

# *Metadata and Standards for Crystallographic Data Dissemination:*

## *Implications for Raw Data Management and Archival*

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**EPSRC**

Engineering and Physical Sciences  
Research Council



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**JISC**



## Current Situation – Data Management



“Data from experiments conducted as recently as six months ago might be suddenly deemed important, but those researchers may never find those numbers – or if they did might not know what those numbers meant”

“Lost in some research assistant’s computer, the data are often irretrievable or an undecipherable string of digits”

“To vet experiments, correct errors, or find new breakthroughs, scientists desperately need better ways to store and retrieve research data”

“Data from Big Science is ... easier to handle, understand and archive. Small Science is horribly heterogeneous and far more vast. In time Small Science will generate 2-3 times more data than Big Science.”

‘Lost in a Sea of Science Data’ S.Carlson, The Chronicle of Higher Education (23/06/2006)



# Experimental Metadata Generation



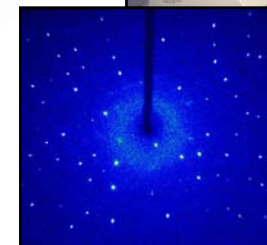
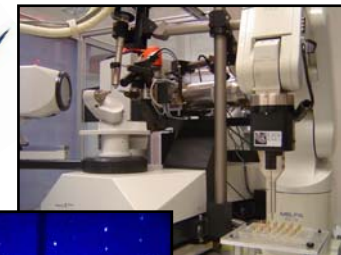
Synthesis



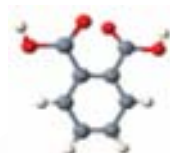
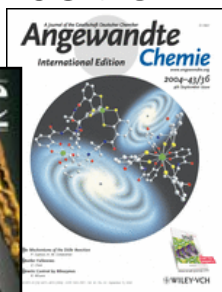
Preparation



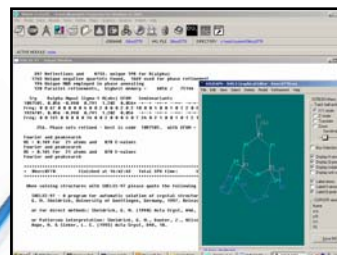
Data Collection



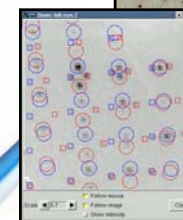
Publication



Structure Solution



Data Processing

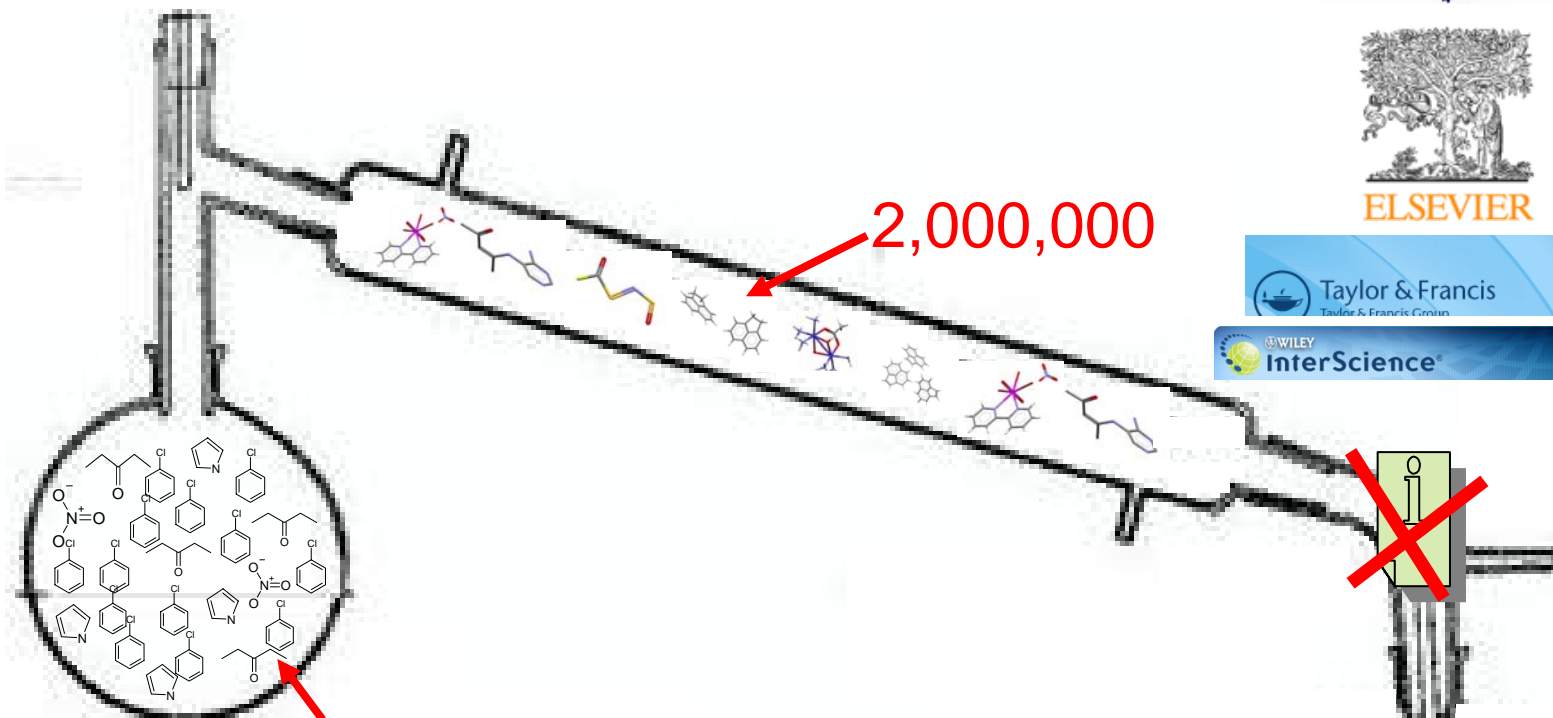




# Current Situation - Data Deluge

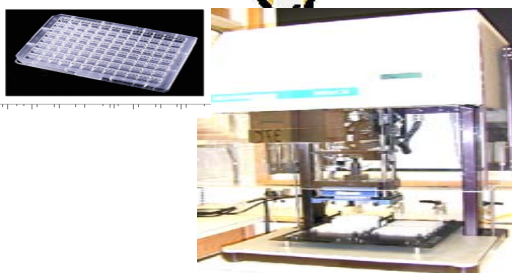
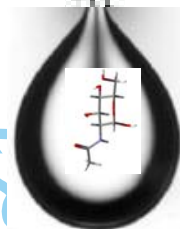
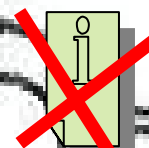


ELSEVIER



30,000,000

2,000,000



450,000



# Separating Data from Interpretations



Intellect & Interpretation (Journal article, report, etc)

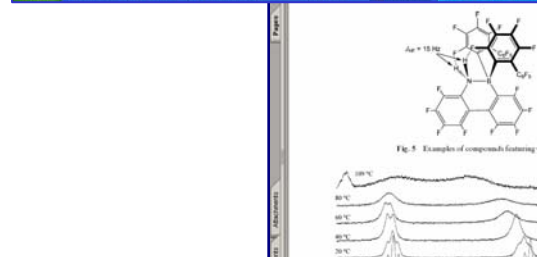
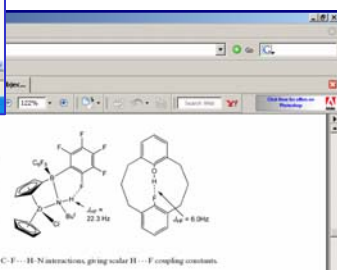
Underlying data (Institutional data repository)

research papers

Structural investigations of phosphorus-nitrogen compounds. 4. Steric and electronic effects in dibenzylamine derivatives of hexachlorocyclophosphazatriene and 4,4,6,6-tetrachloro-2,2-diphenylcyclophosphazatriene<sup>1</sup>

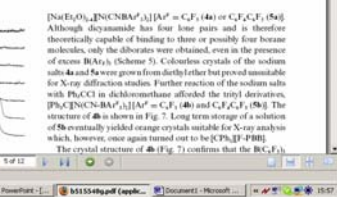
Scraper Book,<sup>a</sup> Simon J. Cole,<sup>b,c</sup> David B. Davies,<sup>b</sup> Michael B. Hursthouse,<sup>b</sup> Adam Klotz,<sup>c</sup> Thomas A. Mierz,<sup>b</sup> Robert A. Shau<sup>a</sup> and Aedin Uhl<sup>b</sup>

A systematic study is presented on the products of aminolysis of N,P<sub>6</sub>F<sub>12</sub> (1) and N,P<sub>6</sub>Cl<sub>4</sub>F<sub>8</sub> (4) with dibenzylamine. Two series of mono- and disubstituted derivatives of compounds (1) and (4), namely N,P<sub>6</sub>F<sub>11</sub>(NCH<sub>2</sub>Ph)<sub>2</sub> (2) and N,P<sub>6</sub>Cl<sub>3</sub>F<sub>9</sub>(NCH<sub>2</sub>Ph)<sub>2</sub> (5) and N,P<sub>6</sub>Cl<sub>3</sub>F<sub>9</sub>(NCH<sub>2</sub>Ph)<sub>2</sub> (6) [where (2), (3), (5) and (6) are new structures], are investigated in order to determine whether steric or electronic effects prevail in the formation of dibenzylamine-substituted cyclophosphoranes. The influence of an electron-releasing group (i.e. phenyl) on the stereochemistry and degree of substitution of the product is analysed by comparison of the above two series. The difference in stereochemically substituted endocyclic P-N bond lengths, A, is used as a measure of the degree of the electronic contribution, in combination with bulky substituents, to quantify the degree of the electron-releasing capacity of the R group. In order to compare geminal versus non-geminal substitution, a difunctional secondary amine was used to form the compound N,P<sub>6</sub>F<sub>11</sub>(NMeC(CH<sub>3</sub>)<sub>2</sub>Me)<sub>2</sub> (7) in stereocage.



particular, we noted that very small changes in structure led to dramatic and unpredictable changes in phase behavior, a frustrating situation. For example, it has been known for almost a decade<sup>23</sup> that poly(methyl acrylate) (PMA) and poly(methyl methacrylate) (PMMA) exhibit miscibility pressures in CO<sub>2</sub> that differ by hundreds of bar – this result would not be predicted by any group contribution thermodynamic model currently in use without purely empirical adjustments. Indeed, the PMA/CO<sub>2</sub> effect is preserved even when material that is for all intents and purposes, insoluble. Again, traditional thermodynamic models provide no guidance here.

We believe that at least part of the answer to these puzzles lies in CO<sub>2</sub>'s ability to act as both Lewis acid and Lewis base, coupled with subtle effects of neighboring substituents on the acidity of carbon precursors. For example, Wallen and colleagues<sup>23</sup> in an analysis of interactions between acylidene groups and CO<sub>2</sub> found that the acidity of the methyl acetate



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Table 1	(1)	(2)	(3)	(4)	(5)
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
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Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
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Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>
Chemical formula	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> P <sub>6</sub> F <sub>12</sub>	C <sub>12</sub> H <sub>12&lt;/</sub>	



# Laboratory Data Management and Archive



 University of Southampton **Crystal Structure Report Archive**

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## 6,7,9,10,12,13,15,16-Octahydro-benzo-1,4,7,10,13-pentaoxacyclopentadecin

**Origination:** Esther Rousay and Jeremy G Frey.

**Data Collection:** Simon J Coles.

**Structure Determination:** Simon J Coles and Micheal B Hursthouse.

University of Southampton

C<sub>14</sub>H<sub>20</sub>O<sub>5</sub>

InChI=1/C14H20O5/c1-2-4-14-13(3-1)18-11-9-16-7-5-15-6-8-17-10-12-19-14/h1-4H,5-12H2



**Available Files**

Final Result



# The eCrystals Public Data Archive



## University of Southampton Crystal Structure Report Archive

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### 6,7,9,10,12,13,15,16-Octahydro-benzo-1,4,7,10,13-pentaoxacyclopentadecin

Simon J Coles, Michael B Hursthouse,  
Jeremy G Frey and Esther Rousay.

University of Southampton

C<sub>14</sub>H<sub>20</sub>O<sub>5</sub>

InChI=1/C14H20O5/c1-2-4-14-13(3-1)18-11-9-16-7-5-15-6-8-17-10-12-19-14/h1-4H,5-12H2

DOI: 10.594/ecrystals.chem.soton.ac.uk/145

**Compound Class:** Organic

**Keywords:** crown ethers

**Creation Date:** 07 October 2004

**Deposited By:** A.N. Admin

**Deposited On:** 20 February 2006



#### Available Files

#### Depositor Comments

Structure already known, but accurately redetermined for a local research project.

#### Data collection parameters

Chemical formula	C14 H20 O5
Crystallisation Solvent	
Crystal morphology	Plate
Crystal system	Orthorhombic
Space group symbol	Pbca
Cell length a	16.4963(18)
Cell length b	8.325(3)
Cell length c	20.061(6)
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	0.0409
R Factor (Obs)	0.0487
R Factor (All)	0.0977
Weighted R Factor (Obs)	0.1008
Weighted R Factor (All)	0.1192

**Citation:** Coles, S.J., Hursthouse, M.B., Frey, J.G. and Rousay, E. (2004), Southampton, UK, University of Southampton, Crystal Structure Report Archive. (doi:10.1594/ecrystals.chem.soton.ac.uk/145)

#### Final Result

04sjc0831.cif	13k
04sjc0831.cml	6k

#### Validation

04sjc0831_checkcif.htm	7k
------------------------	----

#### Refinement

04sjc0831.res	6k
04sjc0831_xl.lst	34k

#### Solution

04sjc0831.prp	6k
04sjc0831_xs.lst	39k

#### Processing

04sjc0831.hkl	702k
04sjc0831.htm	10k
04sjc0831_0kl.jpg	57k
04sjc0831_h0l.jpg	85k
04sjc0831_hk0.jpg	88k

#### Data Collection

04sjc0831_crystal.jpg	17k
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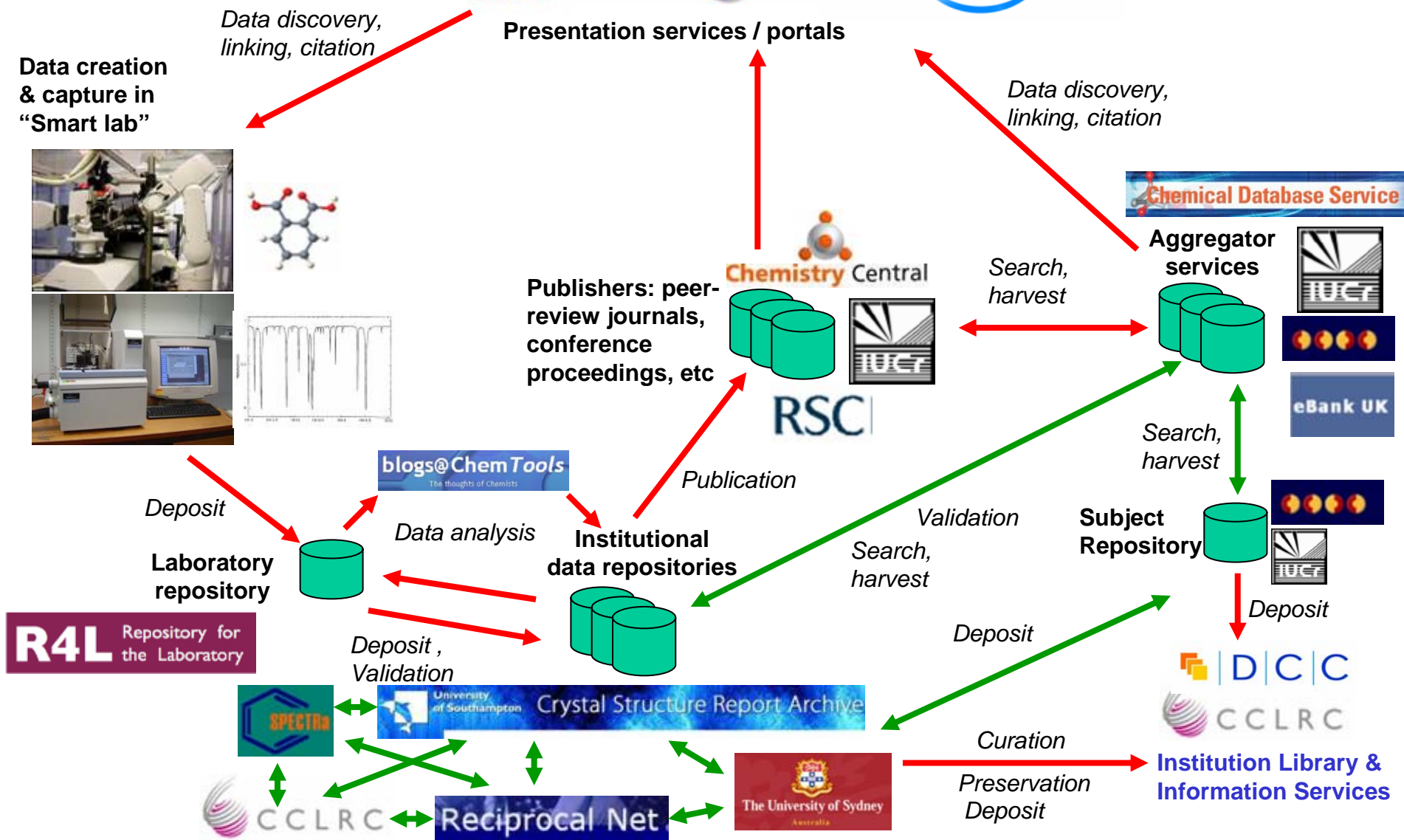
#### Other Files

04sjc0831.doc	78k
04sjc0831.fcf.bt	155k

<http://ecrystals.chem.soton.ac.uk>



# eCrystals 'Global Federation' Model





# Metadata standards: Dublin Core



About 15 core elements

**Dublin Core Metadata Initiative®**

Home > Documents > Dces >

## Dublin Core Metadata Element Set, Version 1.1: Reference Description

**Date Issued:** 2003-06-02  
**Identifier:** <http://dublincore.org/documents/2003/06/02/dces/>  
**Supersedes:** <http://dublincore.org/documents/2003/02/04/dces/>  
**Latest version:** <http://dublincore.org/documents/dces/>  
**Translations:** <http://dublincore.org/resources/translations/>  
**Status of document:** This is a DCMI [Recommendation](#).  
**Description of document:** This document is the reference description, version 1.1

### Introduction

The Dublin Core metadata element set is a standard for cross-domain information to be "anything that has identity". This is the definition used in Internet RFC 2396 by Berners-Lee et al. There are no fundamental restrictions to the types of resource. Three formally endorsed versions exist of the Dublin Core Metadata Element Set:

- ISO Standard 15836-2003 (February 2003): <http://www.niso.org/interchange/15836-2003/>
- NISO Standard Z39.85-2001 (September 2001): <http://www.niso.org/standards/z39-85-2001/>
- CEN Workshop Agreement CWA 13874 (March 2000, no longer available)

For an overview and links to full specifications of all metadata terms maintained by the Dublin Core Metadata Initiative please see: <http://dublincore.org/usage/documents/overview/>.

### The Elements

Element Name: Title
Label: Title
Definition: A name given to the resource.
Comment: Typically, Title will be a name by which the resource is formally known.

Element Name: Creator
Label: Creator
Definition: An entity primarily responsible for making the content of the resource.
Comment: Examples of Creator include a person, an organization, or a service. Typically, the name of a Creator should be used to indicate the entity.

Element Name: Subject
Label: Subject and Keywords
Definition: A topic of the content of the resource.
Comment: Typically, Subject will be expressed as keywords, key phrases or classification codes that describe a topic of the resource. Recommended best practice is to select a value from a controlled vocabulary or formal classification scheme.

Element Name: Description
Label: Description
Definition: An account of the content of the resource.
Comment: Examples of Description include, but is not limited to: an abstract, table of contents, reference to a graphical representation of content or a free-text account of the content.



# Metadata Publication



OAI 2.0 Request Results - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

http://ecrystals.chem.soton.ac.uk/perl/oai2?verb=ListRecords&metadataPrefix=oai\_dc

NCS Interactive Serv... eCrystals Dev Repositories 4 Labs - ... Bb Blackboard Learning ... Calendar WWWgetdata

**OAI Record: oai:ecrystals.chem.soton.ac.uk:19**

**OAI Record Header**

<b>OAI Identifier</b>	oai:ecrystals.chem.soton.ac.uk:19	<a href="#">oai_dc</a>	<a href="#">ebank_mets</a>	<a href="#">formats</a>
<b>Datestamp</b>	2006-02-20			
<b>setSpec</b>	7374617475733D707562	<a href="#">Identifiers</a>	<a href="#">Records</a>	

**Dublin Core Metadata (oai\_dc)**

<b>Title</b>	3,4-Diphenyl-1H-pyrrole-2,5-dicarboxylic acid bis-[(2-amino-ethyl)-amide] hexafluorophosphate dihydrate
<b>Author or Creator</b>	Hursthouse, Michael B.
<b>Author or Creator</b>	Gale, Phil A.
<b>Author or Creator</b>	Navakhun, K.
<b>Author or Creator</b>	Camiolo, S.
<b>Author or Creator</b>	Light, Mark E.
<b>Rights Management</b>	http://ecrystals.chem.soton.ac.uk/rights.html
<b>Publisher</b>	University of Southampton
<b>Date</b>	2002-03-08
<b>Resource Type</b>	Crystal Structure Data Holding
<b>Subject and Keywords</b>	C~22~H~26~N~5~O~2~.F~6~P.H~2~O.HO/c23-11-13-25-21(28)19-17(15-7-3-1-4-8-15)18(16-9-5-2-6-10-16)20(27-19)22(29)26
<b>Resource Identifier</b>	InChI=1/C22H27N5O2.F6P.H2O.HO/c23-11-13-25-21(28)19-17(15-7-3-1-4-8-15)18(16-9-5-2-6-10-16)20(27-19)22(29)26

Done

Start | Inbox for s.j.coles@soto... | Informatics | Tesco.com - Superstore ... | OAI 2.0 Request Resu... | Microsoft PowerPoint - [...]

22:23

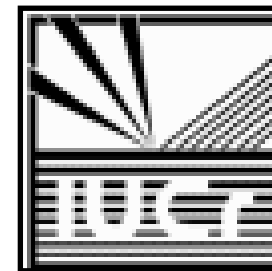
[ecrystals.chem.soton.ac.uk/perl/oai2](http://ecrystals.chem.soton.ac.uk/perl/oai2)



## Metadata Publication



- Using simple Dublin Core
  - Crystal structure
  - Title (Systematic IUPAC Name)
  - Authors
  - Affiliation
  - Creation Date
- Additional **chemical** information through Qualified Dublin Core
  - Empirical formula
  - International Chemical Identifier (InChI)
  - Compound Class & Keywords
- Specifies which 'datasets' are present in an entry
- DOI <http://dx.doi.org/10.1594/ecrystals.chem.soton.ac.uk/145>
- Rights & Citation <http://ecrystals.chem.soton.ac.uk/rights.html>
- Application Profile <http://www.ukoln.ac.uk/projects/ebank-uk/schemas/>





# The New World? Describing and Exchanging Experimental Processes



We are currently seeking further funding and developing collaborations to build myExperiment.

**my**experiment tech

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myExperiment makes it really easy for people to share experiments and discuss them. You will be able to swap workflows and publications as well as documents, photos and videos, all from any web browser.

**We're not ready to launch yet, but if you want to know when we're ready, you can [join our mailing list](#)**

## THE BUZZ

"Their kids may have got there first but scientists will soon have their very own version of MySpace, where they will be able to share preliminary results, ideas and research tools." — [New Scientist Tech](#), October 2006.

Currently, a [lightweight repository of workflows](#) and the [Taverna BioService Finder](#) are available.

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## GET INVOLVED!

myExperiment is a free software project. You can help us by [testing code](#), writing patches and writing



**BLOG**



# The Need for Experimental Metadata



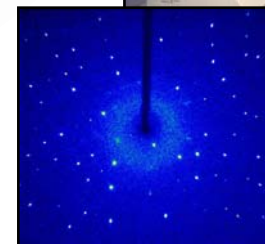
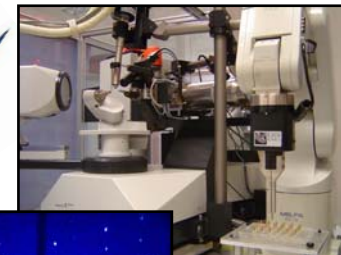
Synthesis



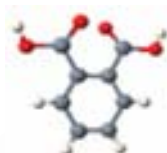
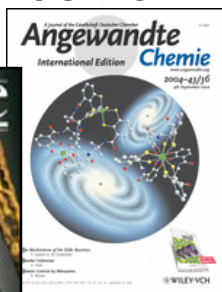
Preparation



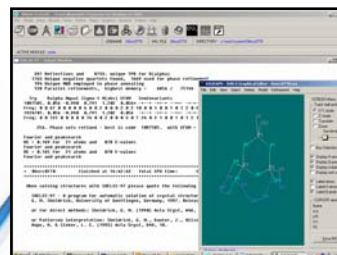
Data Collection



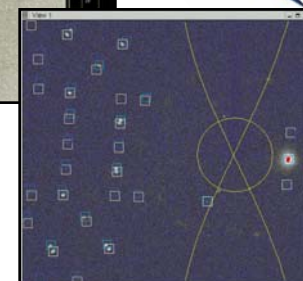
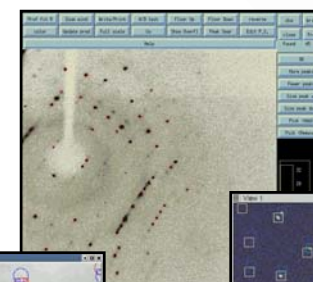
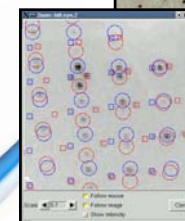
Publication



Structure Solution



Data Processing





## Why do we need metadata for crystallographic raw data?



1. Preservation and curation.  
Description of file types, software (versions).
2. Collaboration and service provision.  
What level of metadata is necessary (if any)?
3. Discovery.  
Is eCrystals level sufficient?
4. Validation and reuse.  
Description of synthesis, sample preparation, data collection process, file types, processing software and methodology.



## Changing Times!



- eCrystals Federation requirements capture (report Jun 2007)
- Robust software & transition to ePrints3 (Summer 2007)
- Capability for 'site configuration' as defined by laboratory working practices (Current)
- Roll out to other laboratories (Summer 2007)
- Collaboration with Sun to link eCrystals to terabyte store for archival and access to raw data (Summer 2007)
- Improve linkage between repository and:
  - desktop /
  - data management systems
  - workflow enactors