



Electronics and  
Computer Science



PSIgate

JISC

## Archiving research data and research publications.

*Dr Leslie Carr, Intelligence, Agents Multimedia, University of Southampton*

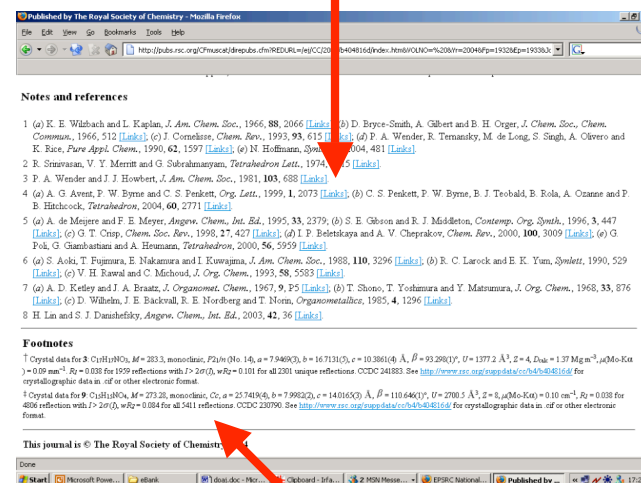
*Dr Simon Coles, School of Chemistry, University of Southampton*

*Dr Liz Lyon, UKOLN, University of Bath*

# Overview

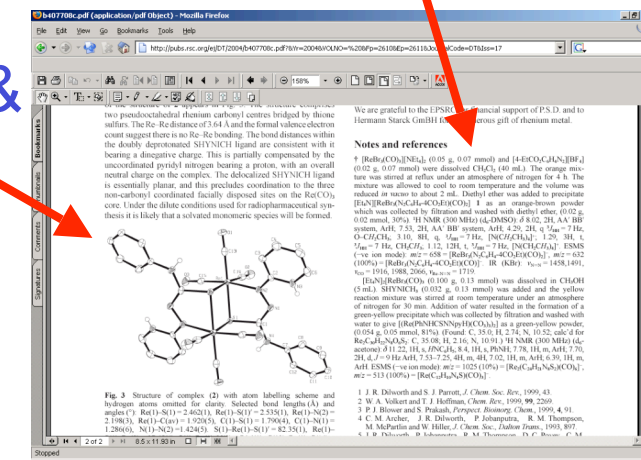
- In an Open Access environment
  - scientific outputs are openly available
  - described by appropriate metadata
  - in Institutional Repositories
  - harvestable by OAI protocols
- Scientists can use the same infrastructure
  - (here eprints.org software and an existing scientific portal service)
  - to provide maximal open access
  - to all their data, as well as their published articles
    - raw data, intermediate calculations, final results
    - in a searchable, accessible form
- BUT this is subject to ongoing investigation.

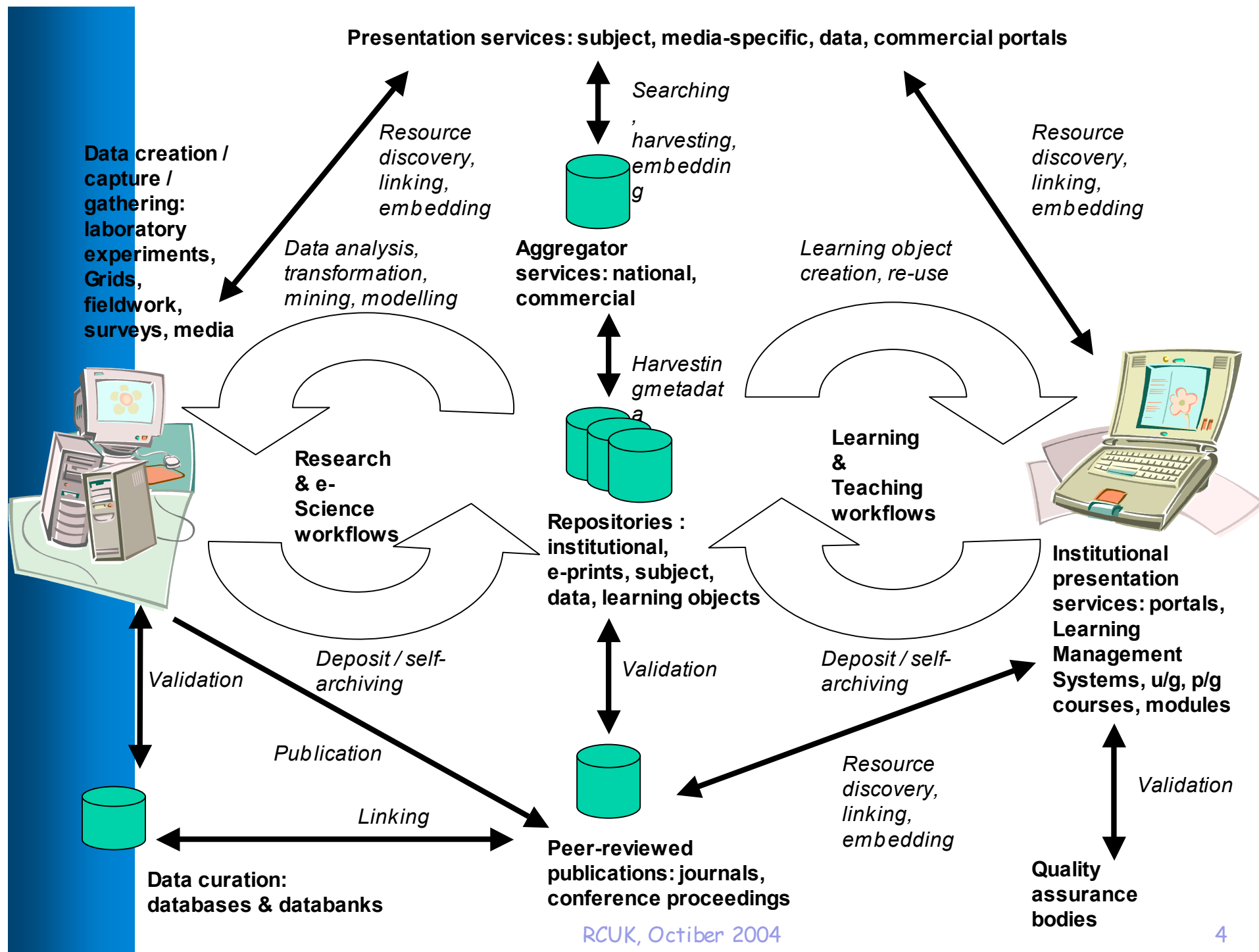
## Hooks into the literature



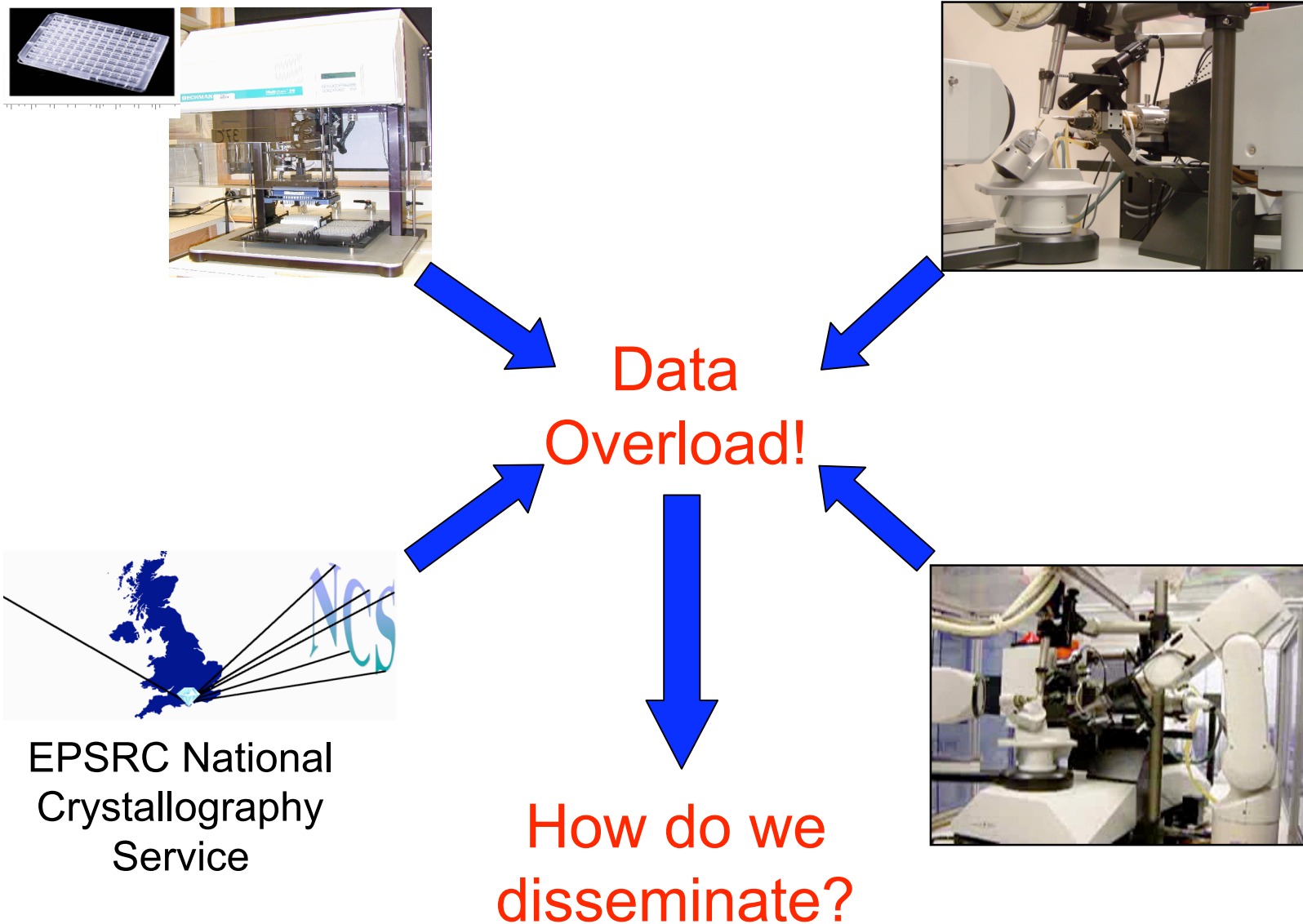
## Raw data!

## Results & derived data

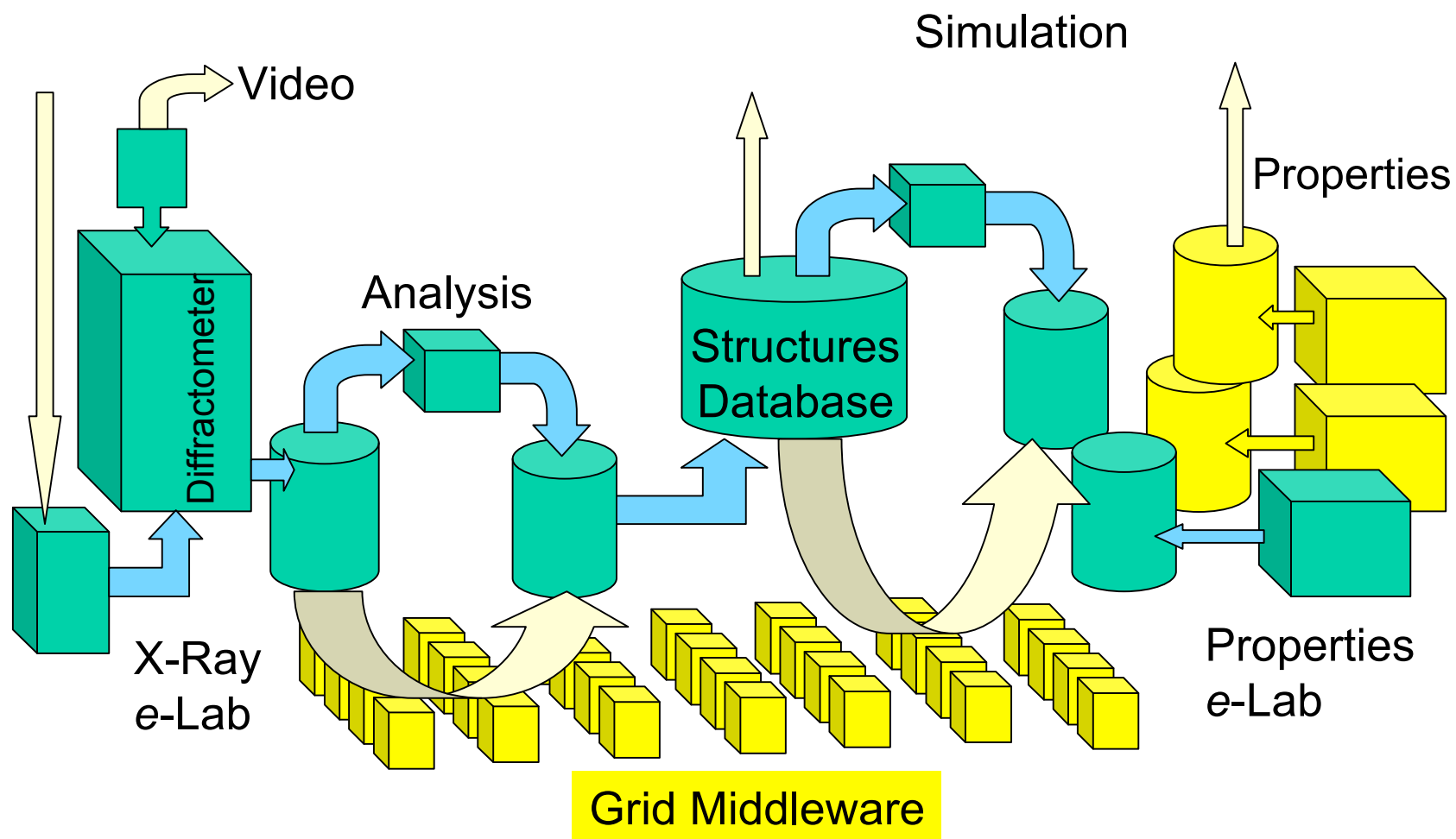




# The data deluge

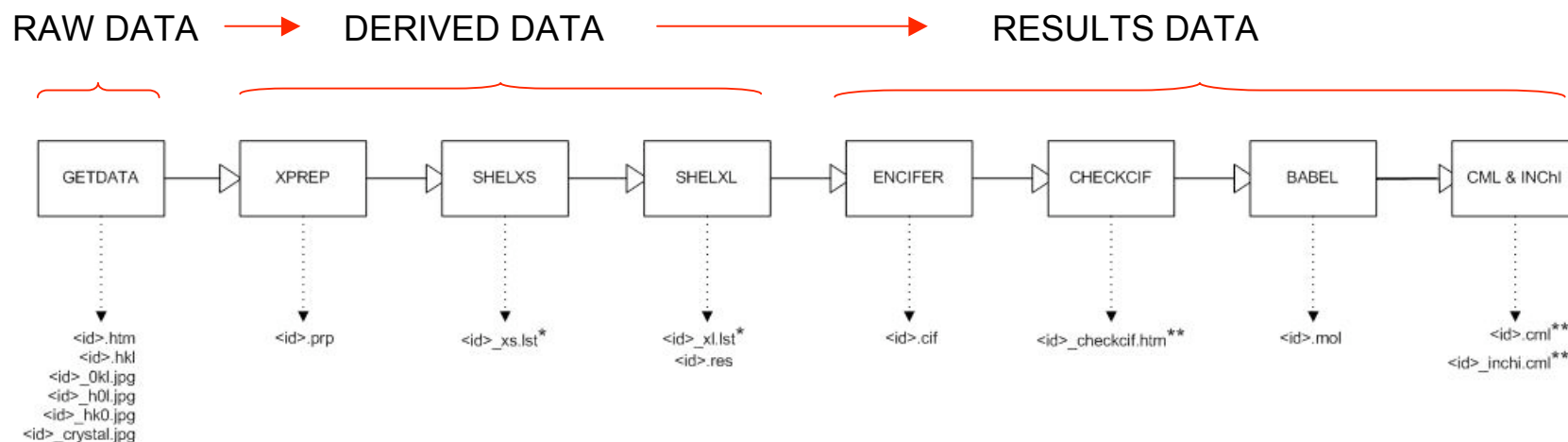


# CombeChem: An EPSRC pilot project



# Crystallography workflow

- **Initialisation:** mount new sample on diffractometer & set up data collection
- **Collection:** collect data
- **Processing:** process and correct images
- **Solution:** solve structures
- **Refinement:** refine structure
- **CIF:** produce CIF (Crystallographic Information File format)
- **Report:** generate Crystal Structure Report





# Deposition into the archive

Southampton Crystal Reports - Core Bibliographic Information - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://ecrystals.chem.soton.ac.uk/perl/users/submit?\_action\_new=1

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 **University of Southampton** Crystal Structure Report Archive 

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### Core Bibliographic Information

Please enter the bibliographic data about your deposit. Fields marked with a \* are fields that must be filled out before your deposit will be accepted.

[< Previous](#) [Save for Later](#) [Next >](#)

**Title of Compound \***  
The title of the Compound  
Example: [N,5-Chloro-pyridin-2-yl-4-fluoro-benzamide](#)

**Authors/Creators \***  
Enter in the format given on the first page or title page. If there are more than four authors, click on the [More Spaces] button.  
Example: [\[Smith\] \[J.P.\] \[j.smith@soton.ac.uk\]](#)  
Example: [\[Chance-Collins\] \[Chris\] \[chris@bar.com\]](#)  
Example: [\[Fu\] \[Yan-Li\] \[\]](#)  
Example: [\[van Hefneer\] \[Ludwig G.\] \[\]](#)

Family Name	Given Name / Initials	Creators email (if known)
1 <a href="#">Coles</a>	<a href="#">Simon J</a>	<a href="#">s.i.coles@soton.ac.uk</a>

Southampton Crystal Reports - Core Bibliographic Information - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://ecrystals.chem.soton.ac.uk/perl/users/submit?\_action\_new=1

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**Institution \***  
Please enter the institution from which the item originated.  
Example: [University of Whitezombia](#)  
[University of Southampton](#)

**Compound Class \***  
[Organic](#)  
[Bio-Organic](#)  
[Organometallic](#)  
[Inorganic](#)

**Empirical Formula \***  
The formula of the compound. Numbers will be displayed as subscript, but not while you are inputting them.

**Uncontrolled Keywords**  
Natural language terms to describe the content of the item

**ICl Code \***  
This code can be obtained from the [Conversion Server at Cambridge](#).



id.zip



# An Archive entry

EBank Southampton - 2-(N-Ferrocenylmethylcarbamoyl)-5-(methoxycarbonyl)-3,4-diphenylpyrrole - Mozilla Firefox

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http://eprints.ebank.ecs.soton.ac.uk/archive/00000025/

**University of Southampton** Crystal Structure Report Archive

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## 2-(N-Ferrocenylmethylcarbamoyl)-5-(methoxycarbonyl)-3,4-diphenylpyrrole

Susanne L. Huth, Michael B. Hursthouse, Simon J. Coles, Mark E. Light, Peter N. Horton, Phil A. Gale, G. Denuault and C. N. Warriner.

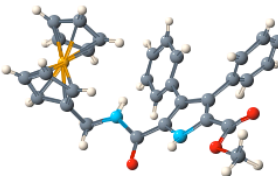
University of Southampton

$C_{30}H_{26}FeN_2O_3$

**CCDC Code:** XUZSUG  
**ICHI Code:** C30H26FeN2O3, 1H3-36-20(35)18-16(14-10H-6H-3H-7H-11H-14)15(13-8H-4H-2H-5H-9H-13)17(33H-18)19(34)32H-12H2-30-28H-26H-27H-29H(30)31(26,27,28,30)21H-22H(31)24H(31)25H(31)23H(21)31

**Compound Class:** Organometallic  
**Keywords:** Supramolecular Chemistry  
**Creation Date:** 31 May 2002  
**Deposited By:** Susanne L. Huth  
**Deposited On:** 10 May 2004

Data collection parameters



Applet: jmol started

Start Pegasus Mail WinGX v1.6... ISSC-XIII - M... EBank Sout... Windows Mes... eBank ISSC a... ECM22EPrint..

### Data collection parameters

Chemical formula	C30 H26 Fe N2 O3
Crystallisation Solvent	
Crystal morphology	
Crystal system	Orthorhombic
Space group symbol	Pbca
Cell length a	6.0816(4)
Cell length b	24.8503(16)
Cell length c	31.120(3)
Cell angle alpha	90.00
Cell angle beta	90.00
Cell angle gamma	90.00
Data collection temperature	120(2)

### Refinement results

Solution figure of merit	
R Factor (Obs)	0.0573
R Factor (All)	0.1185
Weighted R Factor (Obs)	0.1046
Weighted R Factor (All)	0.1243

### Available Files

#### Final Result

02sot064.CIF	19k
02sot064.cml	8k
02sot064_checkcif.html	14k

#### Refinement

02sot064.RES	9k
--------------	----

#### Solution

02sot064.PRP	5k
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#### Processing

02SOT064.HTM	6k
02sot064.HKL	338k

#### Other Files

02sot064.DOC	113k
02sot064.LST	49k

[ecrystals.chem.soton.ac.uk](http://ecrystals.chem.soton.ac.uk)

# All the way back to the underlying data...

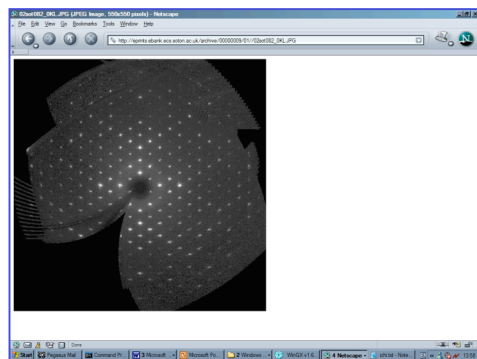
Data collection parameters		Available Files	
Chemical formula	C30 H26 Fe N2 O3	Final Result	
Crystallisation Solvent		02sot064.CIF	19k
Crystal morphology		02sot064.cml	8k
Crystal system	Orthorhombic	02sot064_checkcif.html	14k
Space group symbol	Pbca	Refinement	
Cell length a	6.0816(4)	02sot064.RES	9k
Cell length b	24.8503(16)	Solution	
Cell length c	31.120(3)	02sot064.PRZ	5k
Cell angle alpha	90.00	Processing	
Cell angle beta	90.00	02SOT064.HTM	6k
Cell angle gamma	90.00	02sot064.HKL	338k
Data collection temperature	120(2)	Other Files	
Refinement results		02sot064.DOC	113k
Solution figure of merit		02sot064.LST	49k
R Factor (Obs)	0.0573		
R Factor (All)	0.1185		
Weighted R Factor (Obs)	0.1046		
Weighted R Factor (All)	0.1243		

checkCIF/PLATON report (full structural check)

No syntax errors found. Please wait while processing ....

Datablock: 1

Bond precision:	C-C = 0.0040 Å	Wavelength=0.71073 Å
Cell:	a=8.2045(1) b=10.2618(11) c=10.4118(10)	
	alpha=97.461(1) beta=95.450(1) gamma=98.174(1)	
	Calculated	Reported
Volume	846.14(8)	846.14(8)
Space group	P-1	P-1
Hall group	-P 1	-P 1
Intensity formula	C12 H2 Cl F H2 O	3
Sum formula	C12 H2 Cl F H2 O	3
Mr	230.45	230.45
Mr (calc)	230.45	230.45
Mr (obs)	2	2
Mr (mm)	0.246	0.246
FOOD	206.0	206.0
FOOD	206.41	206.41
Mr (calc)	6.1513	6.1513
Mr (obs)	2059	2059
Mr (calc)	0.966/0.966	0.966/0.966
Mr (obs)	0.966	0.966
Correlation method	"WGT1-SCAN"	
Data completeness	0.97	Theta (max)= 27.49
R(intensity)	0.0331 (1517)	vR2 (reflections)= 0.1292 ( 2449)
R	0.060	Rmax= 135



EPSC National Crystallography Service

Data Collection Summary

Summary report for Directory: diska/02sot082

Report generated 30.09.2002 10:13:51

Unit cell

15124 reflections with 2.91° (data=27.49° (resolution between 7.00Å and 0.77Å) were used for unit cell refinement

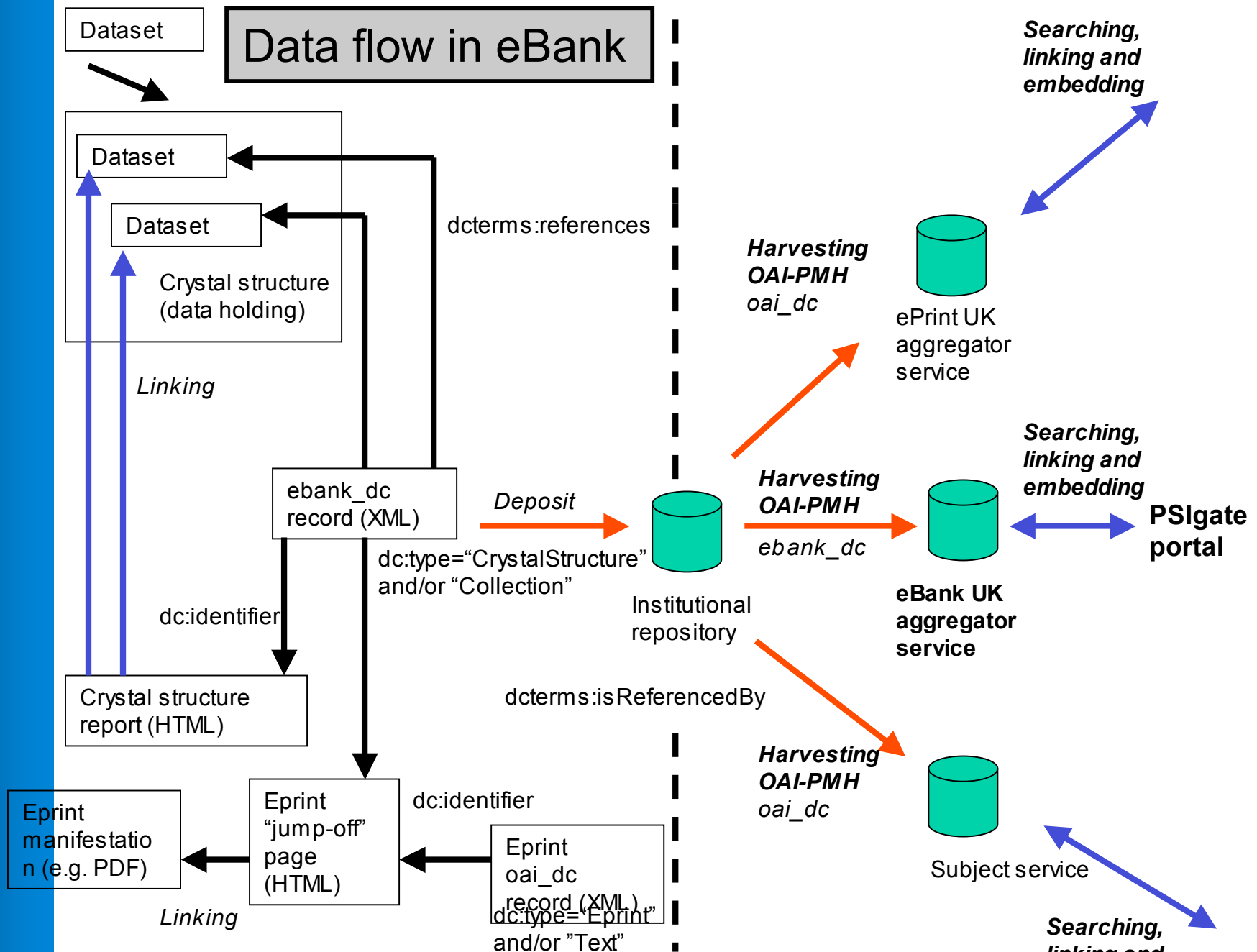
Symmetry used in reduction	P222
a (Angstrom)	9.3113 ± 0.0003
b (Angstrom)	9.8424 ± 0.0003
c (Angstrom)	15.4443 ± 0.0004
alpha (°)	90.000
beta (°)	90.000
gamma (°)	90.000
Volume (Å³)	1415.69 ± 0.07
Minority (°)	0.743 ± 0.002

checkCIF/PLATON report (full structural check)

No syntax errors found. Please wait while processing ....

Datablock: 1

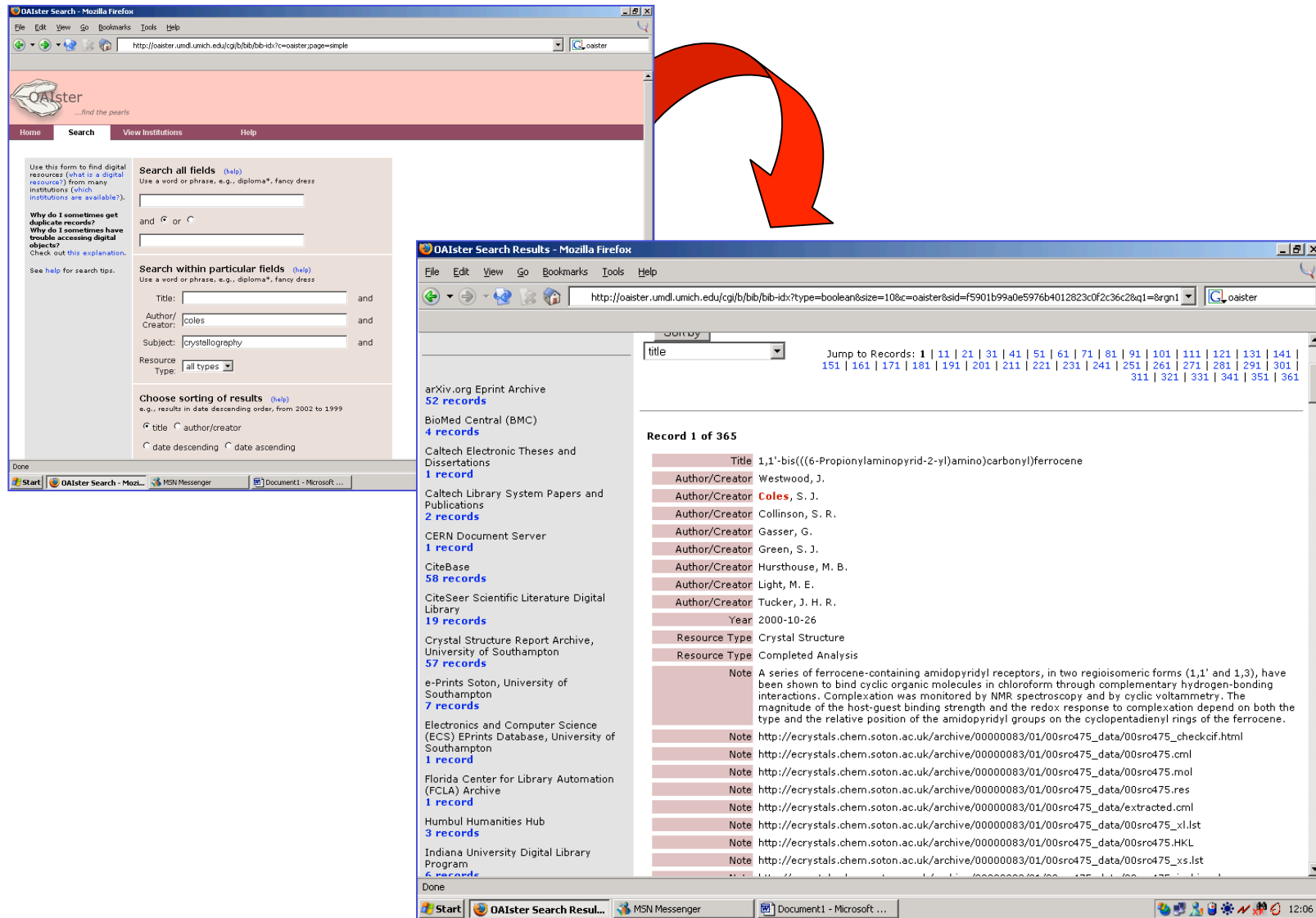
Bond precision:	C-C = 0.0040 Å	Wavelength=0.71073 Å
Cell:	a=8.2045(1) b=10.2618(11) c=10.4118(10)	
	alpha=97.461(1) beta=95.450(1) gamma=98.174(1)	
	Calculated	Reported
Volume	846.14(8)	846.14(8)
Space group	P-1	P-1
Hall group	-P 1	-P 1
Intensity formula	C12 H2 Cl F H2 O	3
Sum formula	C12 H2 Cl F H2 O	3
Mr	230.45	230.45
Mr (calc)	230.45	230.45
Mr (obs)	2	2
Mr (mm)	0.246	0.246
FOOD	206.0	206.0
FOOD	206.41	206.41
Mr (calc)	6.1513	6.1513
Mr (obs)	2059	2059
Mr (calc)	0.966/0.966	0.966/0.966
Mr (obs)	0.966	0.966
Correlation method	"WGT1-SCAN"	
Data completeness	0.97	Theta (max)= 27.49
R(intensity)	0.0331 (1517)	vR2 (reflections)= 0.1292 ( 2449)
R	0.060	Rmax= 135



Model input Andy Powell, UKOLN.

RCUK, October 2004

# Harvesting: OAIster



The screenshot shows the OAIster Search interface in Mozilla Firefox. The search page is on the left, and the search results page is on the right. A red arrow points from the search page to the results page.

**OAIster Search - Mozilla Firefox**

Search all fields (help)  
Use a word or phrase, e.g., diploma\*, fancy dress

Search within particular fields (help)  
Use a word or phrase, e.g., diploma\*, fancy dress

Title:  and  
Author/Creator:  and  
Subject:  and  
Resource Type:

Choose sorting of results (help)  
e.g., results in date descending order, from 2002 to 1999

☐ title ☐ author/creator  
☐ date descending ☐ date ascending

**OAIster Search Results - Mozilla Firefox**

Jump to Records: 1 | 11 | 21 | 31 | 41 | 51 | 61 | 71 | 81 | 91 | 101 | 111 | 121 | 131 | 141 | 151 | 161 | 171 | 181 | 191 | 201 | 211 | 221 | 231 | 241 | 251 | 261 | 271 | 281 | 291 | 301 | 311 | 321 | 331 | 341 | 351 | 361

**Record 1 of 365**

Field	Value
Title	1,1'-bis(((6-Propionylaminopyrid-2-yl)amino)carbonyl)ferrocene
Author/Creator	Westwood, J.
Author/Creator	Coles, S. J.
Author/Creator	Collinson, S. R.
Author/Creator	Gasser, G.
Author/Creator	Green, S. J.
Author/Creator	Hursthouse, M. B.
Author/Creator	Light, M. E.
Author/Creator	Tucker, J. H. R.
Year	2000-10-26
Resource Type	Crystal Structure
Resource Type	Completed Analysis
Note	A series of ferrocene-containing amidopyridyl receptors, in two regioisomeric forms (1,1' and 1,3), have been shown to bind cyclic organic molecules in chloroform through complementary hydrogen-bonding interactions. Complexation was monitored by NMR spectroscopy and by cyclic voltammetry. The magnitude of the host-guest binding strength and the redox response to complexation depend on both the type and the relative position of the amidopyridyl groups on the cyclopentadienyl rings of the ferrocene.
Note	<a href="http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/00sr0475_checkcif.html">http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/00sr0475_checkcif.html</a>
Note	<a href="http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/00sr0475.cml">http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/00sr0475.cml</a>
Note	<a href="http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/00sr0475_xl.lst">http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/00sr0475_xl.lst</a>
Note	<a href="http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/00sr0475.res">http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/00sr0475.res</a>
Note	<a href="http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/extracted.cml">http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/extracted.cml</a>
Note	<a href="http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/00sr0475_xs.lst">http://ecrystals.chem.soton.ac.uk/archive/00000083/01/00sr0475_data/00sr0475_xs.lst</a>

# Linking and aggregating: Search & discover

## eBank UK Demo

This is a prototype interface for the [eBank UK](#) JISC-funded project. It demonstrates an OAI-PMH aggregator service which cross searches a small sample of metadata records describing crystallography experiments (provided by the National Crystallography Service at the University of Southampton), and a small number of metadata records describing articles from the Crystallography literature (made available for use in this demo only by IUCr.) Links to the crystallography data sets and to the articles on line at the IUCr website are available in the search results.

Search for entries matching all the following:

Author =	<input type="text" value="Coles"/>
CCDC Code =	<input type="text"/>
IUPAC name =	<input type="text"/>
Empirical Formula =	<input type="text"/>
Compound Class =	<input type="text" value="All"/>
General keywords =	<input type="text"/>
Date released =	<input type="text"/>
OR published in the last	<input type="text"/>

Search within: ☒ Data Reports ☒ Publications e.g. journal articles

## eBank UK Demo

This is a prototype interface for the [eBank UK](#) JISC-funded project. It demonstrates an OAI-PMH aggregator service which cross searches a small sample of metadata records describing crystallography experiments (provided by the National Crystallography Service at the University of Southampton), and a small number of metadata records describing articles from the Crystallography literature (made available for use in this demo only by IUCr.) Links to the crystallography data sets and to the articles on line at the IUCr website are available in the search results.

Search for entries matching all the following:

Author =	<input type="text"/>
CCDC Code =	<input type="text"/>
IUPAC name =	<input type="text"/>
Empirical Formula =	<input type="text" value="C27H48"/>
Compound Class =	<input type="text" value="All"/>
General keywords =	<input type="text"/>
Date released =	<input type="text"/>
OR published in the last	<input type="text" value="day(s)"/>

Search within: ☒ Data Reports ☒ Publications e.g. journal articles



# Linking and aggregating: Hit browsing

**eBank UK Demo**

## Crystal Structure Data Reports

[Crystal Structure Report of 5alpha-cholestane](#)  
**Creator(s):** Coles, Simon J., Hursthouse, Michael B., Frampton, C. S.  
**Date released:** 23/05/2004  
**Empirical Formula:** C<sub>27</sub>H<sub>48</sub>  
**IUPAC name:** 5alpha-cholestane  
**CCDC code:** ZZZKGI01  
**Compound Class:** Organic  
**Related article:** <http://scripts.iucr.org/cgi-bin/getarticleid?issn=1600-5368&volume=58&fpage=o445&details=yes>

## Publications

**5alpha-Cholestane**  
 The title compound, C<sub>27</sub>H<sub>48</sub>, is a steroid derivative composed of a saturated-carbon fused-ring framework with two methyl substituents and an alkyl side chain.  
**Creator(s):** Coles, S. J., Hursthouse, M. B., Frampton, C. S.  
 Acta Crystallogr E Struct Rep Online Vol 58 Issue Pt 4 pp. o445 - o446  
**DOI:** 10.1107/S1600536802004786  
**Download from:** <http://scripts.iucr.org/cgi-bin/getarticleid?issn=1600-5368&volume=58&fpage=o445&details=yes>  
**Related dataset:** <http://ecrystals.chem.soton.ac.uk/archive/00000051/>

**Available Datafiles**

CIF file  
 processing Dataset  
 refinement Dataset  
 solution Dataset

Your search returned 1 data reports and 1 publications. Viewing 1 to 1

Search for entries matching all the following:  
 Author =

**eBank UK Demo**

## Crystal Structure Data Reports

[Crystal Structure Report of 2-\(N-Ferrocenylmethylcarbamoyl\)-5-\(N-phenylcarbamoyl\)-3,4-diphenyl pyrrole](#)  
**Creator(s):** Hursthouse, Michael B., Light, Mark E., Coles, Simon J., Horton, Peter N., Gale, Phil A., Denuault, G., Warriner, C. N.  
**Date released:** 23/05/2004  
**Empirical Formula:** C<sub>35</sub>H<sub>29</sub>FeN<sub>3</sub>O<sub>2</sub>  
**IUPAC name:** 2-(N-Ferrocenylmethylcarbamoyl)-5-(N-phenylcarbamoyl)-3,4-diphenyl pyrrole  
**CCDC code:** XU2SIU  
**Compound Class:** Organic  
**General keywords:** Supramolecular Chemistry  
**Related article:** [?A URI citation?](#)

## Publications

A supramolecular assembly: aquatris(pentafluorophenyl)borane as its mixed dimethyl sulfone and water solvate, (H<sub>2</sub>O)(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>Me<sub>2</sub>SO<sub>2</sub>H<sub>2</sub>O  
 The title compound, C<sub>18</sub>H<sub>2</sub>BF<sub>15</sub>O<sub>2</sub>H<sub>2</sub>O, obtained by crystallization of a product formed from a reaction mixture containing B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> and Me<sub>2</sub>SO<sub>2</sub> (and H<sub>2</sub>O) in hexane, was characterized in the solid state as a supramolecular assembly containing water adducts of tris(pentafluorophenyl)borane, (H<sub>2</sub>O)B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>, linked together by a network of hydrogen bonds involving one additional H<sub>2</sub>O and one additional Me<sub>2</sub>SO<sub>2</sub> molecule per adduct molecule.  
**Creator(s):** Coles, Simon J., Hursthouse, Michael B., Beckett, Michael A., Dutton, Michael  
 Acta Crystallogr E Struct Rep Online Vol 59 Issue Pt 9 pp. o1354 - o1356  
**DOI:** 10.1107/S1600536802004786  
**Download from:** <http://scripts.iucr.org/cgi-bin/getarticleid?issn=1600-5368&volume=58&fpage=o1354&details=yes>

Structural investigations of phosphorus-nitrogen compounds. 5. Relationships between molecular parameters of 2,2-diphenyl-4,6-cis-oxytetra(ethylenoxy)-4,6-R<sub>2</sub>-cyclophosphazatrienes (R = Cl, OCH<sub>2</sub>CF<sub>3</sub>, OPh, OMe, NHPh, NHBut) and substituent basicity constants  
 The syntheses and crystal structures of six new cis-ansa derivatives N<sub>3</sub>P<sub>3</sub>Ph<sub>2</sub>O(CH<sub>2</sub>CH<sub>2</sub>O)<sub>4</sub> R<sub>2</sub> (R = Cl, OCH<sub>2</sub>CF<sub>3</sub>, OPh, OMe, NHPh, NHBut) are reported and the observed relationship between molecular parameters of the N<sub>3</sub>P<sub>3</sub> ring and substituent basicity constants is discussed.  
**Creator(s):** Besli, S., Coles, S. J., Hursthouse, M. B., Kilic, A., Mayer, T. A., Shaw, R. A.  
 Acta Crystallogr B Vol 58 Pt 6 pp. 1067 - 1073  
**DOI:** 10.1107/S0108768102018608  
**Download from:** <http://scripts.iucr.org/cgi-bin/getarticleid?issn=1600-5368&volume=58&fpage=1067&details=yes>

[Crystal Structure Report of 2-\(N-Ferrocenylcarbamoyl\)-5-\(methoxycarbonyl\)-3,4-diphenylpyrrole](#)  
**Creator(s):** Hursthouse, Michael B., Coles, Simon J., Light, Mark E., Horton, Peter N., Gale, Phil A., Denuault, G., Warriner, C. N.  
**Date released:** 23/05/2004  
**Empirical Formula:** C<sub>29</sub>H<sub>24</sub>FeN<sub>3</sub>O<sub>3</sub>  
**IUPAC name:** 2-(N-Ferrocenylcarbamoyl)-5-(methoxycarbonyl)-3,4-diphenylpyrrole  
**CCDC code:** XU2SOA  
**Compound Class:** Organometallic  
**General keywords:** Supramolecular Chemistry  
**Related article:** [?A URI citation?](#)

## Publications

5alpha-Cholestane  
 The title compound, C<sub>27</sub>H<sub>48</sub>, is a steroid derivative composed of a saturated-carbon fused-ring framework with two methyl substituents and an alkyl side chain.  
**Creator(s):** Coles, S. J., Hursthouse, M. B., Frampton, C. S.  
 Acta Crystallogr E Struct Rep Online Vol 58 Issue Pt 4 pp. o445 - o446  
**DOI:** 10.1107/S1600536802004786  
**Download from:** <http://scripts.iucr.org/cgi-bin/getarticleid?issn=1600-5368&volume=58&fpage=o445&details=yes>  
**Related dataset:** <http://ecrystals.chem.soton.ac.uk/archive/00000051/>

Ethyl (2S<sup>+</sup>)-2-[(2R<sup>+</sup>,2'R<sup>+</sup>,5S<sup>+</sup>)-2',5-dimethyl-5'-oxoperhydro-[2,2']bifuranyl-5-yl]-2-hydroxyethanoate  
 The framework of K<sub>2</sub>Zn(H<sub>2</sub>P<sub>2</sub>O<sub>7</sub>)<sub>2</sub>·2H<sub>2</sub>O contains acid diphosphate-metallate layers linked by KO interactions and weak hydrogen bonds. Zn<sup>2+</sup> cations are coordinated octahedrally by O atoms from two bidentate H<sub>2</sub>P<sub>2</sub>O<sub>7</sub><sup>2-</sup> anions and two water molecules.

**Available Datafiles**

CIF file  
 processing Dataset  
 refinement Dataset  
 solution Dataset

# And finally...

## eBank embedded in a science portal





**PSigate**  
Physical Sciences Information Gateway

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**SEARCH SUBJECTS**

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- Materials science
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This is a prototype test interface to the eBank UK service providing access to data in the University of Southampton eCrystal data repository and elsewhere. eBank UK is a JISC-funded project which is a part of the Semantic Grid Programme. The project is being led by UKOLN in partnership with the Combechem project at the University of Southampton and PSigate.

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**Crystal Structure Data Reports**

**Crystal Structure Report of 2-(N-Ferrocenylmethylcarbamoyl)-5-(N-phenylcarbamoyl)-3,4-diphenyl pyrrole**

**Creator(s):** Hursthouse, Michael B., Light, Mark E., Coles, Simon J., Horton, Peter N., Gale, Phil A., Denuault, G., Warriner, C. N.

**Date released:** 23/05/2004

**Empirical Formula:** C35H29FeN3O2

**IUPAC name:** 2-(N-Ferrocenylmethylcarbamoyl)-5-(N-phenylcarbamoyl)-3,4-diphenyl pyrrole

**Compound Class:** Organic

**General keywords:** Supramolecular Chemistry

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