IUCrData - update on data publication and practices at the IUCr

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‘it is essential that the methods by which the results have been gained, and the data on which they are founded, should be fully published so that they may be subjected to the expert criticism necessary to assess their reliability.’

Editorial preface, *Acta Cryst*. (1948). **1**, 1

History of data publishing at the IUCr

- **1983** Launch of *Acta Crystallographica Section C* (incorporating *Crystal Structure Communications* published by University of Parma since 1972)
- **1987** Vote at Perth Congress to establish Working Party for Crystallographic Information
- **1991** CIF: facilitated machine submission and automatic article generation
- **1996** Mandatory CIF submission
- **1997** CIF-access papers introduced in *Acta C*
- **1999** *Crystallography Journals Online*
- **2000** *Acta C* included in *Crystallography Journals Online*, electronic papers replace CIF-access

CIF access

Acta Cryst. (1997). C**53**, IUC9700001 [doi:10.1107/S0108270197099526]

5-Phenyldibenzophosphole, Polymorph 2

P. R. Meehan, E. C. Alyea and G. Ferguson

Abstract

Polymorph 1 of the title compound, $C_{18}H_{13}P$, has been described previously (Alyea, Ferguson & Gallagher, 1992) and crystallizes in space group $Pca2_1$ with two independent molecules in the asymmetric unit. The present polymorph 2 was obtained serendipitously; it crystallizes in space group $P2_12_12_1$ with one molecule in the asymmetric unit. The pendant phenyl ring of polymorph 2 adopts a slightly different orientation than that reported for the two independent molecules in polymorph 1.

Comment

X-ray analysis of crystals from what proved to be a wrongly labelled sample bottle has shown that they were a second polymorph of 5-phenyldibenzophosphole (I) whose structure we have reported previously (Alyea, Ferguson & Gallagher, 1992) in space group $Pca2_1$ with two independent molecules in the asymmetric unit. The polymorph reported here crystallizes in the chiral space group $P2_12_12_1$ with one molecule in the asymmetric unit.

A view of the molecule is in Fig. 1. Molecular dimensions are very similar to those reported for polymorph 1, with P—C in the range 1.808 (3) to 1.828 (3)Å (1.808 (9) to 1.846 (10)Å in polymorph 1). The orientation of the phenyl ring relative to the benzophosphole ring is defined by *e.g.* the torsion angle C11—P1—C31—C32 68.3 (3)°. In polymorph 1, the corresponding angles for the two independent molecules are 32.0 (5) and 34.1 (6)° respectively. Examination of the structure with *PLATON* (Spek, 1996*a*) showed that there were no solvent accessible voids in the crystal lattice.

Experimental

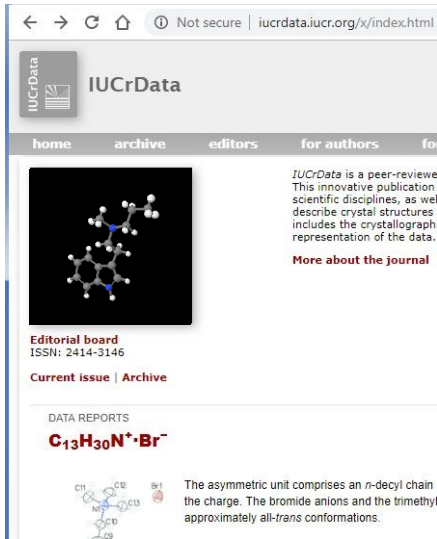
The compound was prepared as described previously (Alyea, Ferguson & Gallagher, 1992) and recrystallized from dichloromethane.

Refinement

Molecules of (I) are achiral but crystallized in the orthorhombic system in the chiral space group $P2_12_12_1$. For the data collection, reflections in the range 0 to +h, 0 to +k and −l to +l were measured to ensure a full Friedel set. During data

History of data publishing at the IUCr

- **2001** *Acta Crystallographica Section E: Structure Reports Online* launched
- **2007** Transition to open access, new shorter format introduced
- **2010** Editorial published reporting systematic scientific fraud in *Acta E*
- **2012** *Acta E* delisted from Science Citation Index
- **2014** Relaunch of *Acta E* with new paper formats, longer *Research Communications* and short *Data Reports*, and new subtitle *Crystallographic Communications*
- **2016** *IUCrData* launched with aim of *'providing short descriptions of crystallographic datasets and datasets from related scientific disciplines*', the first phase providing a home for the short crystal structure reports previously published in *Acta E*



FAIR data

IUCr policy was always to allow free access to data

- Coordinates, anisotropic thermal parameters, structure factors
- In print days, knowledge of the existence of these depended on subscribing to the journal
- Since approximately 1991, these were exposed *via* online tables of contents (*gopher* predating invention of Web!)
- Since 1999 (*Crystallography Journals Online*) fully accessible including historical content
- Structure factors mandatory as electronic files since 1997
- Recommendation for links to primary data following DDDWG activities (2017)

IUCrData objectives

- To provide a new source of revenue
- To develop data publishing at the IUCr
- To get as much data into the public domain as possible
- To create a new home for *Acta E* and other IUCr datasets
- To try to ensure the quality of data in the public domain
- To promote data and journal articles already published by the IUCr
- To investigate ideas for deposition of novel types of data and large data sets
- To provide another mechanism to access the data held by the IUCr

Features of a data article in *IUCrData*

- Title
- Authors
- Abstract
- Keywords
- Peer-reviewed short text
- Figure(s) including an ellipsoid plot
- Chemical scheme
- Tabular information
- Acknowledgements
- References

- Supporting information, *e.g.* text files, videos *etc*.
- PDF version
- Interactive HTML version with integrated supporting information
- CIF or other data set (*e.g.* mmCIF, crystallization data *etc*.)
- Structure factors
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Crystal structure of a
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Tim Peppel, Sabine M. L. Detert, Christian Vo

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wm4108

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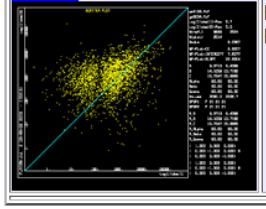
Criteria used for search: cell parameters within 3% of largest cell length and all angles within 2°

Datablock: I						
Co-editor code	**Authors**	**Reference**	**Sum formula**	**Space group**	**Cell parameters**	**Title**
wm4108	**Peppel, Tim; Detert, Sabine M. L.; Vogel, Christian; K\"ockerling, Martin***	**THIS ARTICLE**		**P 21 21 21**	**9.371,14.106,15.735 [90.00,90.00,90.00]**	**Crystal structure of a salt with a cobalt(II) complex anion and a protonated sugar cation: (K(H~2~O)~2~)(GlcN--H)[Co(NCS)~4~]**
Possible Matches						
ya6034 	Peeters, Oswald M.*; Blaton, Norbert M.; De Ranter, Camiel J.	Acta Cryst. E57 (2001), o723--o724	C21 H23 N5 S1	P 21 21 21	9.444,13.725,15.703 [90.00,90.00,90.00]	(+)-N-{4-[(1S,2S)-2-(Dimethylamino)-1-(1H-imidazol-1-yl)propyl]phenyl}-2-benzothiazolamine Internal code of the Janssen Research Foundation: R116010

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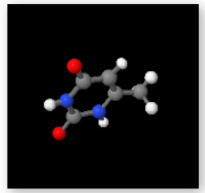

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ISSN: 2414-3146

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These pages give links to instructions on how to prepare your data article for submission and tools to help you do this, details of what to do about supporting information, and utilities to track the status of your data article once it has been accepted and is in production.

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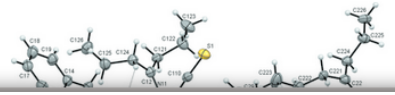
$[Co(NCS)_2(C_{15}H_{22}N_2O_2)_2]$



The title compound, $[Co(NCS)_2(C_{15}H_{22}N_2O_2)_2]$, crystallizes with two half molecules in the asymmetric unit, which are completed by crystallographic

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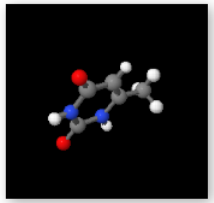

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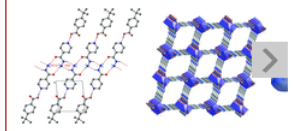

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Andrew R. Chadeayne,[a]* James A. Golen[b] and David R. Manke[b]

[a]CaaMTech, LLC, 58 East Sunset Way, Suite 209, Issaquah, WA 98027, USA, and [b]Department of Chemistry & Biochemistry, University of Massachusetts Dartmouth, 285 Old Westport Road, North Dartmouth, MA 02747, USA

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Edited by I. Brito, University of Antofagasta, Chile (Received 24 June 2019; accepted 4 July 2019; online 9 July 2019)

The title compound {systematic name: [2-(1*H*-indol-3-yl)ethyl](methyl)propylamine}, $C_{14}H_{20}N_2$, has a single molecule in the asymmetric unit. The molecules in the unit cell are held together in infinite one-dimensional chains along [010] through N—H···N hydrogen bonds between indole H atoms and trialkylamine N atoms.

Keywords: **crystal structure**; **tryptamines**; **indoles**; **hydrogen bonding**.

CCDC reference: 1938495

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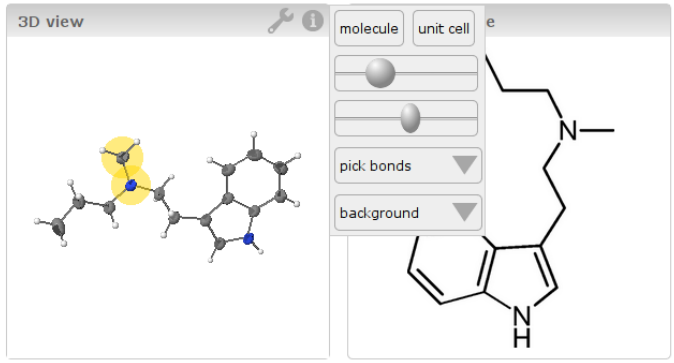

N2-C14 1.467Å

Structure description

N-Methyl-*N*-propyltryptamine (MPT) is a structural analog of *N*,*N*-dimethyltryptamine (DMT), which is a well known `psychedelic' molecule found in a variety of naturally occurring organisms, including plants, animals, and funghi, including mushrooms. In humans, DMT is the only known endogenous mammalian *N*,*N*-dimethylated trace amine (Fontanilla *et al.*, 2009). Naturally occurring tryptamines (*e.g.* DMT, psilocybin, 5-methoxy-*N*,*N*-dimethyltryptamine) and their synthetic derivatives (*e.g.* psilacetin, MPT) have garnered considerable attention of late due to new evidence demonstrating their efficacy in treating mood (*e.g.* anxiety and depression) and post traumatic stress disorders (PTSDs) (Aixalà *et al.*, 2018; Cameron *et al.*, 2019).

Psilocybin, isolated from the so-called `magic' mushrooms, is perhaps the best known prodrug of the serotonin 2a agonist psilocin (Nichols, 2016). Recent studies indicate that psilocin (and its prodrugs like psilocybin and psilacetin) could provide effective treatment for mood

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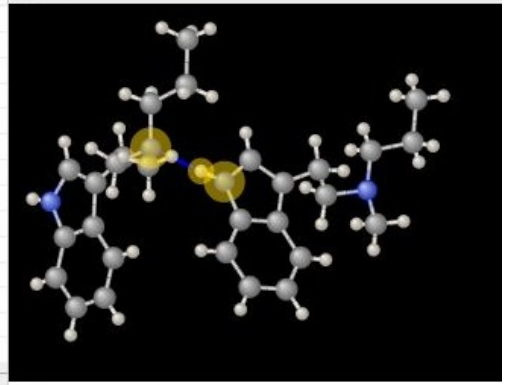
C6—C5—H5	119.4
C7—C6—H6	120.3
C5—C6—C7	119.31 (12)
C5—C6—H6	120.3
C1—C8—C7	105.96 (10)
C1—C8—C9	127.19 (12)
C7—C8—C9	126.70 (11)
C8—C9—H9A	108.9
C8—C9—H9B	
C8—C9—C10	
N1—C1—C8—C7	
N1—C1—C8—C9	
N1—C2—C3—C4	
N1—C2—C7—C6	
N1—C2—C7—C8	
N2—C11—C12—C13	
C1—N1—C2—C3	
C1—N1—C2—C7	
C1—C8—C9—C10	
C2—N1—C1—C8	
C2—C3—C4—C5	
C2—C7—C6—C5	
C2—C7—C8—C1	
C2—C7—C8—C9	

Structure I



N1-H1-N2 = 179.8°

Hydrogen-bond geometry (Å, º)

D—H···*A*

N1—H1···N2^{i}

Symmetry code: (i) −*x*+1/2, *y*+1/2, *z*.

Development of data publishing

- Launch of *IUCrData:* a peer-reviewed service providing a home for the very short articles previously published in *Acta E*
- Enhancement of search and visualisation features across structural data sets housed on the IUCr servers
- Extend data management services to novel types of data
- Host or provide discovery mechanisms for experimental raw data sets (primarily diffraction images)

IUCrData BioData

Crystallization and X-ray analysis of D-threonine aldolase from *Chlamydomonas reinhardtii*

Yuki Hirato,[a] Masaru Goto,[b] Mayumi Tokuhisa,[a] Minoru Tanigawa[a] and Katsushi Nishimura[a,c]*

[a]Department of Materials and Applied Chemistry, College of Science and Technology, Nihon University, 1-8-14 Kanda-Surugadai, Chiyoda-Ku, Tokyo 101-8308, Japan, [b]Department of Biomolecular Science, Faculty of Science, Toho University, 2-2-1 Miyama, Funabashi, Chiba 274-8510, Japan, and [c]Department of Biotechnology and Material Chemistry, Junior College, Nihon University, 7-24-1 Narashinodai, Funabashi, Chiba 274-8501, Japan. *Correspondence e-mail: nishimura.katsushi@nihon-u.ac.jp

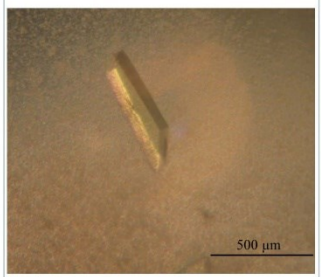
Received 15 November 2016
Accepted 29 December 2016

Edited by A. Nakagawa, Osaka University, Japan

Keywords: D-threonine aldolase; *Chlamydomonas reinhardtii*; D-amino acids; crystallization.

D-Threonine aldolase from the green alga *Chlamydomonas reinhardtii* (CrDTA) catalyzes the interconversion of several β-hydroxy-D-amino acids (*e.g.* D-threonine) and glycine plus the corresponding aldehydes. Recombinant CrDTA was overexpressed in *Escherichia coli* and purified to homogeneity; it was subsequently crystallized using the hanging-drop vapour-diffusion method at 295 K. Data were collected and processed at 1.85 Å resolution. Analysis of the diffraction pattern showed that the crystal belonged to space group *P*1, with unit-cell parameters a = 64.79, b = 74.10, c = 89.94 Å, α = 77.07, β = 69.34, γ = 71.93°. The asymmetric unit contained four molecules of CrDTA. The Matthews coefficient was calculated to be 2.12 Å^3 Da^{-1} and the solvent content was 41.9%.

Crystal



Sequence

```
MRALVSKARLAHSVGGRASQATRCAATISASRAP
  AHLGDALHDVDTPALILDLDAFDRNCEKLKGV
  MAGFPGVAVRPHAKAHKCAEVARRQLQLLGAK
  GVCCQKVIEAEAMAEGGVSDLLLSNEVIAPRK
  IDRLVGLAAAGARVGVCYEREDNLRQLNAAAA
  ARGTHLDVLVELNVGQDRCGVNSADEVVQLAR
  AAAGLDNVRFAGIQAYHGGLQHVRDPRDRAQR
  VGQVVGRARAAVDALKAAGLPCDTVTGGGTGT
  YRVEAASGVFTEVQPGSFAFSDADYARNLQED
  GGVGEWEQSLWVLTQVMSVTPARGLAVVDAGT
  KAVSLDSGPPRLPPAFEAAYGTMMEYGSGGDE
  HGKLMWPQGAYQLPMSLPEVGSLLLLQPGHCD
  PTVNLYDWLVAARRQQGGQQQGGVDGWRVEAV
  WPIRGRGPGQ
```

1. Introduction

Threonine contains two chiral centres and exists as four stereoisomers (L-, L-*allo*-, D- and D-*allo*-threonine). The interconversion of several β-hydroxy-α-amino acids (*e.g.* threonine) and glycine plus the corresponding aldehydes (*e.g.* acetaldehyde) is catalyzed by threonine aldolases (Liu, Dairi *et al.*, 2000). In general, threonine aldolases are classified into L- and D-type enzymes according to their stereospecificity at the α-carbon. Depending on their stereospecificity at the β-carbon of threonine, L-type threonine aldolases can be further classified into three types (Dückers *et al.*, 2010):

biodata reports

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Crystallization and X-ray analysis of D-threonine aldolase from *Chlamydomonas reinhardtii*

Yuki Hirato,[a] Masaru Goto,[b] Mayumi Tokuhisa,[a] Minoru Tanigawa[a] and Katsushi Nishimura[a,c]*

[a]Department of Materials and Applied Chemistry, College of Science and Technology, Nihon University, 1-8-14 Kanda-Surugadai, Chiyoda-Ku, Tokyo 101-8308, Japan, [b]Department of Biomolecular Science, Faculty of Science, Toho University, 2-2-1 Miyama, Funabashi, Chiba 274-8510, Japan, and [c]Department of Biotechnology and Material Chemistry, Junior College, Nihon University, 7-24-1 Narashinodai, Funabashi, Chiba 274-8501, Japan. *Correspondence e-mail: nishimura.katsushi@nihon-u.ac.jp

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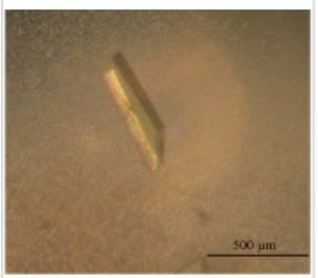
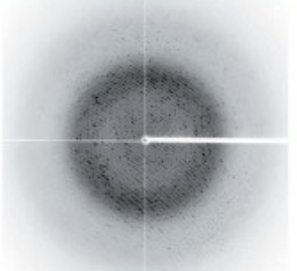
Crystal



Diffraction pattern



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Ambiguity of DOIs

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- Does not guarantee that the **content** is persistent
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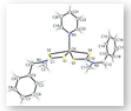


Bis(*N*-benzyl-*N*-methyldithiocarbamato-$\kappa^2 S,S'$)(pyridine-κN)cadmium(II)

M. A. Ehsan, M. Mazhar and E. R. T. Tiekink

The title compound, $[Cd(C_9H_{10}NS_2)_2(C_5H_5N)]$, features a five-coordinate Cd^{II} atom, being coordinated by two nearly symmetrically chelating dithiocarbamate ligands and a pyridine N atom. The resulting NS_4 donor set defines a distorted coordination geometry tending toward square pyramidal. In th packing, centrosymmetric ten-membered $\{\cdots HCNCS\}_2$ synthons arise as a result of methylene-C-H···S int These are connected into layers parallel to (10-2) *via* weak methyl-C-H···π(phenyl) interactions.

Keywords: **crystal structure**; **cadmium**; **dithiocarbamate**.

Read article **Similar articles**

Supporting information

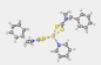
CIF _data — Crystallographic Information File (CIF) https://doi.org/10.1107/S2414314615024293/sj4002sup1.cif
Contains datablocks I, global

HKL _index_h — Structure factor file (CIF format) https://doi.org/10.1107/S2414314615024293/sj4002Isup2.hkl
Contains datablock I

CCDC reference: 851623

checkCIF report

3D view



Full crystallographic data

Supporting information

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Contains datablocks I, global

HKL _index_h — Structure factor file (CIF format) https://doi.org/10.1107/S2414314615024293/sj4002Isup2.hkl
Contains datablock I

Where does the DOI point?

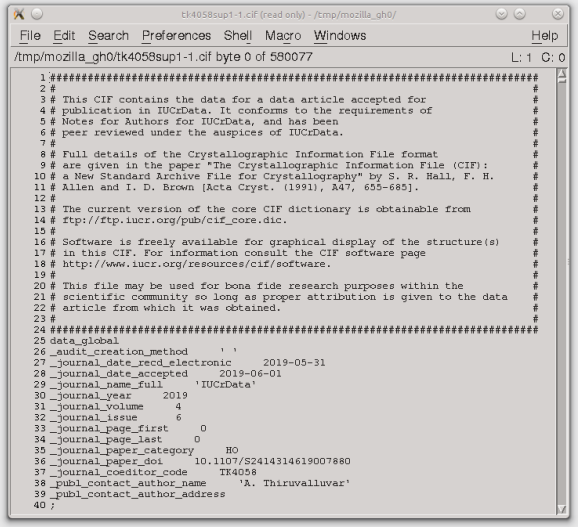
- Following a CrossRef link associated with an IUCr data set DOI downloads the data file immediately
- Same is true of PDB files

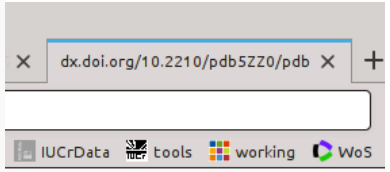
BUT

- https://doi.org//10.1107/S2414314619007880/tk4058sup1.cif downloads a CIF directly from IUCr journals
- http://dx.doi.org/10.2210/pdb5ZZ0/pdb downloads a compressed PDB file directly from PDB
- https://dx.doi.org/10.5517/ccdc.csd.cc20vdhs takes the user to the WebCSD landing page

IUCr journals:

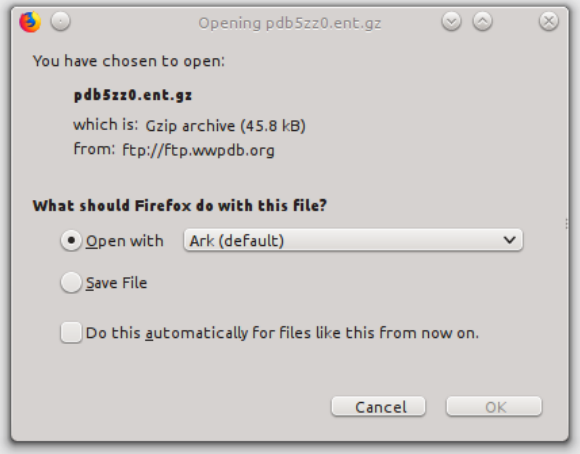
https://doi.org//10.1107/S2414314619007880/tk4058sup1.cif





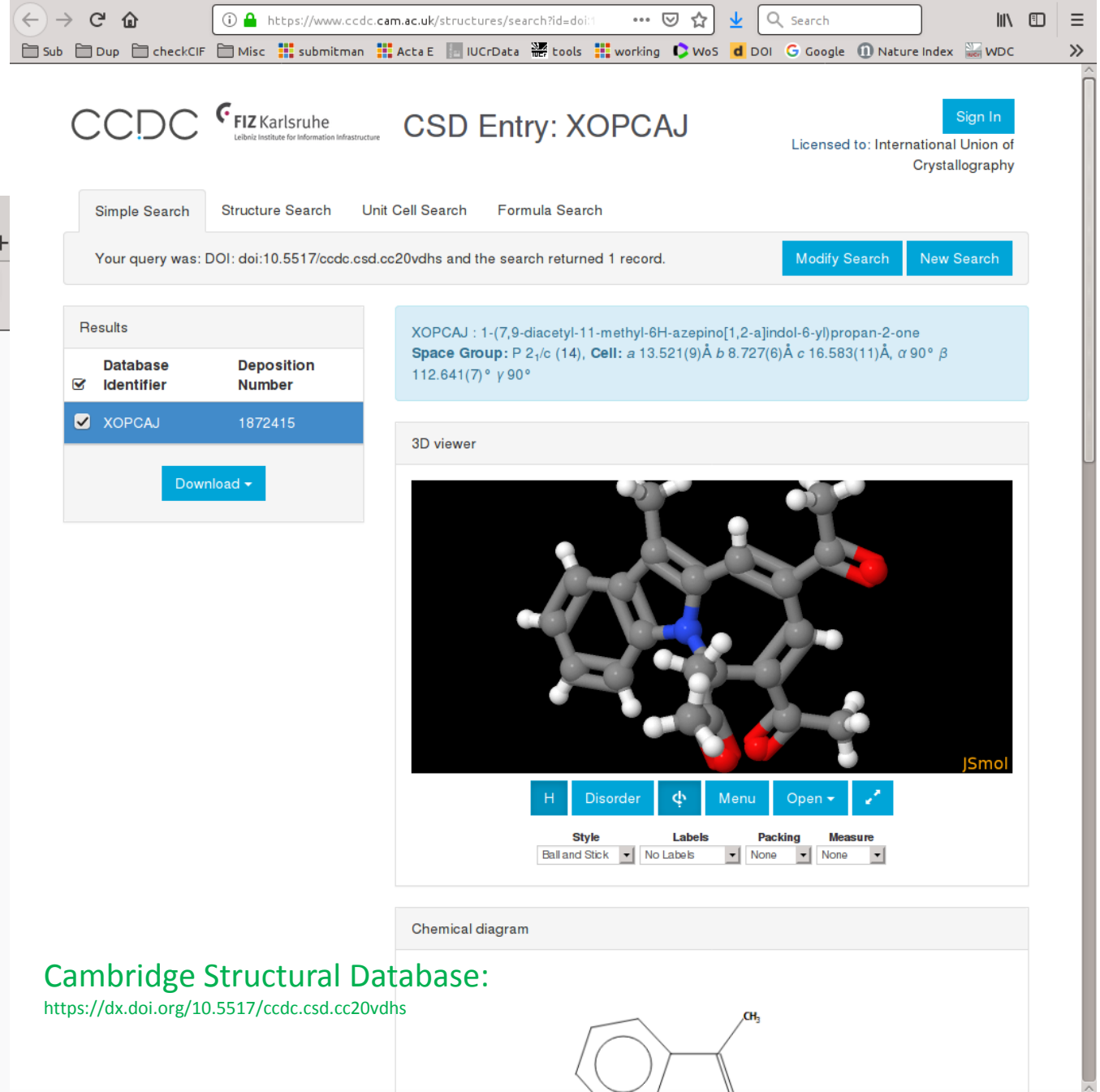
Protein Data Bank:

http://dx.doi.org/10.2210/pdb5ZZ0/pdb



Cambridge Structural Database:

https://dx.doi.org/10.5517/ccdc.csd.cc20vdhs



Towards an API

- Regardless of the decision on the canonical presentation of a DOI, it would be useful to develop an application programming interface:
  - Keyed on DOI
  - Load data in multiple (arbitrary?) formats
    - CIF1
    - CIF2
    - CIF-JSON
    - PDB and alternative macromolecular formats
  - Retrieve data sets matching specific criteria

Pilot project

- IUCr Chester will work on a prototype data harvesting API
- This will inform the direction of development effort in related fields
- Any suggestions for useful features of such an API welcomed

Summary

- The IUCr has always recognised the importance of data
- The journals require deposition of supporting data for published crystal structures - these data sets are thoroughly assessed as part of the publication process.
- *IUCrData* currently publishes short structure reports and is looking to expand into new areas
- The IUCr is participating in a pilot project on a data harvesting API
- We wish to work with the community and welcome suggestions for future developments