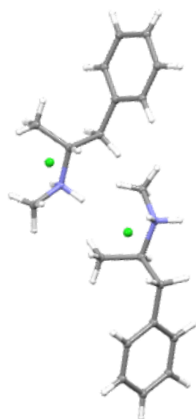
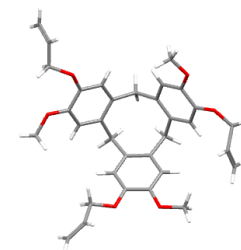
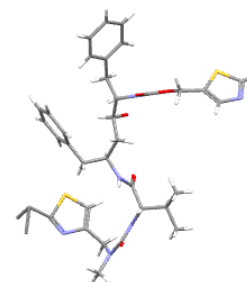
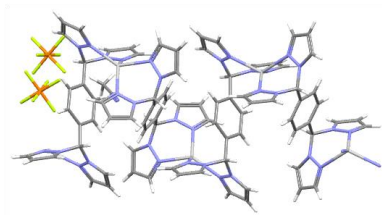
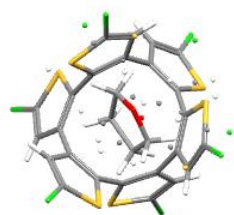
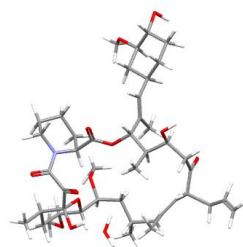


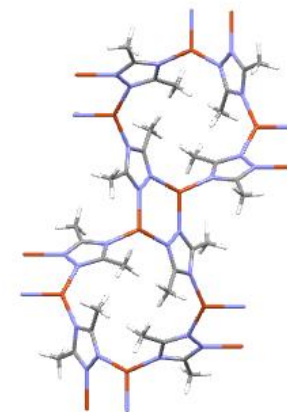


# A Journey from Data to Knowledge



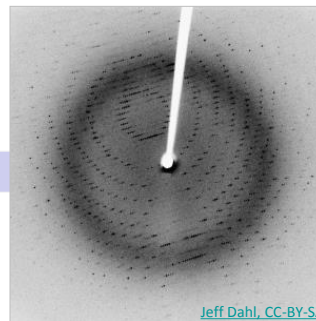
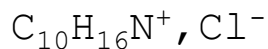
**Ian Bruno**  
**Cambridge Crystallographic Data Centre**

@ijbruno  
@ccdc\_cambridge



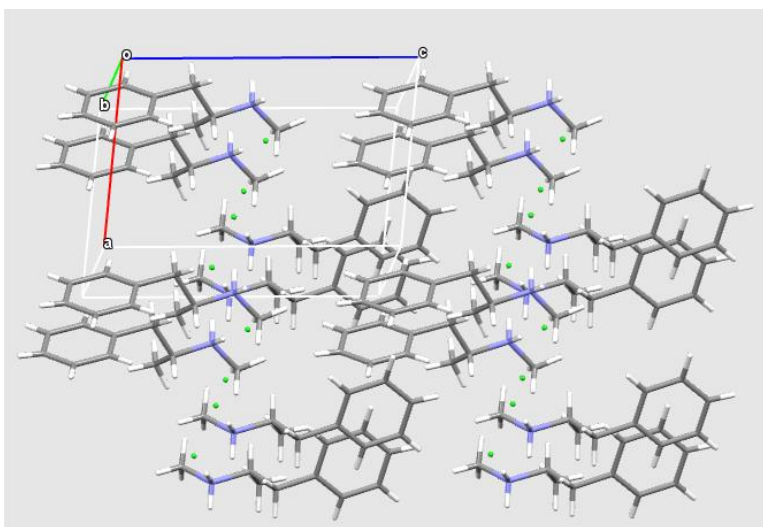


## Experimental Data



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_diffrn_radiation_monochromator graphite
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_diffrn_measurement_method '\psi and \omega'
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_diffrn_reflns_number 5892

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_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_occupancy
_atom_site_disorder_group
_atom_site_refinement_flags
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_disorder_group
_atom_site_disorder_group
C1 Cl 0.23185(8) 0.78305(9) 0.55574(6) 0.02213(16) Uani d 1 1 . . .
N M1 0.8091(3) 0.6811(3) 0.8969(2) 0.0172(4) Uani d U 1 1 . . .
C C1 0.6984(4) 0.7807(5) 0.4387(2) 0.0224(6) Uani d U 1 1 . . .
C C2 0.7610(6) 0.8922(8) 0.7089(3) 0.0256(6) Uani d U 1 1 . . .
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C C4 0.8703(4) 0.5637(4) 0.7481(3) 0.0236(6) Uani d U 1 1 . . .
```



- Experimentally determined 3D coordinates of atoms
- Arrangement of molecules in the crystal
- Captured in a CIF file



# Crystallographic Information Framework (CIF)

*Acta Cryst.* (1991), **A47**, 655–685

**International Union of Crystallography**

**Commission on Crystallographic Data  
Commission on Journals**

**Working Party on Crystallographic Information**

**The Crystallographic Information File (CIF): a New Standard  
Archive File for Crystallography\***

BY SYDNEY R. HALL

*Crystallography Centre, University of Western Australia, Nedlands 6009, Australia*

FRANK H. ALLEN

*Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England*

AND I. DAVID BROWN

*Institute for Materials Research, McMaster University, Hamilton, Ontario L8S 4M1, Canada*

(Received 8 April 1991; accepted 28 June 1991)

## Abstract

The specification of a new standard Crystallographic Information File (CIF) is described. Its development is based on the Self-Defining Text Archive and Retrieval (STAR) procedure [Hall (1991), *J. Chem. Inf. Comput. Sci.* **31**, 326–333]. The CIF is a general, flexible and easily extensible free-format archive file; it is human and machine readable and can be edited by a simple text editor. The CIF is designed for the electronic transmission of crystallographic data between individual laboratories, journals and databases: it has been adopted by the International Union of Crystallography as the recommended medium for this purpose.

## Introduction

There is an increasing need in many branches of science for a uniform but flexible method of archiving and exchanging data in electronic form. Rapid advances in computer technology, coupled with the expansion of local, national and international networks, have fuelled the need for such a facility. The variety and relative inflexibility of existing data exchange formats have inhibited their effective use. This is true even in fields where the basic data requirements are well defined. Problems of data exchange are further exacerbated if the number and nature of data types change rapidly and continuously. Under these conditions specialized and local file formats have proliferated. This diversity was tolerable when electronic data

- Standard format for capturing data about structure and experiment
- Maintained by the International Union of Crystallography (IUCr)
- Widely adopted by crystallographic and publishing communities



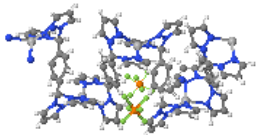
# Crystal Structure Deposition

PICK A STRUCTURE TO EDIT

612345-612345.cif

- data\_rw010605para

3D VISUALISER





JSmol


FILE CONTENTS


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30
31 _audit_creation_method      SHELXL-97
32 _chemical_name_systematic
33 ;
34 ?
35 ;
36 _chemical_name_common      ?
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39 _chemical_formula_sum      'C21 H19.50 Ag F6 N8.50 P'
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42 loop_
43 _atom_type_symbol
44 _atom_type_description
45 _atom_type_scatter_dispersion_real
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CSD FIELDS


Compound name 


Synonyms/other names 


Crystal colour 


Crystal habit 

Space group 

Study temperature (K) 

Formula moiety 

Formula sum 

Melting point (K) 

- Researchers deposit CIFs with CCDC
- Deposition services provide basic validation checks
- Depositor receives a unique accession ID
- Pre-publication access for trusted reviewers



# Data Deposition Challenges



Name	Status Reason	Depositor	Deposition Co.	Subject (Email)
1283376-DEP	Awaiting CCDC Numbers	Shun-W Wang	CCDC Deposit	New valid web deposit
1283374-DEP	Awaiting Correction	Konstantin Doma	CCDC Deposit	Re: CCDC Depository Req
1283365-DEP	Awaiting CCDC Numbers	Michael Jennings	CCDC Deposit	New valid web deposit
1283362-DEP	Awaiting CCDC Numbers	Laura Cañadilla	CCDC Deposit	pre-publication of file
1283363-DEP	Awaiting Correction	Dra. Victoria Cast	CCDC Deposit	Deposited Data - CCDC P
1283360-DEP	In progress of assigning ...	Mareike Johnke	CCDC Deposit	Deposit of 7 X-ray struc
1283356-DEP	Awaiting Correction	Chang Hong	CCDC Deposit	Re:CCDC Depository Req
1283136-DEP	Awaiting Correction	D. Stemborn	CCDC Deposit	CCDC submission - chang
1283440-DEP	Awaiting Correction	mouayedabdulale	CCDC Deposit	Re: CCDC Depository Req

Name	Deposit	CCDC Number	Source File (External Format)	Status Reason	Register Decisions Present
1643223-C...	1000218-DEP	929,193	structure_1999264231.txt	Added to WebCSD	No
1762050-C...	1274796-DEP	929,193	ccdc.cif	Added to WebCSD	No
1762051-C...	1274796-DEP	929,193	dvshtou11vls_mach.cif	Added to WebCSD	No
1643224-C...	1000218-DEP	929,192	structure_1999264230.txt	Inactive	No
1643225-C...	1000218-DEP	929,191	structure_1999264240.txt	Inactive	No

- Syntax errors
- Inaccuracies
- Revisions
- Republications
- Timely release

Over 60,000 structures deposited annually



# Crystal Structure Dissemination

Your query was: Doi: 10.1023/A:1011052932607 and returned 4 records

Results

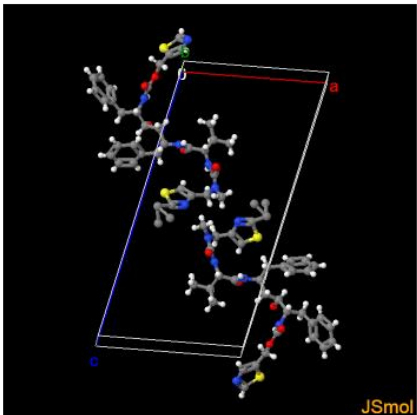
← PREV    NEXT →

CCDC #	Refcode
<input checked="" type="checkbox"/>	710528 YIGPIO
<input checked="" type="checkbox"/>	710530 YIGPIO01
<input checked="" type="checkbox"/>	710527 YIGPIO02
<input checked="" type="checkbox"/>	710529 YIGPIO03

Download ▾

YIGPIO : (5S-(5R\*,8R\*,10R\*,11R\*))-10-Hydroxy-2-methyl-5-isopropyl-1-(2-isopropyl-4-thiazolyl)-3,6-dioxo-8,11-dibenzyl-2,4,7,12-tetra-azatridecan-13-  
oic acid 5-thiazolyl methyl ester  
Spacegroup: P21, Cell: *a* 13.438(3)Å *b* 5.288(1)Å *c* 27.055(5)Å,  $\alpha$  90°  $\beta$  103.15(2)°  $\gamma$  90°

3D viewer



JSmol

H   Disorder   ↻   Menu   Open ▾

Style   Labels   Packing   Measure

Ball and Stick ▾   No Labels ▾   Unit Cell ▾   None ▾

- On publication, deposited data sets freely available for anyone to download
- Individual structures accessible via CCDC Summary Page\*
- Web services enable structure lookup and retrieval

\* New Summary Page scheduled for launch December 2014



# Linking articles and data

**ACS Publications**  
MOST TRUSTED. MOST CITED. MOST READ.

Cu(II) metal organic frameworks (MOFs) using pyrazole and aromatic carboxylic MOFs are synthesized based on a hexanuclear Cu-pyrazolate unit as a secondary intriguing structural networks like (4,4) type herringbone grid or an archetypal MOFs showed highly encouraging photocatalytic degradation of toxic organic dyes in wastewater purification. On the other hand, magnetic behaviors of MOF-2 and Cu6 unit have also been investigated.

Organic Chemicals and Reactions

Author of this Article  
 Any Author  
 Research Topic (Now with patent search)

Bala, Sukhen

Search

Accession Codes

CCDC: 1019417  
CCDC: 1019418  
CCDC: 1019419

History

Just Accepted Manuscript  
October 22, 2014  
Received August 18, 2014

...ine from 2-chloropyridine is described via a Directed mechanism in 26–28% yields. By performing sequential, a variety of functionalised heteroaryl and arylboronic ne scaffolds have been accessed in synthetically tives. 2-Chloro-4-heteroaryl-3-iodopyridines and rted. The synthesis of 5-[3,4-bis(2- a two-step Sonogashira/Suzuki-Miyaura reaction nylacetylene and 6-fluoropyridin-3-yl-3-boronic acid

- Divergent synthesis of arylated pyridin-2(1H)-one deriv... *Tetrahedron*
  - Combined directed ortho metalation-halogen dance (HD) s... *Organic Letters*
  - ▶ View details of all 3 citing articles in Scopus
- Provided by Scopus*

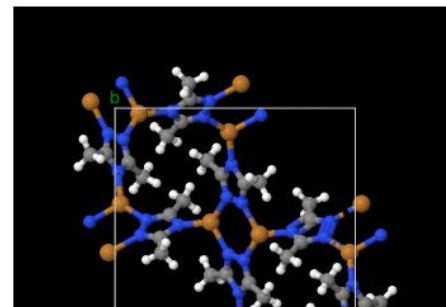


View Record in Scopus

ELSEVIER

ASUQIO : catena-(( $\mu^3$ -3,5-Dimethyl-1,2,4-triazolato-N,N')-copper(i))  
Spacegroup: P42/n, Cell: a 13.470(2)Å b 13.470(2)Å c 6.142(2)Å,  $\alpha$  90°  $\beta$  90°  $\gamma$  90°

3D viewer



Associated publications

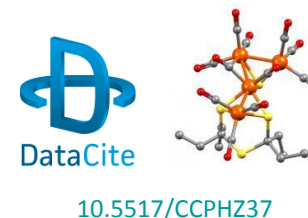
- Jie-Peng Zhang, Shao-Liang Zheng, Xiao-Chun Huang, Xiao-Ming Chen, *Angewandte Chemie, International Edition*, 2004, 43, 206, DOI: [10.1002/anie.200352627](https://doi.org/10.1002/anie.200352627)
- Jie-Peng Zhang, Yan-Yong Lin, Xiao-Chun Huang, Xiao-Ming Chen, *Journal of the American Chemical Society*, 2005, 127, 5495, DOI: [10.1021/ja042222t](https://doi.org/10.1021/ja042222t)
- Jie-Peng Zhang, Yan-Yong Lin, Xiao-Chun Huang, Xiao-Ming Chen, *Dalton Transactions*, 2005, 3681, DOI: [10.1039/b509615d](https://doi.org/10.1039/b509615d)

Links are in place for ACS, RSC, Elsevier and IUCr journals



# DOIs and Data Citation

- Unambiguous and persistent identification of datasets
- Over 500,000 DOIs registered since April 2014
- Foundation for formalising data citation and interoperability



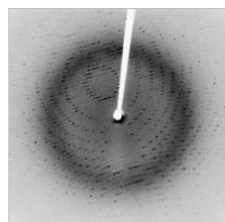
**DC<sup>1</sup>**  
Data Citation Principles

Data should be considered legitimate, citable products of research...

<https://www.force11.org/datacitation>

## Dataset Publication

CCDC 892348: Experimental Crystal Structure Determination. **A. Crystallographer**, *Cambridge Crystallographic Data Centre* (2013)  
<http://dx.doi.org/10.5517/CCYYKFV>



Potential for linking between derived data at CCDC and raw data stored at STFC based on DOIs.



Coverage of CCDC data by the Thomson Reuters Data Citation Index to be achieved via the DataCite metadata store.

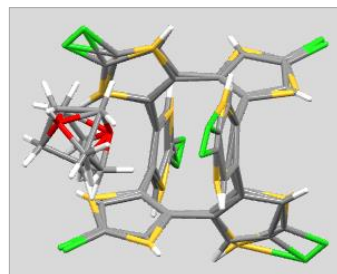




# Assigning Chemistry

## Data deposited with CCDC

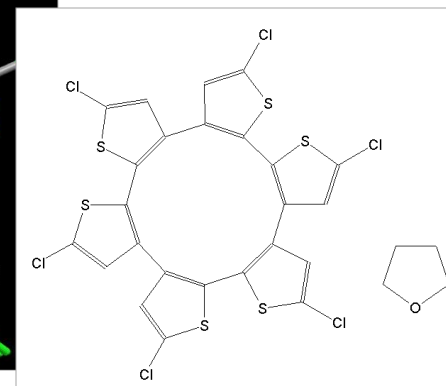
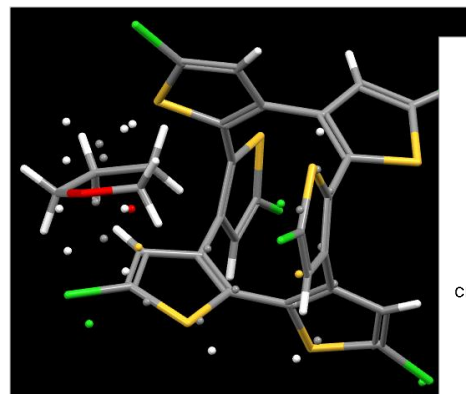
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_atom_site_fract_z  
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_atom_site_occupancy  
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_atom_site_disorder_assembly  
_atom_site_disorder_group
```



```
C11 Cl 0.5993(2) 1.0007(7) 0.8131(17) 0.044(3) Uani 0.50 1 d PDU A 1  
S1 S 0.5321(3) 0.8260(6) 0.9322(3) 0.0327(11) Uani 0.50 1 d PDU A 1  
C2 C 0.5529(4) 0.8802(9) 0.8184(9) 0.029(4) Uani 0.50 1 d PDU A 1  
C3 C 0.5286(7) 0.8174(18) 0.7440(7) 0.031(4) Uani 0.50 1 d PDU A 1  
H3A H 0.5350 0.8343 0.6771 0.037 Uiso 0.50 1 calc PR A 1  
C4 C 0.4918(8) 0.7220(19) 0.7783(8) 0.027(4) Uani 0.50 1 d PDU A 1  
C5 C 0.4900(6) 0.7171(14) 0.8779(9) 0.029(4) Uani 0.50 1 d PDU A 1  
C12 Cl 0.3202(2) 0.4982(6) 1.0830(5) 0.0586(15) Uani 0.50 1 d PDU A 1  
S2 S 0.38755(19) 0.6658(5) 0.9578(5) 0.0400(10) Uani 0.50 1 d PDU A 1
```

- Unambiguous identification of datasets
- Correction of syntax errors
- Provenance and attribution

## Entry in Cambridge Structural Database



Identifier	ABOWOD
Literature Reference	M.J.Marsella, Kunsang Yoon, F.S.Tham, <i>Org.Lett.</i> (2001), <b>3</b> , 2129, doi: <a href="https://doi.org/10.1021/ol016122t">10.1021/ol016122t</a>
Formula	C <sub>24</sub> H <sub>6</sub> Cl <sub>6</sub> S <sub>6</sub> ·2(C <sub>4</sub> H <sub>8</sub> O)
Compound Name	trans-1 <sup>5</sup> ,2 <sup>5</sup> ,3 <sup>5</sup> ,4 <sup>5</sup> ,5 <sup>5</sup> ,6 <sup>5</sup> -Hexachloro-1,2,4,6(3,2),3,5(2,3)-hexathiophenacyclohexaphane tetrahydrofuran solvate
Disorder	The whole cyclophane molecule and the tetrahydrofuran solvent molecule are disordered equally over two sites.

- Assignment of chemistry
- Additional scientific data and metadata
- Review by editorial staff

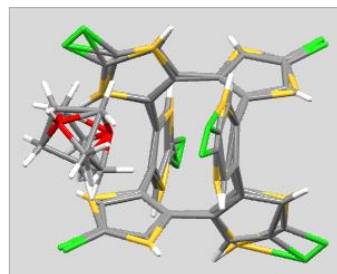
Assignment of chemistry is required to make data findable, interoperable and reusable



# Assigning Chemistry

## Data deposited with CCDC

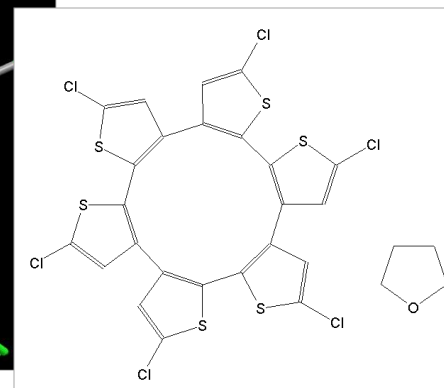
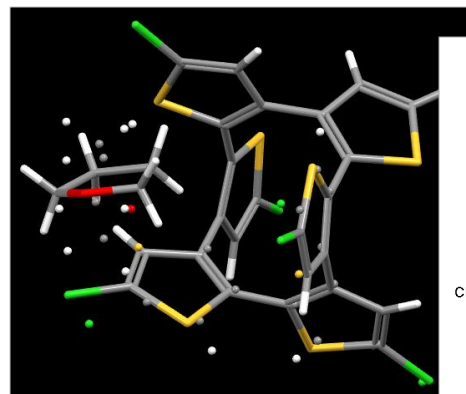
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_atom_site_fract_y  
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_atom_site_U_iso_or_equiv  
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_atom_site_symmetry_multiplicity  
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```



```
C11 Cl 0.5993(2) 1.0007(7) 0.8131(17) 0.044(3) Uani 0.50 1 d PDU A 1  
S1 S 0.5321(3) 0.8260(6) 0.9322(3) 0.0327(11) Uani 0.50 1 d PDU A 1  
C2 C 0.5529(4) 0.8802(9) 0.8184(9) 0.029(4) Uani 0.50 1 d PDU A 1  
C3 C 0.5286(7) 0.8174(18) 0.7440(7) 0.031(4) Uani 0.50 1 d PDU A 1  
H3A H 0.5350 0.8343 0.6771 0.037 Uiso 0.50 1 calc PR A 1  
C4 C 0.4918(8) 0.7220(19) 0.7783(8) 0.027(4) Uani 0.50 1 d PDU A 1  
C5 C 0.4900(6) 0.7171(14) 0.8779(9) 0.029(4) Uani 0.50 1 d PDU A 1  
C12 Cl 0.3202(2) 0.4982(6) 1.0830(5) 0.0586(15) Uani 0.50 1 d PDU A 1  
S2 S 0.38755(19) 0.6658(5) 0.9578(5) 0.0400(10) Uani 0.50 1 d PDU A 1
```

- Unambiguous identification of datasets
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Formula	C <sub>24</sub> H <sub>6</sub> Cl <sub>6</sub> S <sub>6</sub> ·2(C <sub>4</sub> H <sub>8</sub> O)
Compound Name	trans-1 <sup>5</sup> ,2 <sup>5</sup> ,3 <sup>5</sup> ,4 <sup>5</sup> ,5 <sup>5</sup> ,6 <sup>5</sup> -Hexachloro-1,2,4,6(3,2),3,5(2,3)-hexathiophenacyclohexaphane tetrahydrofuran solvate
Disorder	The whole cyclophane molecule and the tetrahydrofuran solvent molecule are disordered equally over two sites.

- Assignment of chemistry
- Additional scientific data and metadata
- Review by editorial staff

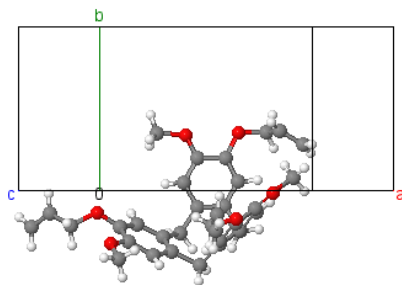
Assignment of chemistry is required to make data findable, interoperable and reusable



Crystal CIFs

- Associated Hyperlink: [http://www.ccdc.cam.ac.uk/services/structure\\_request?pid=ccdc:148418&sid=ChemSpider](http://www.ccdc.cam.ac.uk/services/structure_request?pid=ccdc:148418&sid=ChemSpider)  
Comments: Structure reported in RSC article <http://dx.doi.org/10.1039/B000825G> and hosted by CCDC with reference 148418  
Unit cell:  $a=14.4429(5)\text{\AA}$ ,  $b=8.0609(3)\text{\AA}$ ,  $c=24.3908(7)\text{\AA}$ ,  $\alpha=90.00^\circ$ ,  $\beta=99.510(2)^\circ$ ,  $\gamma=90.00^\circ$ ,  $T=123(2)\text{K}$ , space group  $P21/n$ ,  $Z=4$   
Approved: No  
Submitted by: Aileen Day

HM: P21/n  
a=14.443Å  
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c=24.391Å  
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 $\beta=99.510^\circ$   
 $\gamma=90.000^\circ$

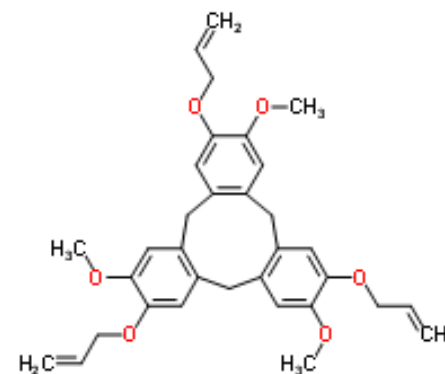


Bulk identification of links between ChemSpider molecules and CCDC Crystal Structures will be facilitated by InChIs.

Other opportunities:

- PubChem
- UniChem (EBI)
- Wikipedia
- Chemical Abstracts

I U P A C



Standard InChI:

InChI=1S/C33H36O6/c1-7-10-37-31-19-25-13-23-17-29(35-5)33(39-12-9-3)21-27(23)15-24-18-30(36-6)32(38-11-8-2)20-26(24)14-22(25)16-28(31)34-4/h7-9,16-21H,1-3,10-15H2,4-6H3

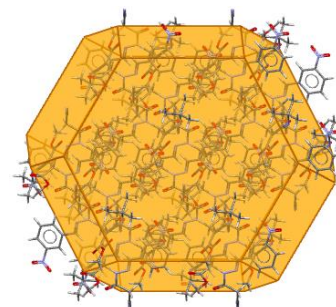
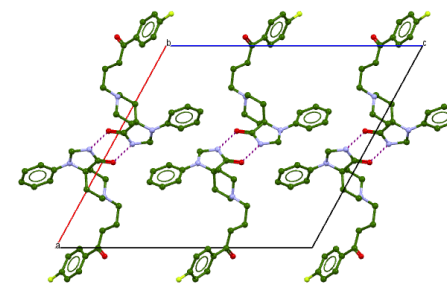
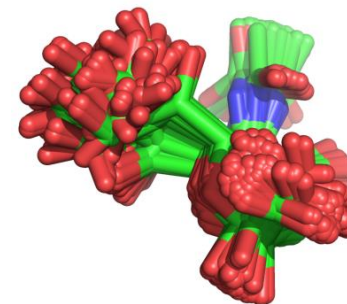
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# Knowledge-based Solutions

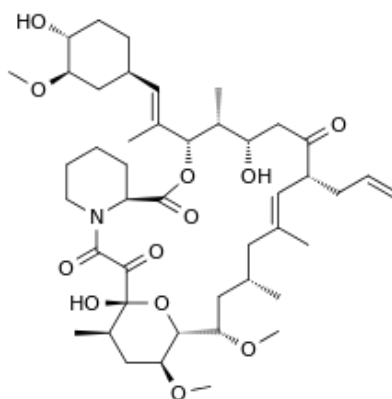
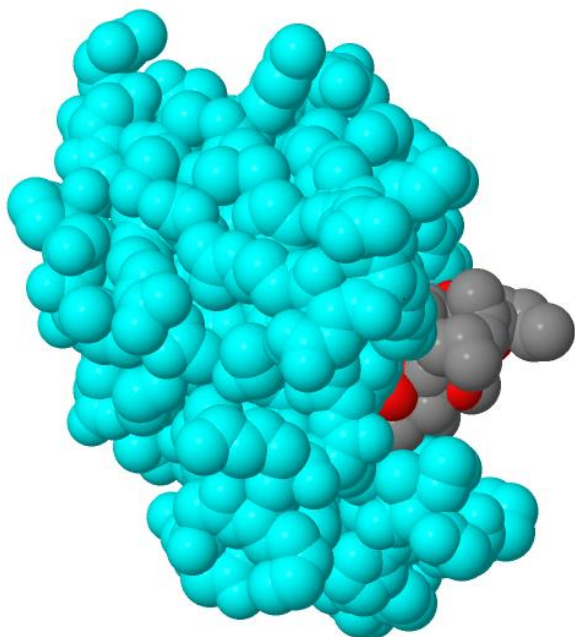
- Provide insights into
  - molecular dimensions and shape
  - molecular interactions
- Applicable to
  - drug design and development
  - design of new materials
  - crystal engineering
  - structure validation





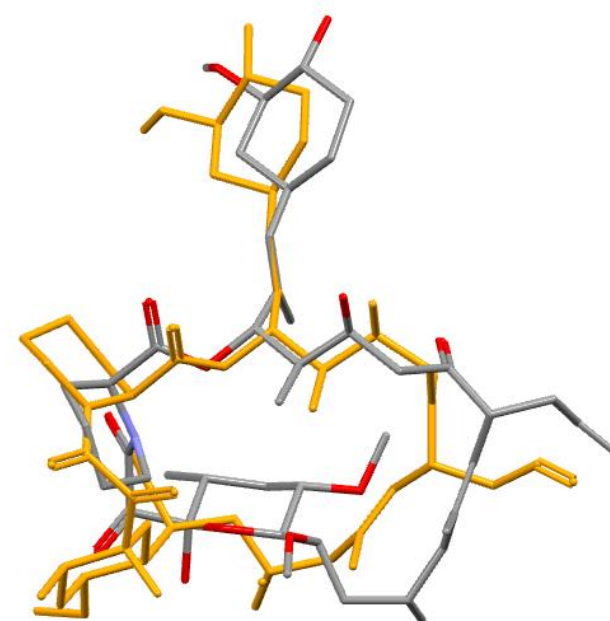
# Crystal Structure Knowledge Helps Drug Design

PDB 1BKF complexed with PDB Ligand FK5



Tacrolimus: An immunosuppressive drug. Also used in the treatment of skin conditions.

CSD FINWEE10 overlayed on PDB Ligand FK5



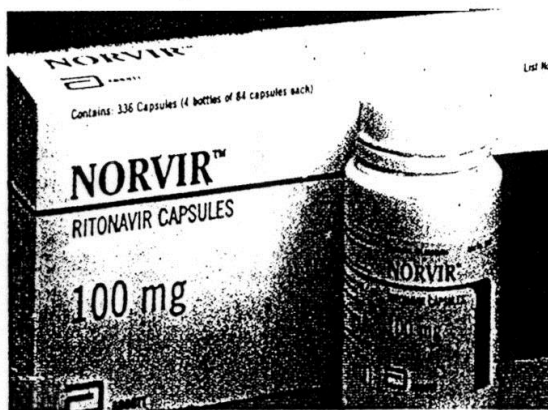
Understanding factors that influence the shape of molecules helps identify better drug candidates



# Crystal Structure Knowledge Mitigates Risk

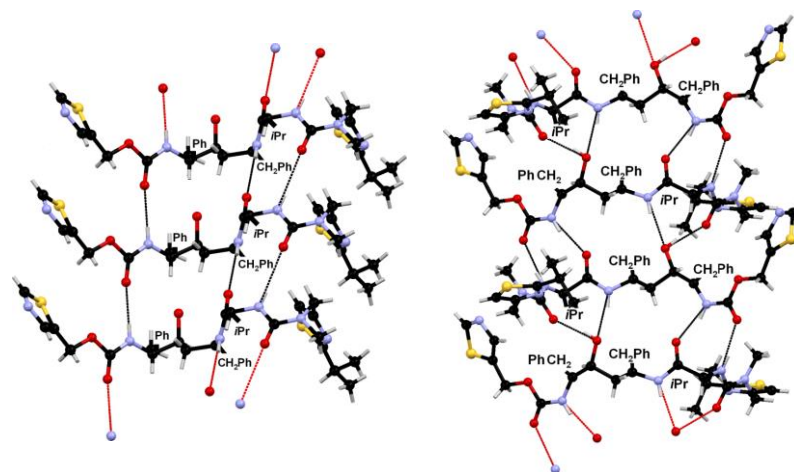
## Manufacturing problems hit Abbott's HIV drug ritonavir

Capsules of Abbott Laboratories' protease inhibitor Norvir (ritonavir) are likely to become unavailable by the middle of August. The company has a problem with the manufacture of the anti-HIV capsules which it cannot resolve at present.



*Capsules unlikely to be available from mid-August*

The problem relates to “undesirable” crystal formation. Abbott says that a series of capsules from a number of marketed batches of capsules were examined and there was no

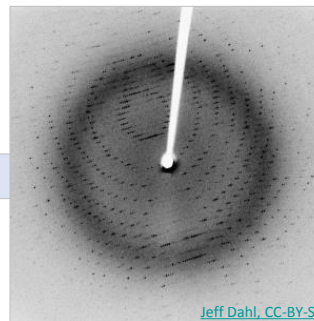
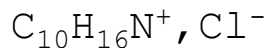


Different crystal forms, different interactions, different solubility, different stability.

Knowing the likelihood of specific molecular interactions occurring helps assess the risk of undesirable crystal formation

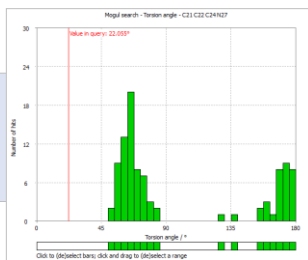
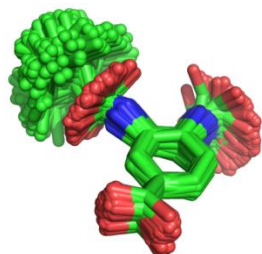


# Experimental Data



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  _atom_site_refinement_flags
  _atom_site_occupancy
  _atom_site_symmetry_multiplicity
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  _atom_site_disorder_group
Cl C1 0.23185(8) 0.78305(9) 0.55574(6) 0.02213(16) Dani d 1 1 . . .
N N1 0.8081(3) 0.6811(3) 0.5969(2) 0.0572(4) Dani d U 1 1 . . .
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```



MIVCUT: (+)-Methamphetamine hydrochloride  
Spacegroup: P21, Cell: a / 7.1022(11)Å b / 7.2949(11)Å c / 10.0121(17)Å, α 90°, β 97.220(4)°, γ 90°

3D viewer

**organic compounds**

Acta Crystallographica Section E  
Structure Reports  
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**Redetermination of (+)-methamphetamine hydrochloride at 90 K**

Patrick Hakey, Wayne Ouellette, Jon Zubieta and Timothy Korter\*

Department of Chemistry, Syracuse University, Syracuse, New York 13244, USA  
Correspondence e-mail: timothy@corry.syr.edu

Received 20 March 2008; accepted 22 April 2008

Key indicators: single-crystal X-ray study; T = 90 K; mean σ(C–C) = 0.004 Å; R factor = 0.052; wR factor = 0.116; data-to-parameter ratio = 13.6.

The title crystal structure (systematic name: N-methyl-1-phenylpropan-2-aminium chloride),  $C_{10}H_{16}N^+Cl^-$ , was originally determined by Simon, Bocskai & Torok [Acta Pharm. Hung. (1987), 67, 75–79] and Nov. K. et al. [Methamphetamine hydrochloride, 1987, 1988, 1989, 1990, 1991, 1992, 1993, 1994, 1995, 1996, 1997, 1998, 1999, 2000, 2001, 2002, 2003, 2004, 2005, 2006, 2007, 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019, 2020].

**Data collection**  
Bruker APEX CCD area-detector  
diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{min} = 0.022$ ,  $T_{max} = 0.971$

**Refinement**  
 $R_{int} = 0.051$   
 $wR_{int} = 0.117$   
 $S = 1.05$   
2720 reflections  
174 parameters  
1 restraint

**Table 1**  
Hydrogen-bond geometry (Å, °).

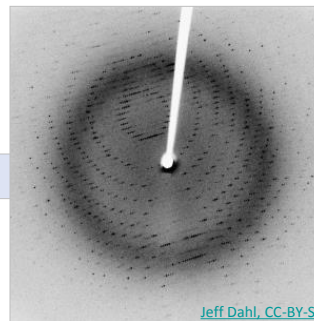
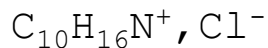
D—H...A	D—H	H...A	D...A
N1—H1D...Cl1 <sup>a</sup>	0.08 (4)	0.234 (6)	0.312 (6)
N1—H1E...Cl1 <sup>a</sup>	0.08 (5)	0.222 (6)	0.304 (6)

Symmetry codes: (i)  $x \rightarrow x + 1, y \rightarrow y - 1, z \rightarrow z + 1$ ; (ii)  $x \rightarrow x + 1, y \rightarrow y, z \rightarrow z + 1$ .

# Structural Knowledge

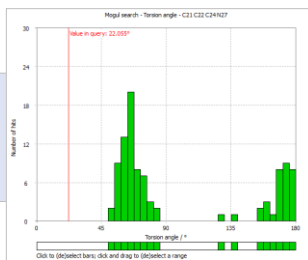
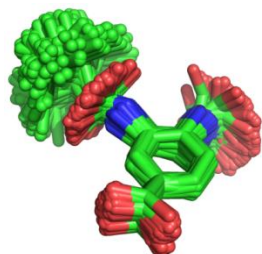


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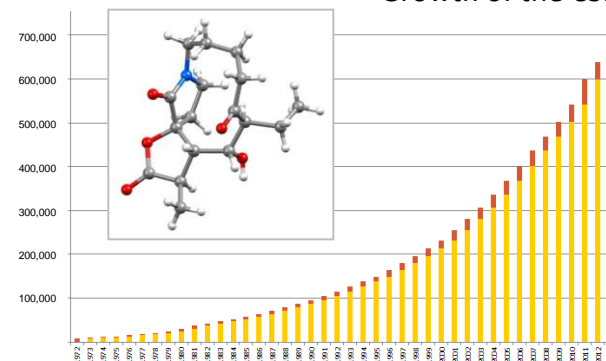
# Crystal Structure Growth

- Cambridge Structural Database
  - organic and metal-organic compounds
  - **750,422 structures**
- Inorganic Crystal Structure Database
  - inorganic compounds
  - **173,473 structures**
- Protein Data Bank
  - biological macromolecules
  - **105,025 structures**

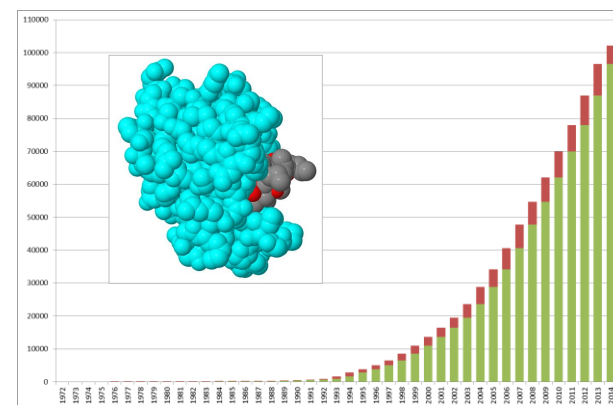
ESTABLISHED 1965



Growth of the CSD



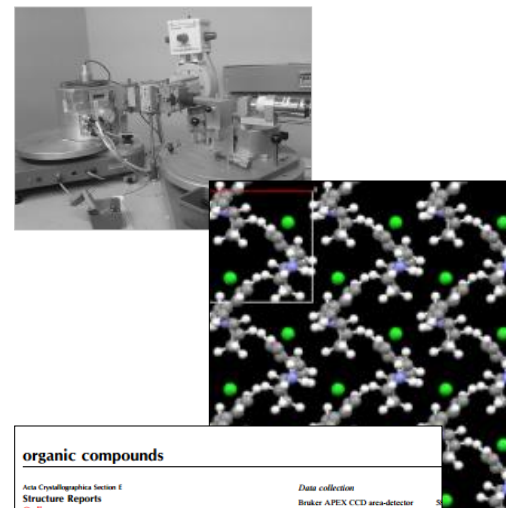
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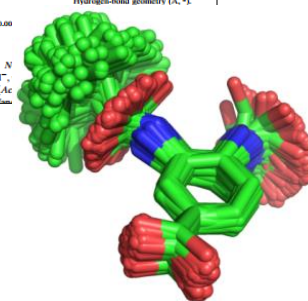


# A Collaborative Journey

- Academic research community
- Instrument manufacturers
- Publishers
- Data repositories
- Industrial partners
- Scientific software vendors



organic compounds	
<small>Acta Crystallographica Section E Structure Reports Online ISSN 1600-5388</small>	<small>Data collection Bruker APEX CCD area-detector diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2002) <math>T_{min} = 0.022</math>, <math>T_{max} = 0.971</math></small>
<b>Redetermination of (+)-methamphetamine hydrochloride at 90 K</b>	<small>Refinement <math>R[F^2 &gt; 2\sigma(F^2)] = 0.051</math> <math>wR(F^2) = 0.117</math> <math>S = 1.05</math> 2720 reflections 174 parameters 1 restraint</small>
<small>Patrick Hakey, Wayne Ouellette, Jon Zubieta and Timothy Korter*</small>	<small>Table 1 Hydrogen-bond geometry (Å, °)</small>
<small>Department of Chemistry, Syracuse University, Syracuse, New York 13244, USA Correspondence e-mail: inkorter@sy.edu Received 20 March 2008; accepted 22 April 2008</small>	
<small>Key indicators: single-crystal X-ray study; T = 90 K; mean <math>\sigma(C) = 0.00</math> 0.052; <math>wR</math> factor = 0.118; data-to-parameter ratio = 15.6.</small>	
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## We've come a long way...

- Essential foundations
  - standard file formats
  - rich metadata
  - standard identifiers
  - interoperable services
  - sustainability

### RDA-WDS Data Publishing Activities

- Workflows
- Publishing Data Services
- Data Bibliometrics
- Cost Recovery





## ... there are new roads ahead

- Essential foundations
  - standard file formats
  - rich metadata
  - standard identifiers
  - interoperable services
  - sustainability
  
- Future opportunities
  - unpublished data
  - enhanced deposition services
  - new publication pathways
  - data metrics and impact

### RDA-WDS Data Publishing Activities

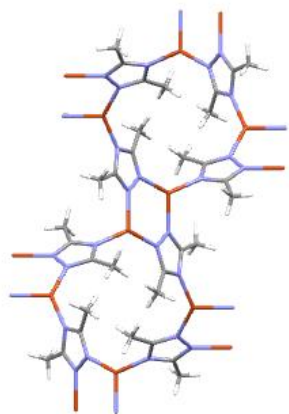
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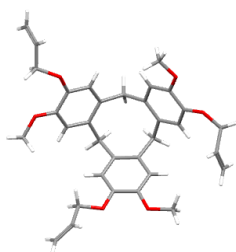
# Time's Up!

- **About your speaker:**

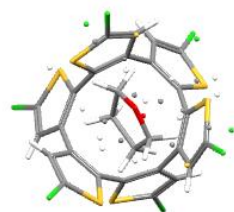
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- **Company:** Cambridge Crystallographic Data Centre
- **Email:** [bruno@ccdc.cam.ac.uk](mailto:bruno@ccdc.cam.ac.uk)
- **Social Media:** @ijbruno @ccdc\_cambridge



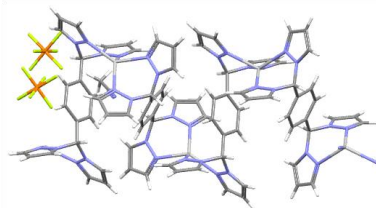
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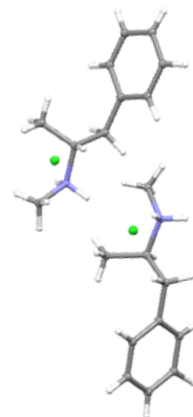
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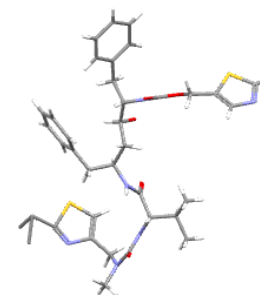
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