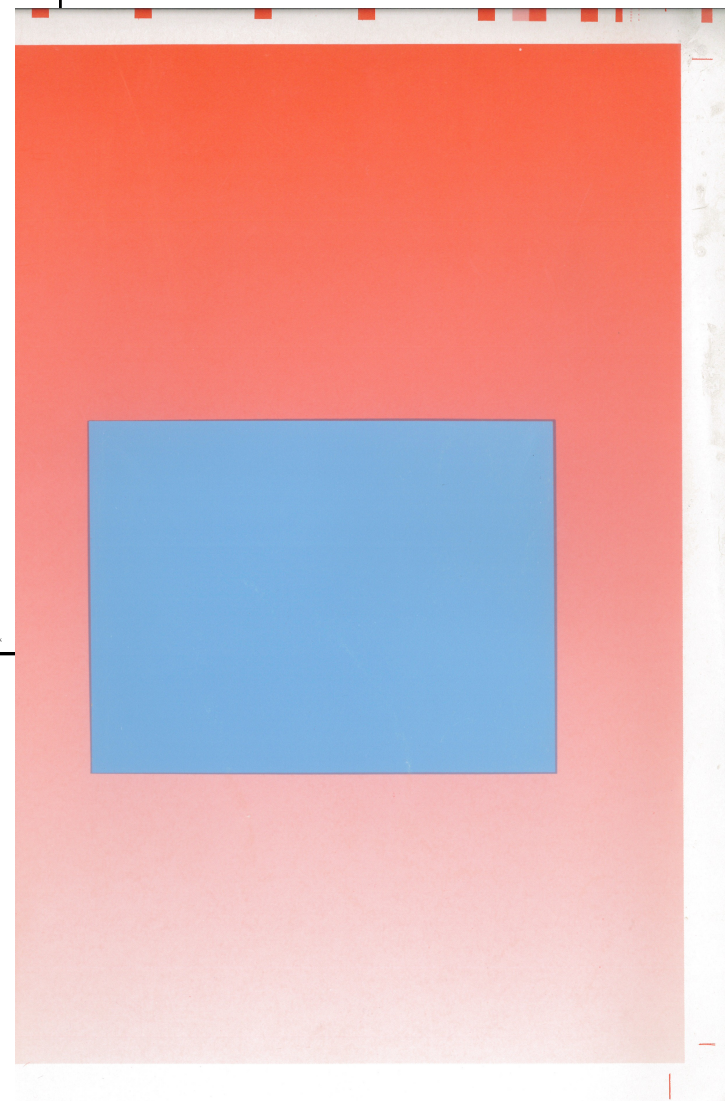
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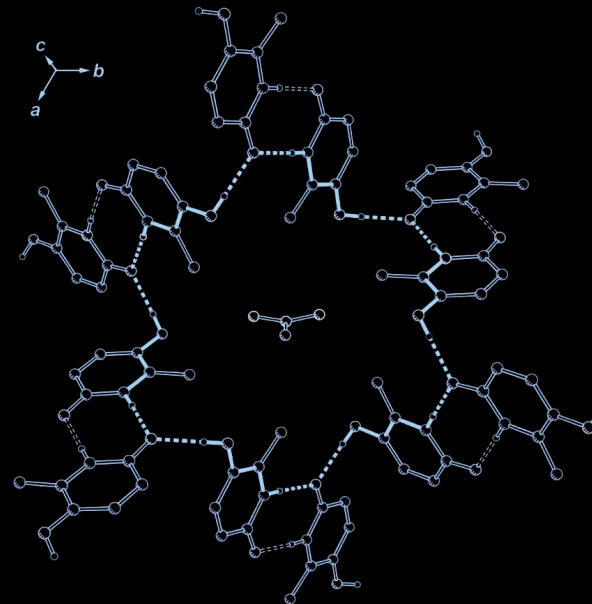


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