

The “CombeChem” Project

Semantic Support for the Chemical Information
Life cycle

Jeremy Frey
School of Chemistry
University of Southampton

The CombeChem Project

- ✦ End to End linking of data and information
 - ✦ Laboratory to publication and back again
 - ✦ Very long data chains can be involved e.g. from a chemistry lab to mouse genetic expression
- ✦ The exponential world of combinatorial synthesis and high throughput analysis meets the exponentially growing power of computing
 - ✦ “Automation, Semantics & the Grid”

Smart Laboratory

Smart HCI

Goal

Literature

Knowledge

CombeChem Data and Knowledge Cycle
End-to-End Management

Digital Model

Analysis

Synthesis

Smart Storage

Smart Dissemination

e-Science

- ★ 'e-Science is about global collaboration in key areas of science, and the next generation of infrastructure that will enable it.'

John Taylor, DG of UK OST

- ★ '[The Grid] intends to make access to computing power, scientific data repositories and experimental facilities as easy as the Web makes access to information.'

Tony Blair, 2002

- ★ What is the web?

The concept of Publication@Source

- ✦ Trace all the way back from publication to the original data - provenance
- ✦ The data is the key - DataGrid
- ✦ Start as you mean to go on - ELNs are a necessity

necessary if a calculation or discussion is changed; the section to be deleted is simply removed by drawing a neat "x" through it.

In view of the fact that a notebook is a primary record, data are not copied into it from other sources (such as this manual or a lab partner's notebook, in a joint experiment) without clear acknowledgment of the source. Observations are never collected on note pads, filter paper, or other temporary paper for later transfer into a notebook. If you are caught using the "scrap of paper" technique, your improperly recorded data may be confiscated by your TA or instructor at any time. It is important to develop a standard approach to using a notebook routinely as the primary receptacle of observations.

Each week at the beginning of lab lecture, you will turn in your prelab problems from the manual for grading. Problems not turned in at the beginning of lab lecture will be

Observations are never collected on note pads, filter paper or other temporary paper for later transfer into a notebook



If you are caught using the "scrap of paper" technique, your improperly recorded data may be confiscated by your TA

Lab books are a big block to publication@source: if it's not digital, it is more difficult to share



This is where it all starts: The Lab & The Lab Book

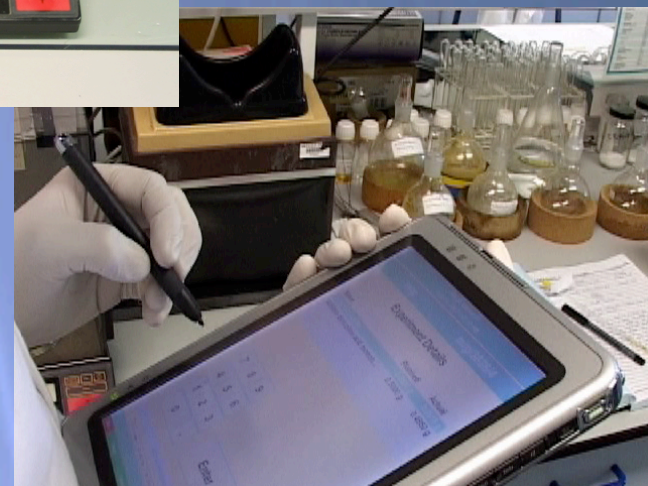
Need a usable digital lab book. Design by analogy to help Chemists and Computer Scientists work together.

ACS 10 Sept 06

Cyberinfrastructure



Only some equipment is networked



COSHH

leverage off things we already have to do

COSHH ASSESSMENT FORM				Record No.
SUBSTANCE NAME	PHYSICAL FORM	QUANTITY	NATURE OF HAZARD	
Water	liquid	1000ml	None	
Dextrose	Solids	<20g	possible irritation to eyes and skin	
Caffeine	Solids (tea)	<1g	Harmful if swallowed, induce vomiting.	
Milk	liquid	<100ml	No particular hazards	
NATURE OF PROCESS liquid extraction of caffeine, followed by combination with dextrose to produce a sweet drink				
Is there a less hazardous substance? <i>No</i> If so, why not use it?				
CONTROL MEASURES REQUIRED <i>No specific measure required</i> (Local exhaust ventilation, personal protection, etc.)				

Perhaps computational chemists should be made to do the same!
 Statistical modelling and design requires planning to be most effective

TOL
LIS

PLAN

Process
Record

PLAN
Process
Record

Ingredient List	
Fluorinated biphenyl	0.9 g
Br11OCB	1.59 g
Potassium Carbonate	2.07 g
Butanone	40 ml

Dissolve 4-fluorinated biphenyl in butanone

Add K2CO3 powder

Heat at reflux for 1.5 hours

Cool and add Br11OCB

Heat at reflux until completion

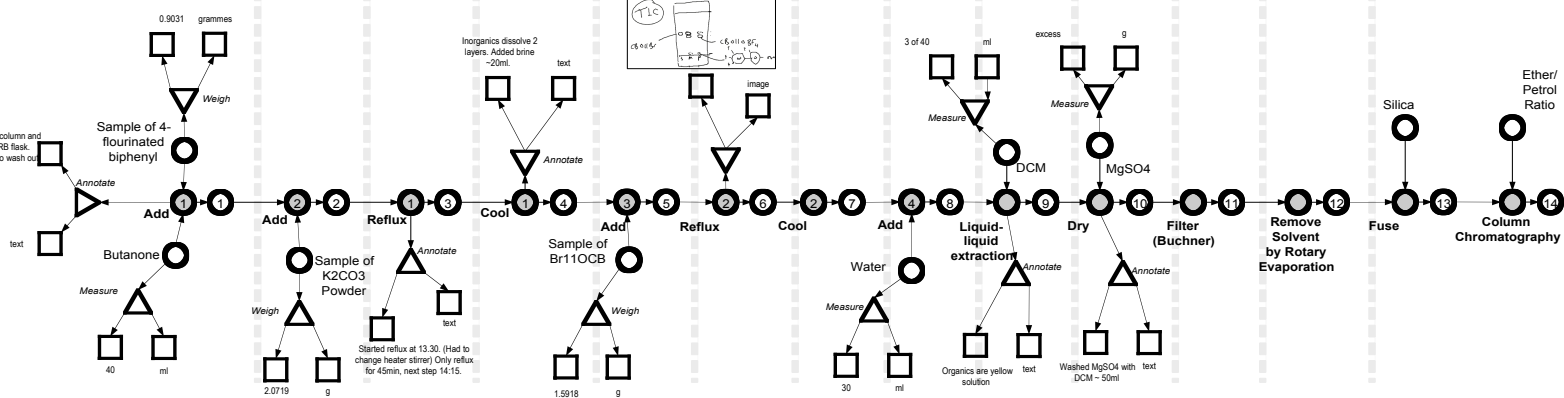
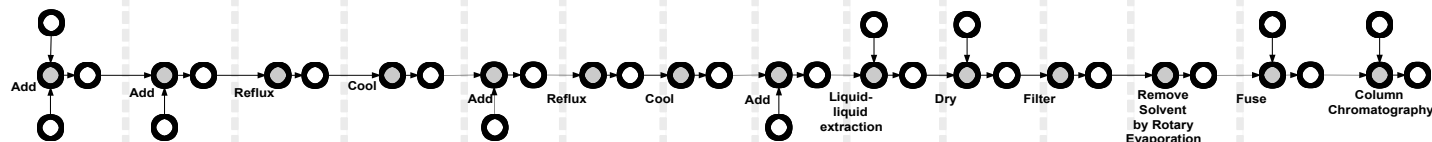
Cool and add water (30ml)

Extract with DCM (3x40ml)

Combine organics, dry over MgSO4 & filter

Remove solvent in vacuo

Fuse compound to silica & column in ether/petrol



Key	
Process	○
Input	○○
Literal	□
Observation	▽

Observation Types	
weight - grammes	
measure - ml, drops	
annotate - text	
temperature - K, °C	

Future Questions
Whether to have many subclasses of processes or fewer with annotations
How to depict destructive processes
How to depict taking lots of samples
What is the observation/process boundary? e.g. MRI scan

Combechem
30 January 2004
gvh, hrm, gms

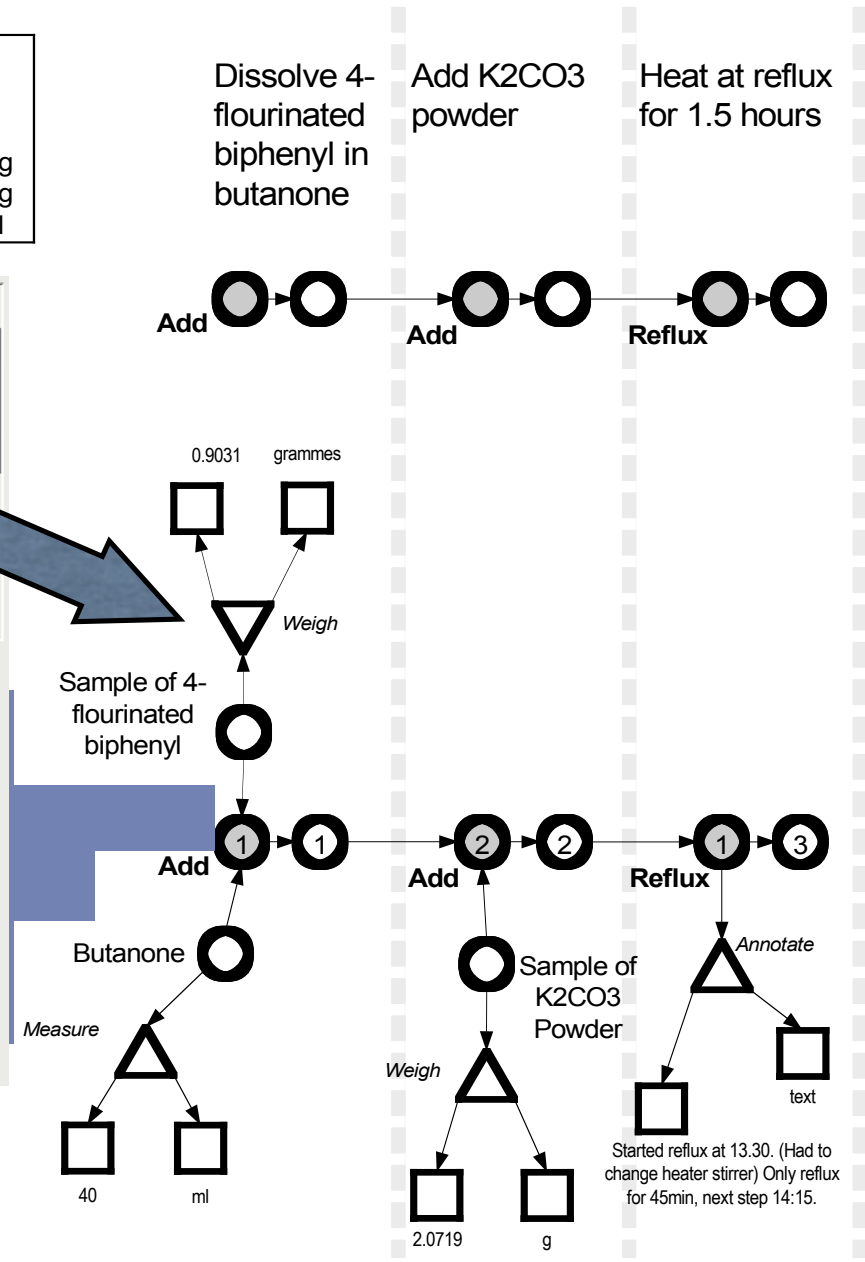
ACS

Ingredient List	
Fluorinated biphenyl	0.9 g
Br11OCB	1.59 g
Potassium Carbonate	2.07 g
Butanone	40 ml

Name	Planned	Actual
Fluorinated biphenyl	0.9000 g	0.9031 g
Br11OCB	1.5900 g	1.5918 g
Potassium Carbonate	2.0719 g	2.0719 g
Butanone	40.0 ml	40.0 ml

7	8	9
4	5	6
1	2	3
0	.	

Enter	Del
-------	-----

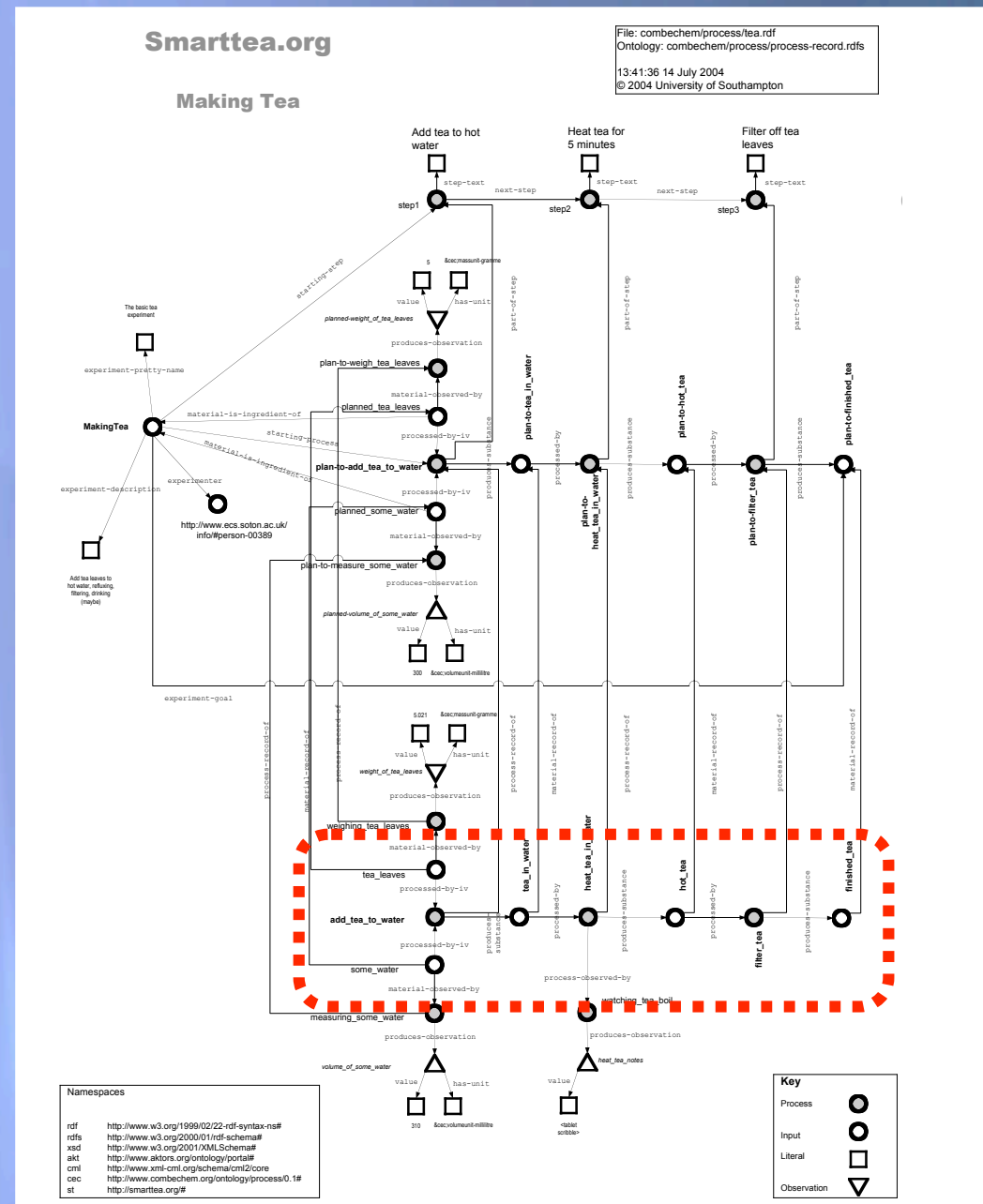


getRecord()

There is a potential containment problem in pulling back partial RDF graphs from the triple store.

Solved by using multiple triple stores but boundaries are a major issue for the future.

ACS 10 Sept 06

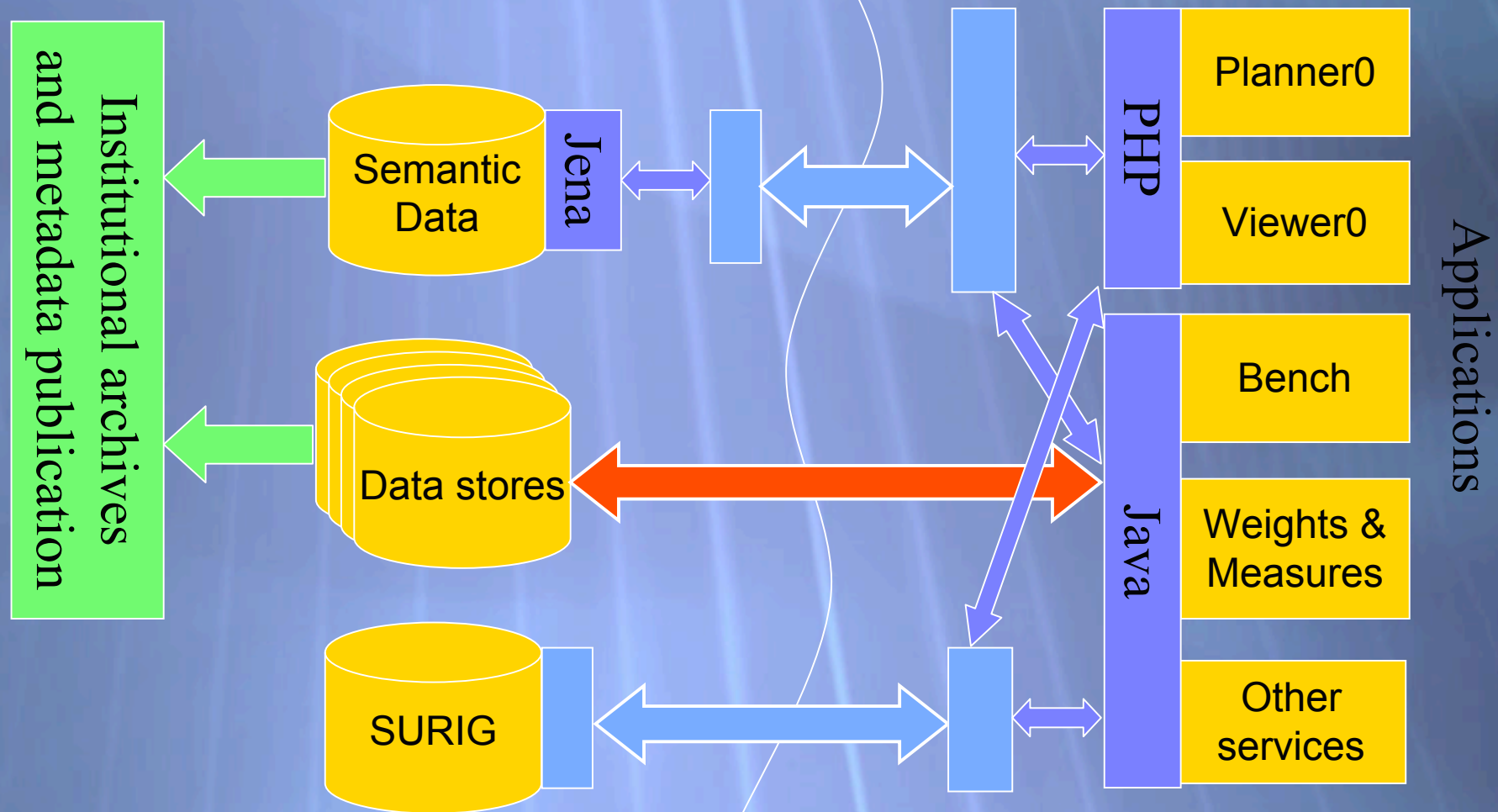


Cyberinfrastructure

Jeremy Frey 11

Architecture

“Client” Libraries
SOAP

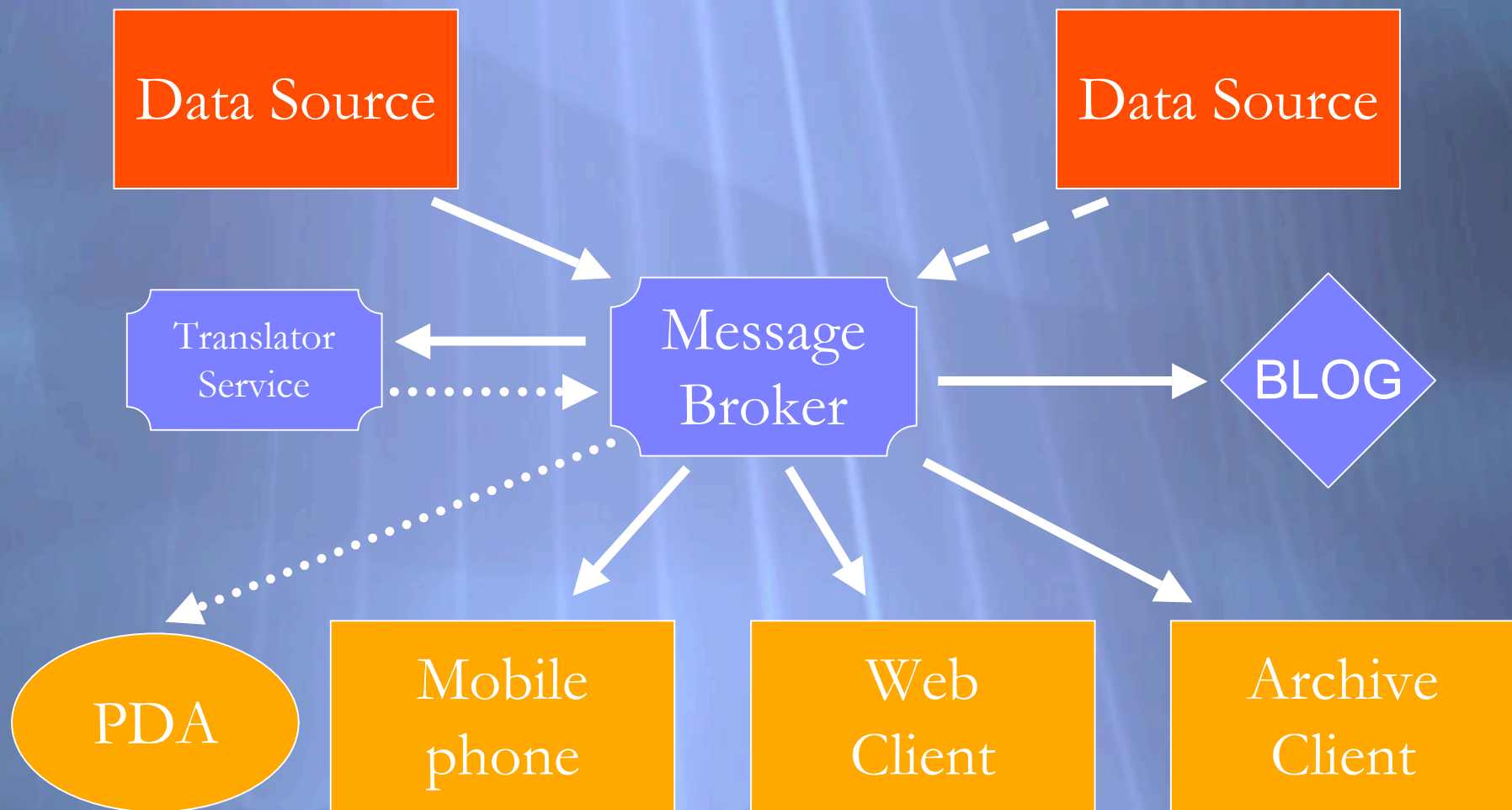


The Laboratory

- ✦ Capture information from places you would not want to put your eyes
- ✦ Capture environmental data automatically
- ✦ Capture people and movements
- ✦ Provide this information in real time as well as for the laboratory record

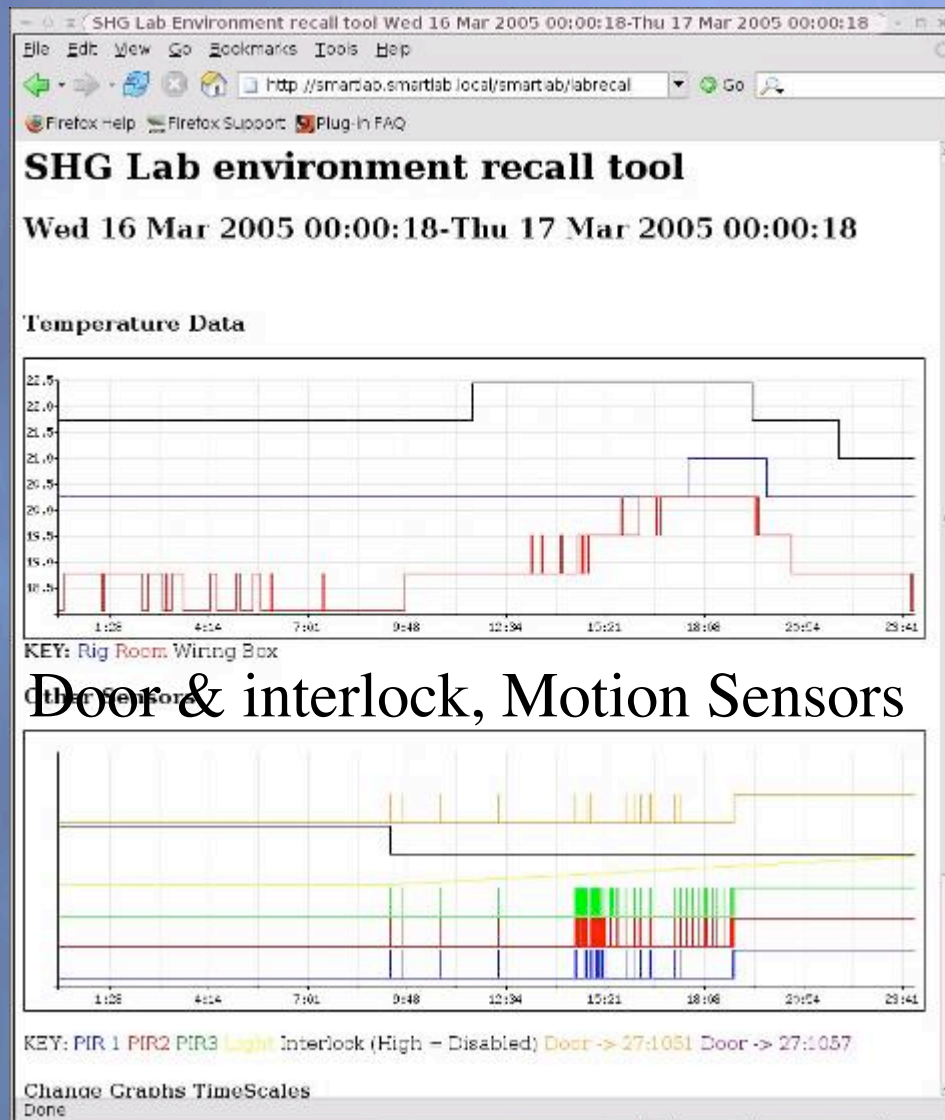


Pub-Sub systems provide the flexible & extensible approach to distribution



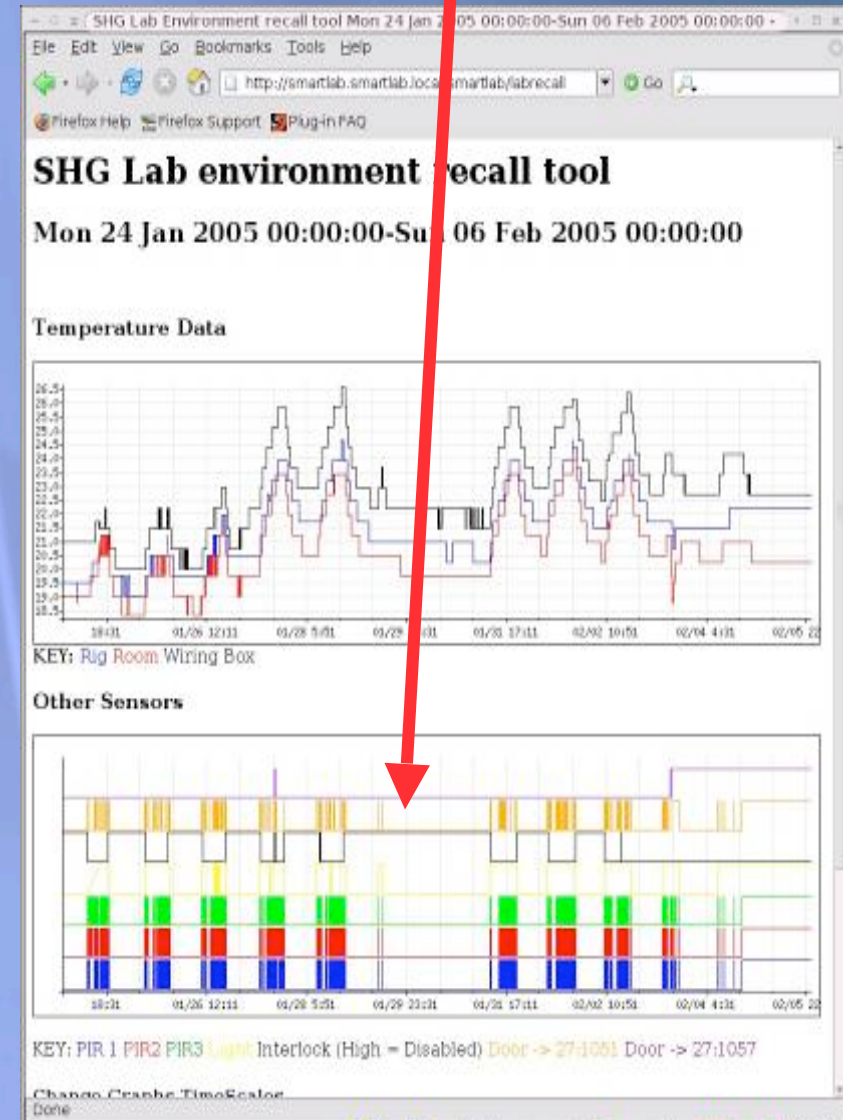
Temperature – room, laser

Air Conditioning failed



ACS 10 Sept 06

Cyberinfrastructure



Jeremy Frey 15

BBC NEWS | Science/Nature | Chemists escape labs via mobiles - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <http://news.bbc.co.uk/1/hi/sci/t>

bbc.co.uk

Low Graphics version | Change edition

News Front Page
World
UK
England
Northern Ireland
Scotland
Wales
Business
Politics
Health
Education
Science/Nature
Technology
Entertainment

Have Your Say
Magazine
In Pictures
Week at a Glance
Country Profiles
In Depth

Last Updated: Fr
E-mail this to
Chemists
By Jo Twist
BBC News sci

A blend of mobile and award-winning technology is letting scientists escape the lab

The software, "middleware", computer system, other securely instantaneous

As part of a new project in the university used to let Scientists

Address <http://news.bbc.co.uk/1/hi/sci/tech/4233757.stm>

experiment in more detail.

PDAs everywhere

Members of Dr Frey's non-linear laser spectroscopy group, working as part of the Combechem project, successfully trying out the system at conferences at the university bar.

The next step is to evolve the system so that at a button on a mobile, scientists will be able to remove the conditions in the lab, like turning down the temperature.

It could also realise the promise of controlling home environments from phones easily and seamlessly.

But there are many other potential applications for the monitoring jobs done by the power industries, healthcare professions and other labs.



Chemists enjoy a drink at the bar while keeping an eye on the lab

IBM won the Royal Academy of Engineering's MacRobert prize which rewards technological and engineering innovation for the program in June last year.

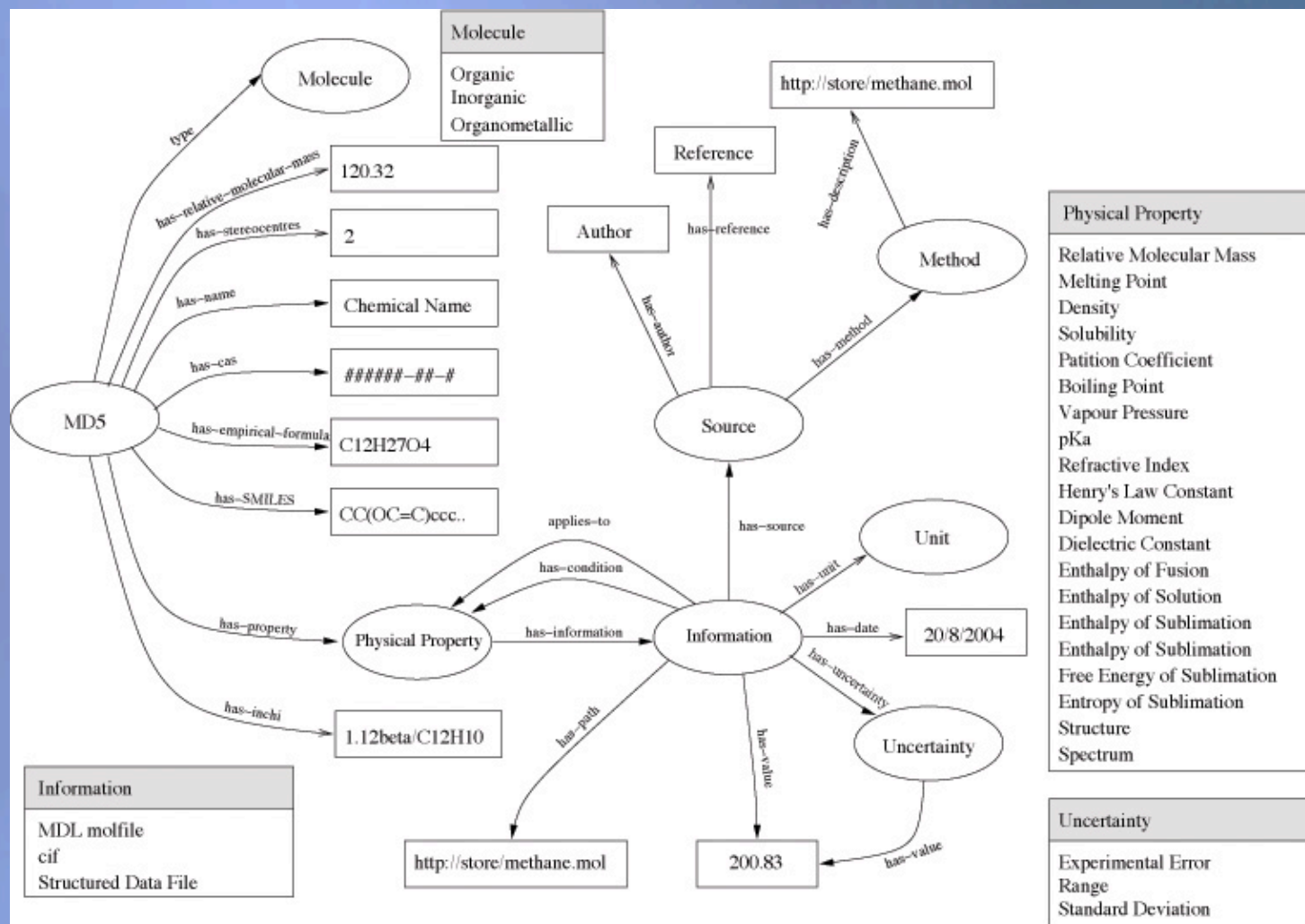
Used by top global banks, the WebSphere MQ family is a decade old.



Databases - Our experience

- ✦ What do you do when the actual users keep changing their mind?
- ✦ Is a traditional relational database suitable?
- ✦ Danger of re-enforcing scientific bias against relational database for laboratory data.
- ✦ RDF & Triple stores were again the solution

RDF/RDFS High level Schema for chemical properties



Property in RDF

- ★ `<c:OrganicMolecule`
`rdf:about="file:///storage/ba8efc2ce0edada69d63b02d1b8630c6.rdf">`
- ★ `<c:has-inchi>1.12Beta/C12H13NO2/c1-2-15-8-9-5-6-11(14)12-10(9)4-3-7-`
`13-12/h1H3,2H2,3-7H,8H2,14H</c:has-inchi>`
- ★ `<c:has-cas>22049-19-0</c:has-cas>`
- ★ `<c:has-empirical-formula>C12H13NO2</c:has-empirical-formula>`
- ★ `<c:has-stereocentres>0</c:has-stereocentres>`
- ★ `<c:has-property>`
- ★ `<c:MeltingPoint>`
- ★ `<c:has-information>`
- ★ `<c:Information>`
- ★ `<c:has-value>150`
- ★ `</c:has-value>`
- ★ `<c:has-uncertainty>`
- ★ `<c:Range>`
- ★ `<c:has-value>16`
- ★ `</c:has-value>`
- ★ `</c:Range>`
- ★ `</c:has-uncertainty>`
- ★ `</c:Information>`
- ★ `</c:has-information>`
- ★ `</c:MeltingPoint>`
- ★ `</c:has-property>`
- ★ `</c:OrganicMolecule>`
- ★ `<rdfs:Class rdf:about="&c;OrganicMolecule">`
- ★ `<rdfs:label>Organic Molecule</rdfs:label>`
- ★ `<rdfs:subClassOf rdf:resource="&c;Molecule" />`
- ★ `</rdfs:Class>`
- ★ `<rdfs:Class rdf:about="&c;PhysicalProperty">`
- ★ `<rdfs:label>Property</rdfs:label>`
- ★ `</rdfs:Class>`
- ★ `<rdfs:Class rdf:about="&c;PartitionCoefficient">`
- ★ `<rdfs:label>Paritition Coefficient</rdfs:label>`
- ★ `<rdfs:subClassOf rdf:resource="&c;PhysicalProperty" />`
- ★ `<rdfs:description>Ratio of substance dissolved in octan-`
`1-ol and water`
- ★ `</rdfs:description>`
- ★ `</rdfs:Class>`

TRIANGLE

CAS INCHI NAME SMILES EMPIR

1202-32-0

Search the DB Canned Example

query number = [10]

MOLECULE

type	Resource
type	Molecule
has-SMILES	<chem>c1cccc1C=C(CCN(=O)=O)</chem>
has-name	B-ETHYL-B-NITROSTYR
has-mmm	177.2
has-stereocentres	0
has-empirical-formula	C10H11NO2
has-cas	1202-32-0

has-property

48.29587

type PhysicalProperty

type BoilingPoint

type Resource

has-information

49.29587

type Resource

type Information

has-date 2005-2-28

has-value 307.5

has-uncertainty

has-unit

has-source

63.29587

type Source

type PhysProp

type Resource

has-method

54.29587

type Resource

type Laboratory

of-quality

has-condition

has-property

16.29587

type PhysicalProperty

type Solubility

type Resource

has-property

26.29587

type PhysicalProperty

type Information

type Resource

has-information

has-property

6.29587

type PhysicalProperty

type Solubility

type Resource

has-information

3mol

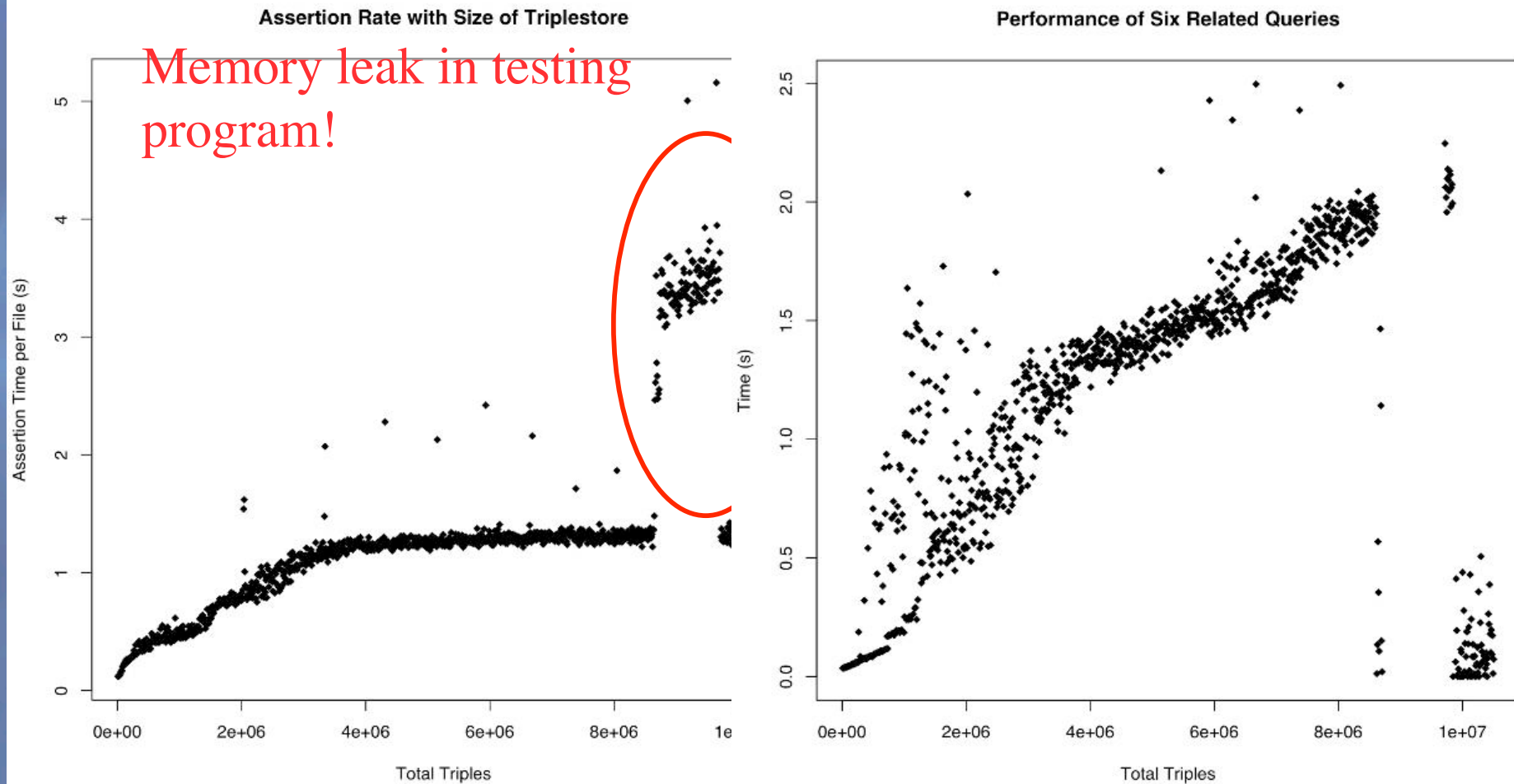
© University of Southampton 2005
ACCESS RESTRICTED
Version 1.0.4

ACS 10 Sept 06

Cyberinfrastructure

Triple Stores - The Heart of the Semantic Web

Scaling - 3Store response



Scaling the triplestores

Moved from...

- ✦ A model of harvesting data from multiple sources into one scalable store

to

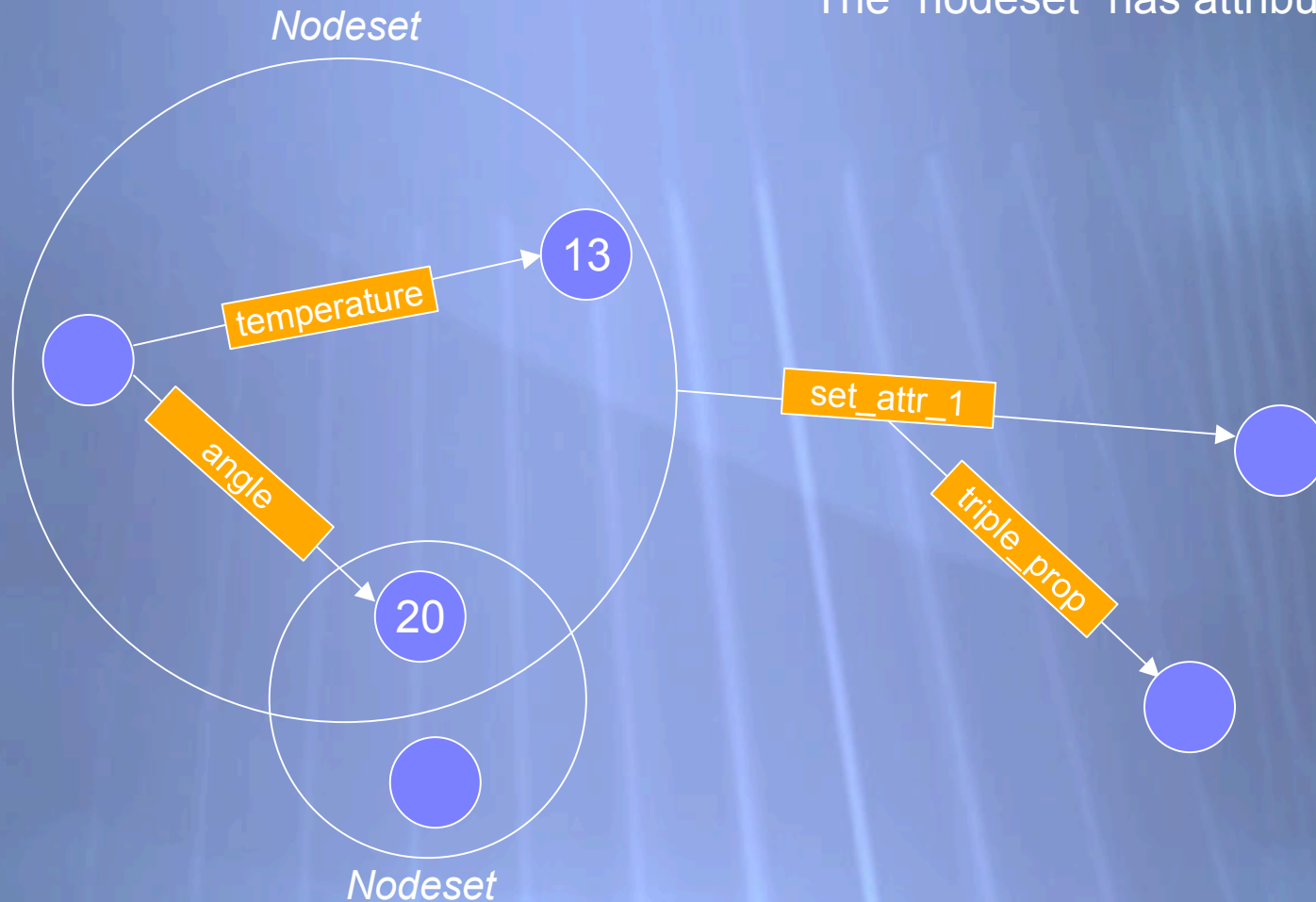
- ✦ A model of distributed RDF sources and caching what is needed for the task at hand into multiple stores fit-for-purpose



The Semantic Web!

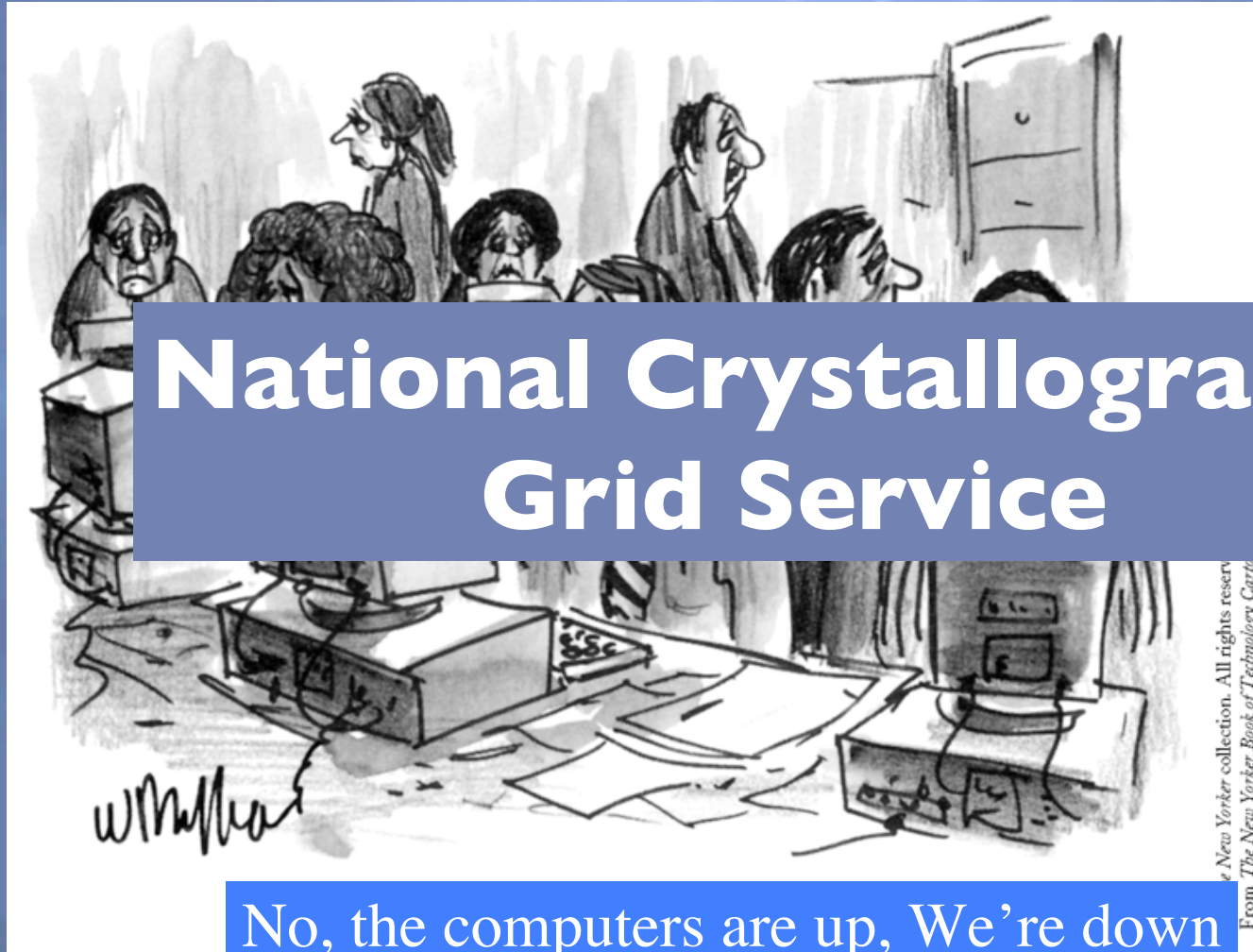
- ✦ Very Complex RDF
- ✦ Use a graph-based model.
 - ✦ Base on RDF ideas
 - ✦ Actual data is stored as a graph
 - ✦ Contrast with models like E-R, where the graph “models” the data, rather than actually being the data.
 - ✦ A node in E-R might be “customer”, and represent the class of entities that are customers, rather than any specific customer.
- ✦ The pseudograph model:
 - ✦ Each node is a datum.
 - ✦ Each edge denotes an association/attribute/property.
 - ✦ Nodes can be grouped into nodesets, which are also nodes.
 - ✦ A node may be in more than one nodeset.
 - ✦ A node-edge-node triple can also be a node.
 - ✦ Main difference from RDF is an attempt to build reification into the model.

The “nodeset” has attributes



- ★ The edge with the attribute name `set_attr_1` is an attribute of a nodeset.
- ★ The edge with the attribute name `triple_prop` is an attribute of the above edge.

Experiments on the Grid



National Crystallography Grid Service

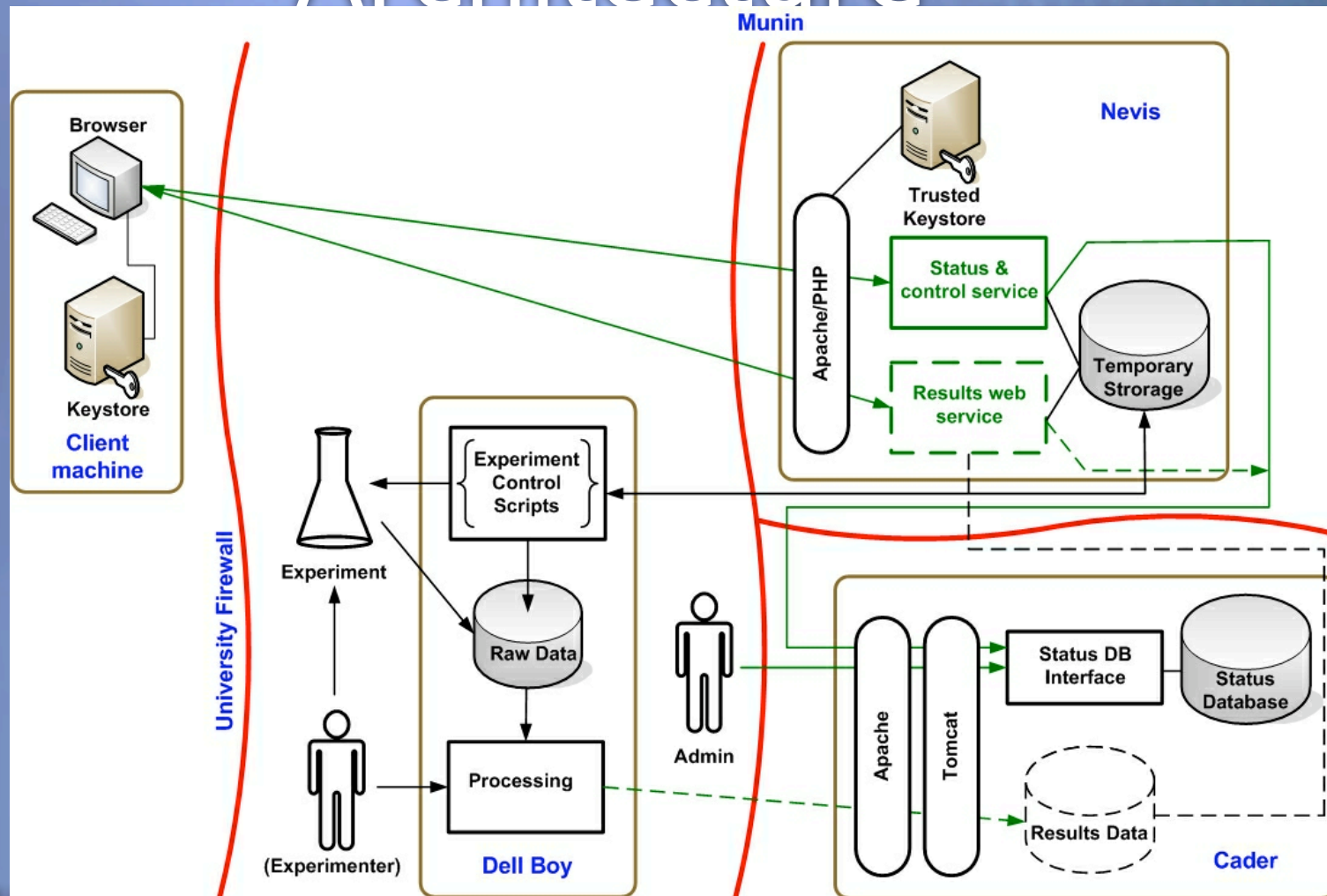
No, the computers are up, We're down

Security and
trust for
experiments
and data

Role based
authorisation
needed for
experiments
not entirely
the same as
for
computers



NCS Grid Service Architecture




Combechem status - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Media

Address <https://interact.xservice.soton.ac.uk/status/index.php> Go Links



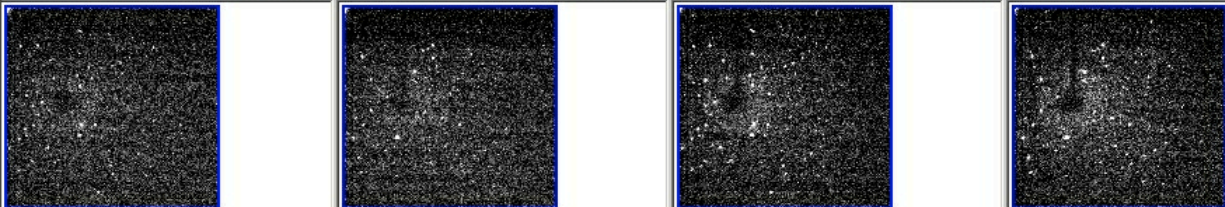
National Crystallography Service – Sample Status

Viewing samples for M E Light (light@soton.ac.uk)

NCS ID	Customer ID	Received	Collection	Status	Details
04MEL0098	2nd test	2004-02-12	001	Succeeded	HKL file / Report
04MEL0093	mel01	2004-02-06	001	Succeeded	HKL file / Report
04SRC0104	#13-123	2004-03-08	001	Next	Due at 00:00:00 (est)
04SRC0103	#12-01	2004-03-08	001	Failed (Referred)	Diffraction too weak
			002	Failed (No Further Action)	Crystals too small
04SRC0105	HSF-HCl				

Done

X-Ray Diffractometer Images



Status Log

ACS 10 Sept 2004 Users can follow and interact with experiment

David Fraser

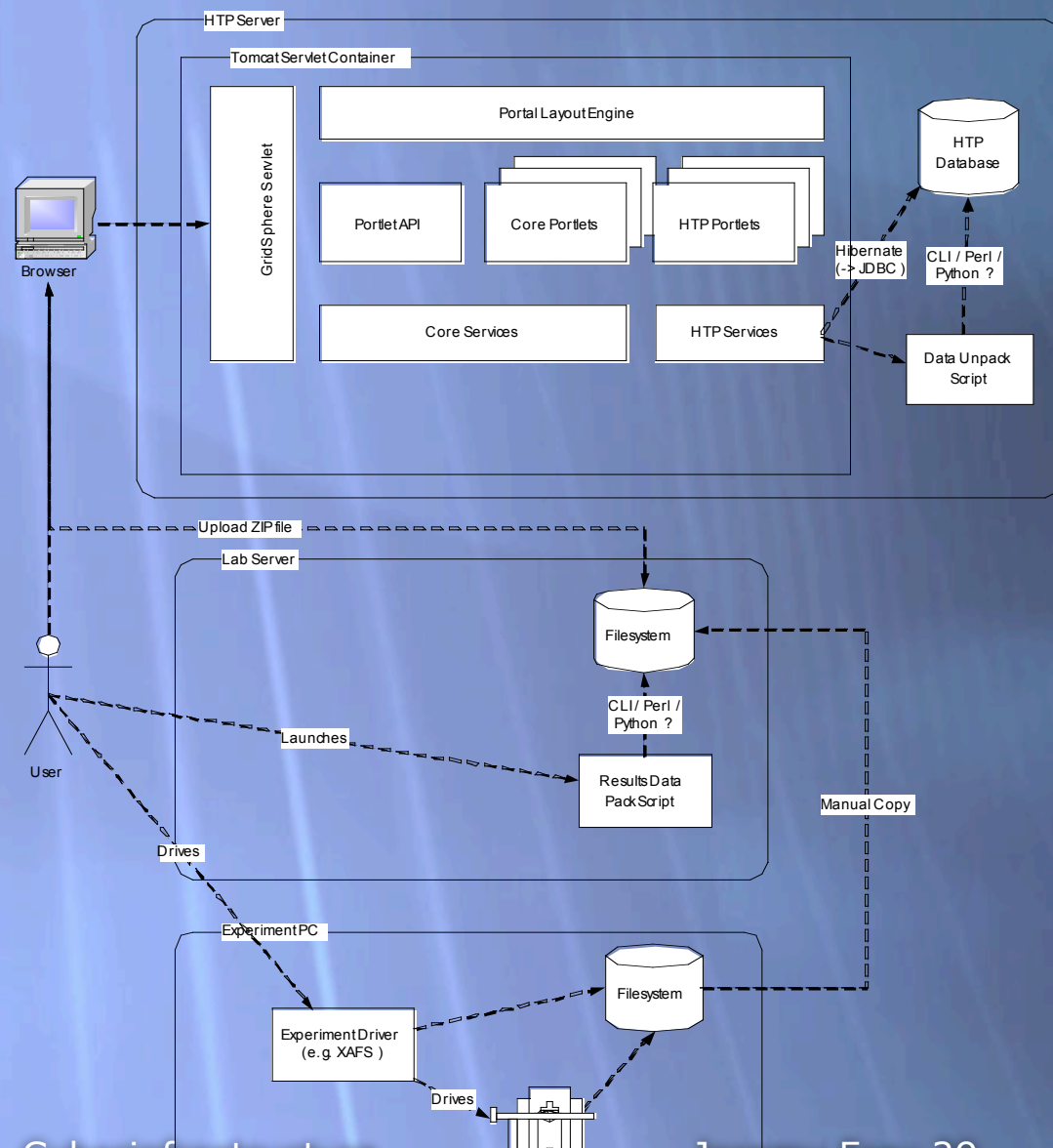
May 28

HTP Sample Tracking

Using ideas from the NCS Grid Service we have produced a prototype for a high throughput catalyst experiment involving array samples investigated by Raman, MS, EXAFS with the samples manufactured at one site and tested at several others

ACS 10 Sept 06

HTP Architecture (First Prototype)

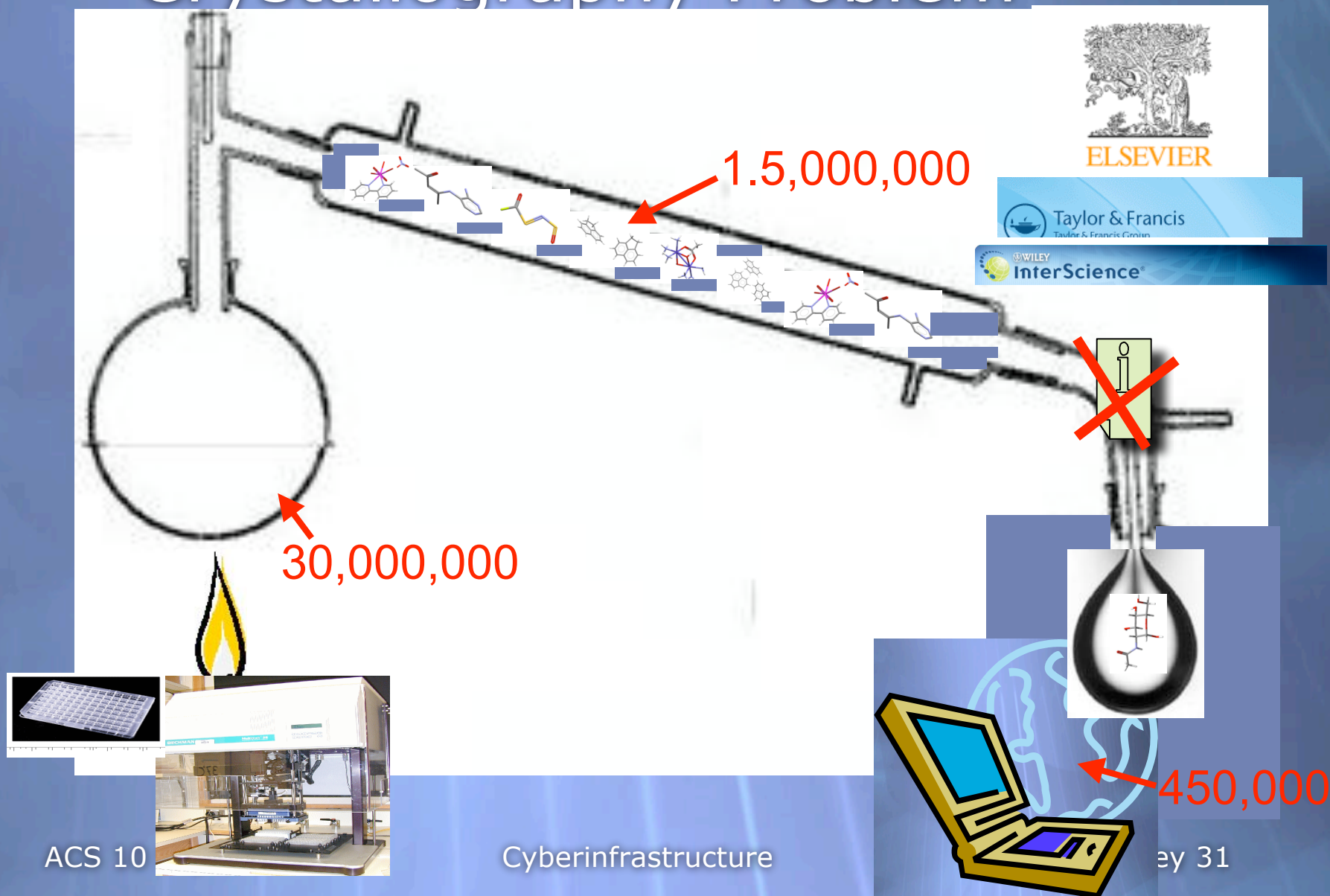


Cyberinfrastructure


Jeremy Frey 29

Dissemination

A Data-Rich Subject – the Crystallography Problem



The eCrystals Data Archive


University of Southampton Crystal Structure Report Archive

[Home](#)
[About](#)
[Browse](#)
[Search](#)
[Register](#)
[User Area](#)
[Help](#)

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

C₁₄H₂₀O₅

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

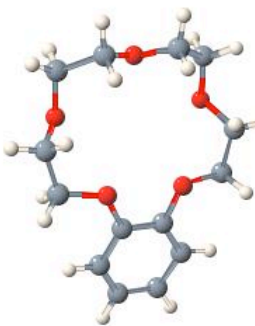
Compound Class: Organic

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
---------------------------------------	-----

Other Files

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

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

ACS 10 Sept 06

Cyberinfr

Access to the underlying data

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

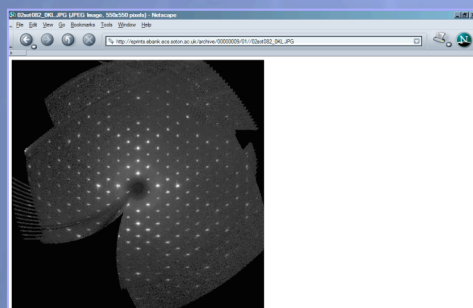
02sot064:PRP 5k

Processing

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

Other Files

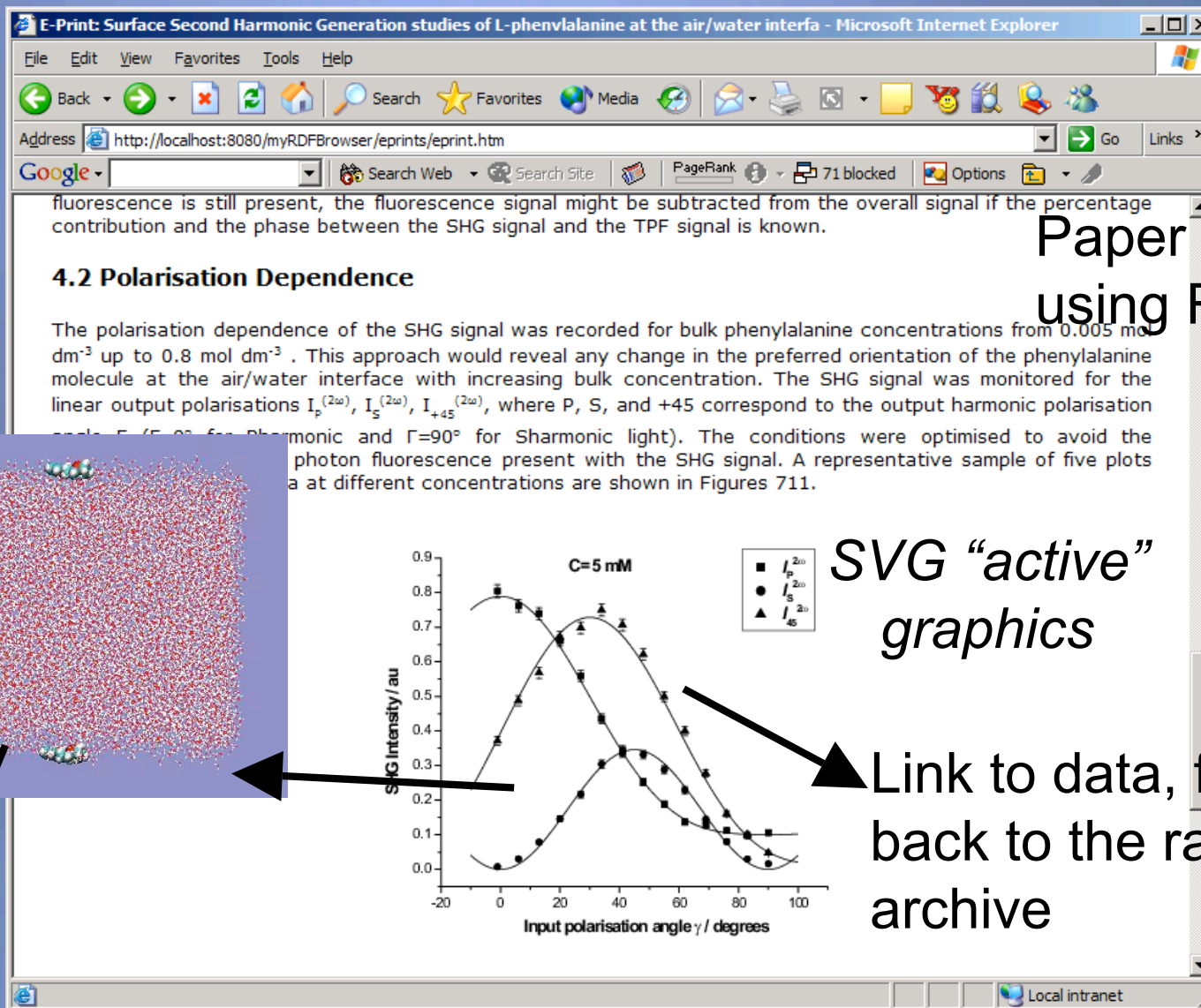
02sot064.DOC	113k
02sot064.LST	49k



AC

Cyberi

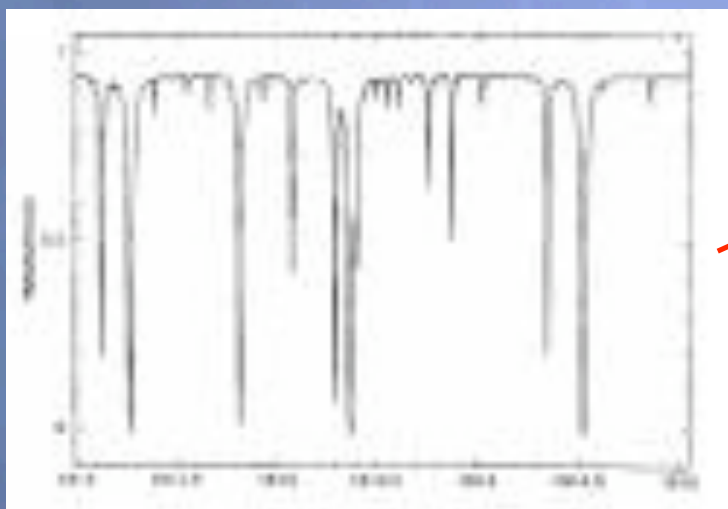
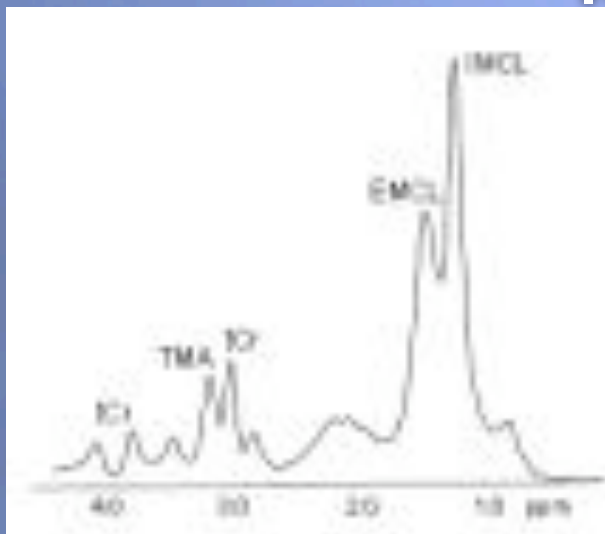
Jeremy Frey 33



Paper organized using RDF

Link to simulation, full simulation data archived in BioSimGrid

Need for a data archive in the laboratory



by passing through columns of P_2O_5 with moisture indicator and 4 Å molecular sieves and permeation chromatography (GPC) measurements were performed on a Polymer Laboratories PL-GPC-220 instrument equipped with a PL-gel 5 Å Mixed-C column, a refractive index detector, and a PD2040 light scattering detector. The GPC column was calibrated using eight monodisperse polystyrene standards in the range 580–48300 Da.

Preparation of $CPh_3[NCPBB](1)$

Potassium cyanide (33.6 mg, 0.5 mmol) was ground to a powder using a pestle and mortar in a dry box. PBB (0.478 g, 0.5 mmol) and 50 mL diethyl ether were then added, and the mixture was heated to reflux for 12 h. The solvent was removed *in vacuo* to leave a off-white foam which was washed with warm hexane (50 mL) to give $K[NCPBB]$ as a white powder (0.495 g, 48% yield). This solid was stirred with triphenylchloromethane (0.135 g, 0.485 mmol) in dichloromethane (15 mL) for 3 h. The solution was filtered to remove KCl, concentrated to ca. 5 mL and cooled to $-26^\circ C$ to give an orange crystalline solid, yield: 0.324 g (0.315 mmol, 63% with respect to KCN). IR (nujol): 2189 cm^{-1} (ν_{CN}). 1H NMR (CD_2Cl_2 , $20^\circ C$, 300.13 MHz): δ 8.28 (t, 3 H, $J = 7.5$ Hz, *p*-Ph), 7.90 (t, 6 H, $J = 7.5$ Hz, *m*-Ph), 7.70 (d, 6 H, $J = 7.3$ Hz, *o*-Ph). ^{13}C NMR (CD_2Cl_2 , $20^\circ C$, 75.48 MHz): δ 211.4 (CPh_3), 144.0 (*p*-C), 143.0 (*m*-C), 140.3 (*ipso*-C), 131.0 (*o*-C), 153.6, 150.3, 147.5, 146.4, 140.3, 139.6, 136.9, 136.3, 128.3, 113.5, 109.5 (Ar C-F). ^{11}B NMR (CD_2Cl_2 , $20^\circ C$, 96.3 MHz): δ -16.2 (br s). ^{19}F NMR (CD_2Cl_2 , $20^\circ C$, 282.4 MHz): δ -118.72 (br, s, 1 F), -120.22 (br, s, 1 F), -121.99 (br, s, 1 F), -122.50 (s, 1 F), -132.20 (s, 1 F), -133.94 (br, 6 F, *o*-F on $B(C_6F_5)_3$), overlapping signals (-134.15, -134.39, -134.95, -135.27, -135.64), 136.89 (br, 1 F), -137.81 (br, 3 F), -138.79 (d, 1 F), -144.73 (t, 1 F), -149.78 (t, 1 F), -151.11 (t, 1 F), -154.65 (t, 1 F), -154.93 (t, 1 F), -155.32 (t, 1 F), -156.86 (t, 1 F), -157.24 (t, 1 F), -157.55 (t, 1 F), -158.29 (m, 1 F), -158.90 (t, 1 F), -159.57 (t, 3 F, $J = 20$ Hz, *p*-F on $B(C_6F_5)_3$), -159.98 (t, 1 F), -161.44 (br, 2 F), -164.0 to -164.4 (overlapping signals, 3 F), -165.33 (br, 2 F), -166.12 (t, 3 F, $J = 20$ Hz, *m*-F on $B(C_6F_5)_3$). Anal. Calcd for $C_{24}H_{15}B_2F_8N$:

Preparation of $CPh_3[(C_6F_5)_3BCNPBB](2)$

$Me_3SiNCB(C_6F_5)_3$ (0.51 g, 0.84 mmol) and Ph_3CCl (0.23 g, 0.84 mmol) were stirred in 20 mL of dichloromethane for 0.5 h to give a yellow solution. After removal of volatiles *in vacuo*, the residue was washed with pentane (30 mL), PBB (0.81 g, 0.84 mmol) and dichloromethane (30 mL) were added, and the mixture was stirred for 2 h. The solvent was then removed. The product was washed again with 30 mL of pentane and dried *in vacuo* to yield a yellow-orange powder (yield 1.01 g, 5.8 mmol, 69%). Attempts to recrystallise the product from dichloromethane were not successful. IR (nujol): 2284 cm^{-1} (ν_{CN}). 1H NMR (CD_2Cl_2 , $20^\circ C$, 300.13 MHz): δ 8.56 (t, 3, $J = 8.0$ Hz *p*-Ph), 7.90 (t, 6 H, $J = 7.5$ Hz, *m*-Ph), 7.70 (d, 6 H, $J = 7.2$ Hz, *o*-Ph). ^{13}C NMR (CD_2Cl_2 , $20^\circ C$, 75.48 MHz): δ 211.0 (CPh_3), 144.1 (*p*-C), 143.0 (*m*-C), 140.1 (*ipso*-C), 130.9 (*o*-C). ^{11}B NMR (CD_2Cl_2 , $20^\circ C$, 96.3 MHz): δ -4.35 (br, 1 B, N- $B(C_6F_5)_3$), -18.27 (s, 1 B, $C-B(C_6F_5)_3$). ^{19}F NMR (CD_2Cl_2 , $20^\circ C$, 282.4 MHz): δ -118.72 (br, s, 1 F), -120.22 (br, s, 1 F), -121.99 (br, s, 1 F), -122.50 (s, 1 F), -132.20 (s, 1 F), -133.94 (br, 6 F, *o*-F on $B(C_6F_5)_3$), overlapping signals (-134.15, -134.39, -134.95, -135.27, -135.64), 136.89 (br, 1 F), -137.81 (br, 3 F), -138.79 (d, 1 F), -144.73 (t, 1 F), -149.78 (t, 1 F), -151.11 (t, 1 F), -154.65 (t, 1 F), -154.93 (t, 1 F), -155.32 (t, 1 F), -156.86 (t, 1 F), -157.24 (t, 1 F), -157.55 (t, 1 F), -158.29 (m, 1 F), -158.90 (t, 1 F), -159.57 (t, 3 F, $J = 20$ Hz, *p*-F on $B(C_6F_5)_3$), -159.98 (t, 1 F), -161.44 (br, 2 F), -164.0 to -164.4 (overlapping signals, 3 F), -165.33 (br, 2 F), -166.12 (t, 3 F, $J = 20$ Hz, *m*-F on $B(C_6F_5)_3$). Anal. Calcd for $C_{24}H_{15}B_2F_8N$:

Not just the published spectra!
Cyberinfrastructure Jeremy Frey 35

The R4L Repository

Deposit

Chemical Name *
The name of the chemical compound which is the subject of the experiment.

InChI *
InChI (International Chemical Identifier) code describing the chemical compound which is the subject of the experiment.

Experimental Technique *
The technique used to produce data about the chemical compound.

Single Crystal Diffraction
Powder X-Ray Diffraction
Infra-Red Spectroscopy
Ultra-Violet Spectroscopy
Mass Spectroscopy
Raman Spectroscopy
Optical Microscopy
Differential Scanning Calorimetry
Thermogravimetric Analysis
Nuclear Magnetic Resonance

Instrument *
Manufacturer and model of instrument used.

Date *
The date that the experiment was carried out.
"Day" or both "Month" and "Day" may be omitted if appropriate.
Year: Month: Unspecified Day:

Time *
The time that the experiment was carried out.

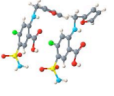
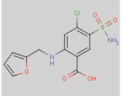
Experimenters *
The research worker(s) who conducted the experiment.

Family Name	Given Name / Initials	Email (if known)
<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="text"/>	<input type="text"/>	<input type="text"/>
<input type="text"/>	<input type="text"/>	<input type="text"/>

[More Spaces](#)

R4L Repository for the Laboratory Home About Browse Search Register User Area Help

Furosemide Form1
Furosemide Form1 (Single Crystal Diffraction): 10 December 2003 14:05. Hughes, David S and Karami, Sohrab (for: Hursthouse, Michael B and Coles, Simon J).

Experiment data files:

- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)

InChI: CC1=CC=C(C=C1)NC(=O)C2=CC(=C(C=C2)S(=O)(=O)N)C(=O)O

Instrument: Bruker Nexus 3000 Area Detector

ID Code: 6

Deposited By: [Dr Simon Coles](#)

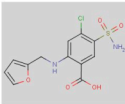
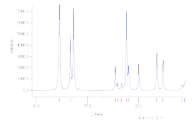
Deposited On: 06 October 2005

File: [furosemide_form1.pdf \(17.1 kb\)](#)

Repository Staff Only: [edit this item](#)

R4L Repository for the Laboratory Home About Browse Search Register User Area Help

Furosemide Form1
Furosemide Form1 (Powder X-Ray Diffraction): 14 September 2004 10:19. Hughes, David S and Light, Mark E (for: Hursthouse, Michael B and Coles, Simon J).

Experiment data files:

- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)
- [furosemide_form1.pdf \(17.1 kb\)](#)

InChI: CC1=CC=C(C=C1)NC(=O)C2=CC(=C(C=C2)S(=O)(=O)N)C(=O)O

Instrument: Bruker D5000

ID Code: 7

Deposited By: [Dr Simon Coles](#)

Deposited On: 06 October 2005

File: [furosemide_form1.pdf \(17.1 kb\)](#)

Repository Staff Only: [edit this item](#)

[Contact Information](#)

R4L Repository for the Laboratory Home About Browse Search Register User Area Help

InChI:
InChI=1/2C12H11ClN2O5S/c2*13-9-5-10(15-6-7-2-1-3-20-7)8(12(16)17)4-11(9)21(14,18)19/h2*1-5,15H,6H2,(H,16,17)(H2,14,18,19)

Number of items: 4.

[Furosemide Form1](#). (Optical Microscopy): 30 September 2004 15:57. Hughes, David S (for: Hursthouse, Michael B and Coles, Simon J).

[Furosemide Form1](#). (Powder X-Ray Diffraction): 14 September 2004 10:19. Hughes, David S and Light, Mark E (for: Hursthouse, Michael B and Coles, Simon J).

[Furosemide Form1](#). (Infra-Red Spectroscopy): 29 July 2004 12:09. Hughes, David S (for: Hursthouse, Michael B and Coles, Simon J).

[Furosemide Form1](#). (Single Crystal Diffraction): 10 December 2003 14:05. Hughes, David S and Karami, Sohrab (for: Hursthouse, Michael B and Coles, Simon J).

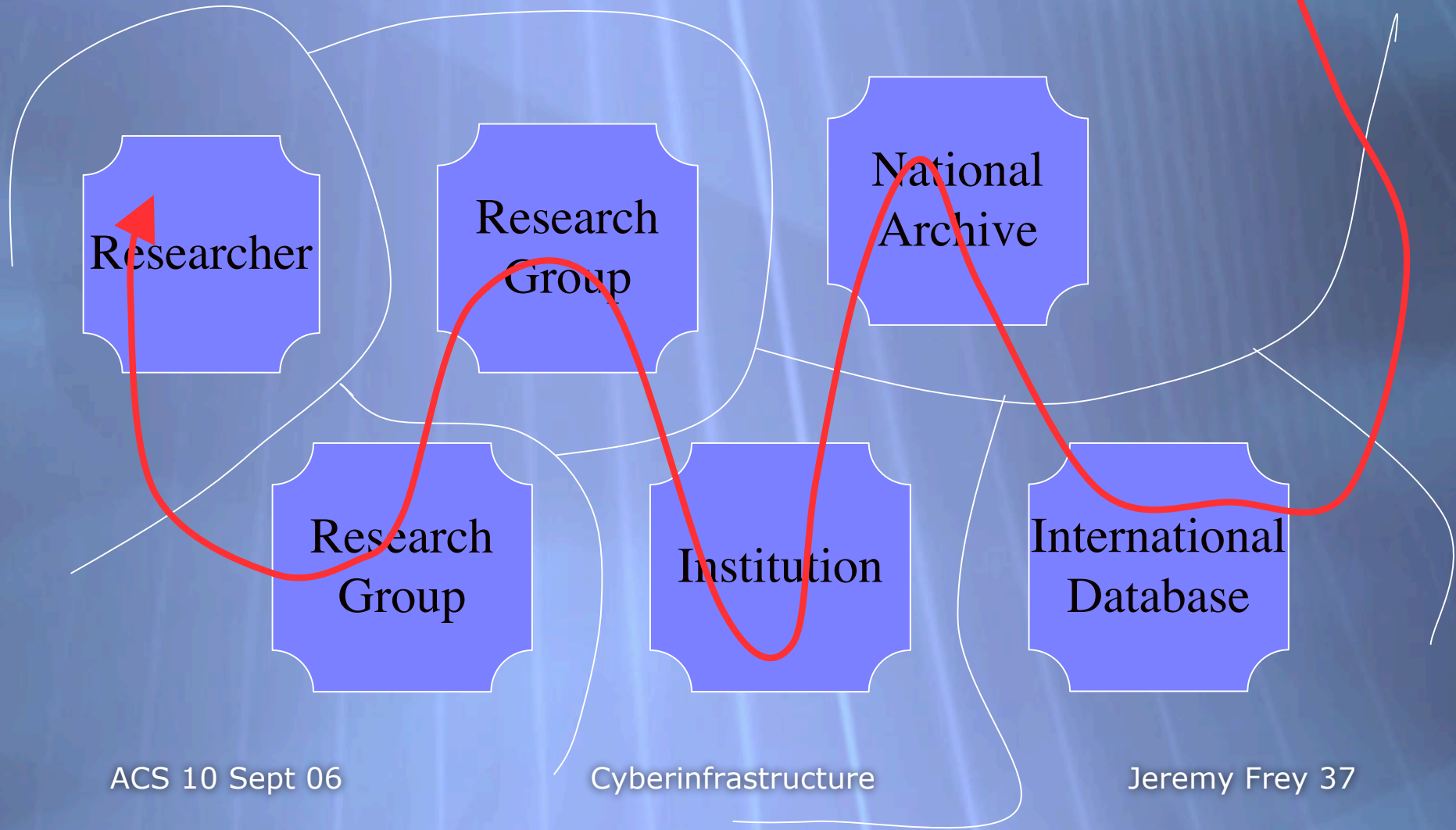
This list was generated on **Sun Nov 6 19:30:03 GMT 2005**.

[Contact Information](#)

Search

Jeremy Frey 36

Several groups making and analysing the library Administrative Domains transfer or share the data



Summary:

- ✦ Making sure other people can find, understand and re-use your data easily and with confidence (even when there is a huge amount of it!)
- ✦ Make use of Plans to inform the digital context - metadata in advance
- ✦ Have concern for the “End-to-End life cycle” of chemistry information from the start.
- ✦ Understanding Usability and Human Computer Interaction is vital for adoption

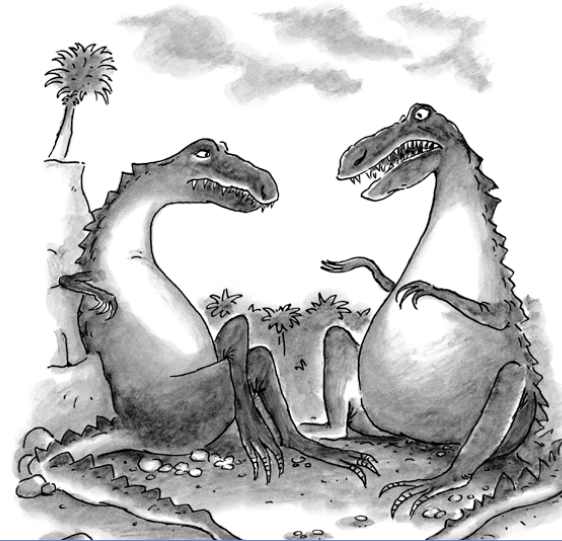
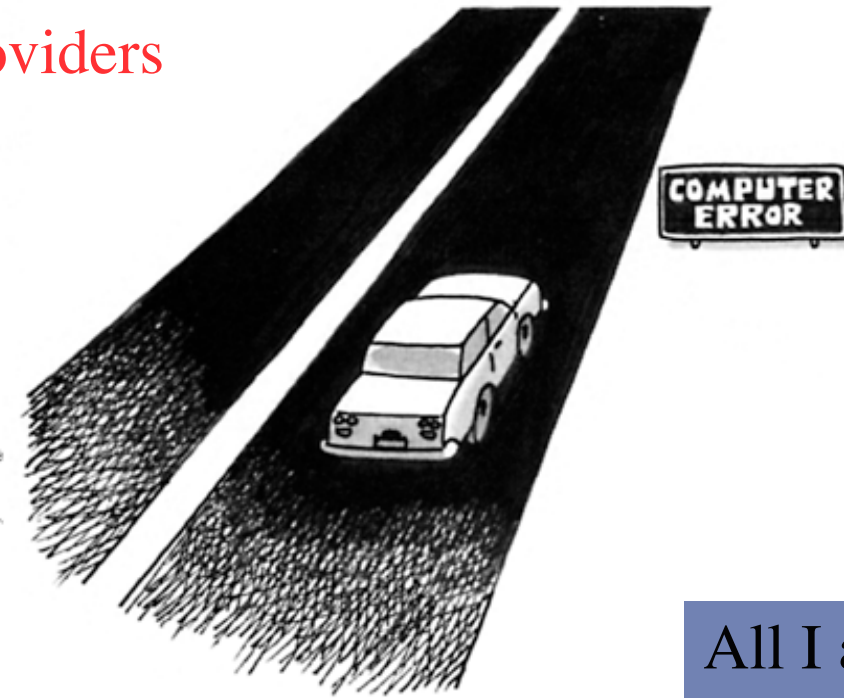
Summary:

- ✦ Is the semantic web/grid enough
- ✦ It is sufficient to evolve and improve the practice of chemistry
- ✦ It is not enough - 'Pictures are worth a thousand words' more like 10,000 words of metadata
- ✦ The Semiotic Web will be needed to improve the communication of models

Information
Consumers

Information
Providers

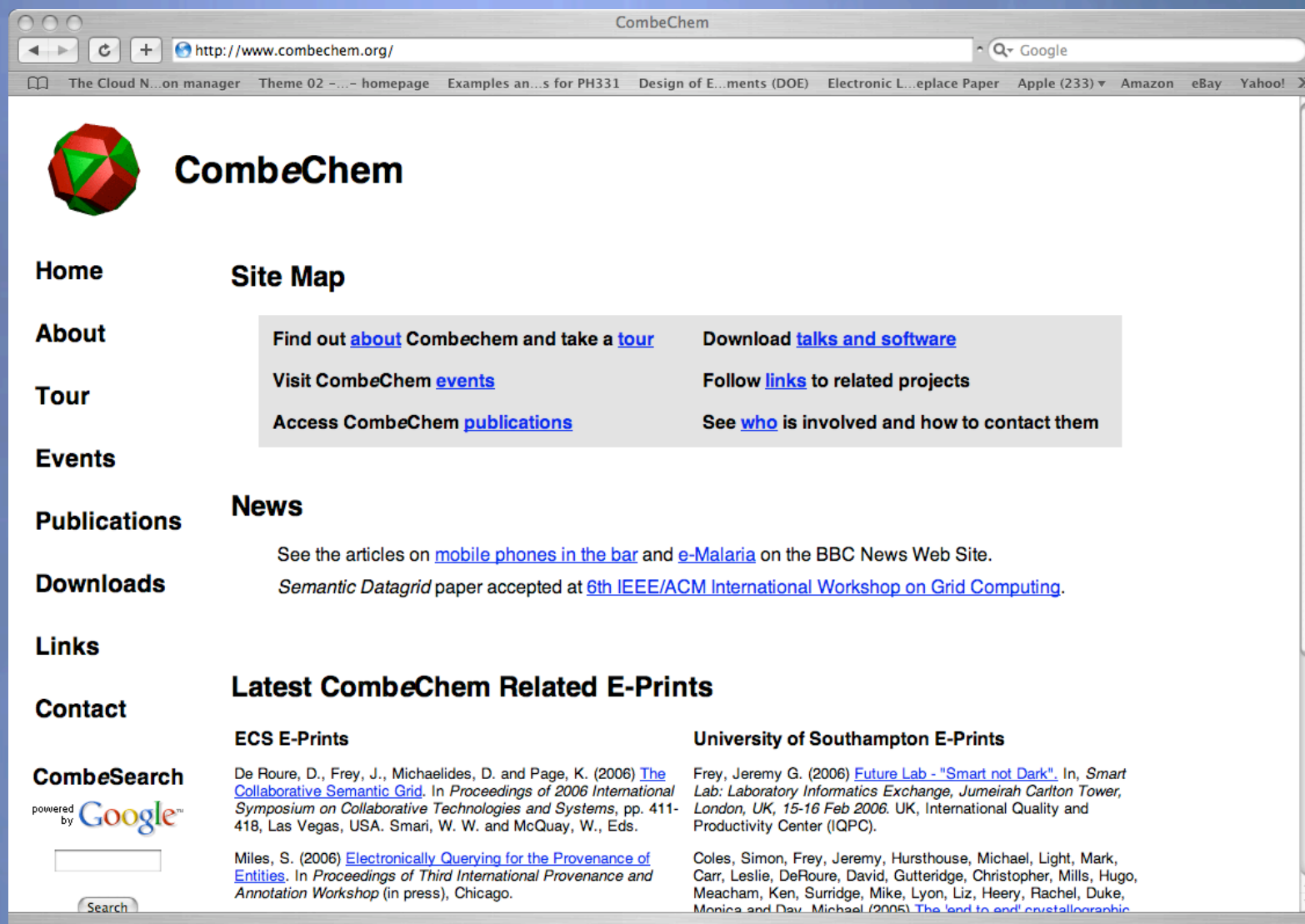
© The New Yorker collection. All rights reserved.
From *The New Yorker Book of Technology Cartoons*.



© The New Yorker collection. All rights reserved.
from *The New Yorker Book of Technology Cartoons*.

All I am saying is that now is the
time to develop the technology to
deflect an asteroid

www.combechem.org



The screenshot shows a web browser window titled "CombeChem" with the address bar displaying "http://www.combechem.org/". The browser's address bar also includes a Google search icon. The website's navigation menu includes links for Home, About, Tour, Events, Publications, Downloads, Links, and Contact. The main content area features a "Site Map" section with links to "about", "tour", "events", "publications", "talks and software", "links", and "who". Below this, there is a "News" section with two articles: "mobile phones in the bar" and "e-Malaria" on the BBC News Web Site, and "Semantic Datagrid paper accepted at 6th IEEE/ACM International Workshop on Grid Computing". The "Latest CombeChem Related E-Prints" section is divided into two columns: "ECS E-Prints" and "University of Southampton E-Prints". The "ECS E-Prints" column lists two papers: "The Collaborative Semantic Grid" by De Roure, D., Frey, J., Michaelides, D. and Page, K. (2006) and "Electronically Querying for the Provenance of Entities" by Miles, S. (2006). The "University of Southampton E-Prints" column lists two papers: "Future Lab - 'Smart not Dark'" by Frey, Jeremy G. (2006) and "The 'end to end' crystallographic" by Coles, Simon, Frey, Jeremy, Hursthouse, Michael, Light, Mark, Carr, Leslie, DeRoure, David, Gutteridge, Christopher, Mills, Hugo, Meacham, Ken, Surridge, Mike, Lyon, Liz, Heery, Rachel, Duke, Monica and Dav, Michael (2005). At the bottom left, there is a "CombeSearch" section powered by Google, with a search input field and a "Search" button.

CombeChem

Home

About

Tour

Events

Publications

Downloads

Links

Contact

Site Map

Find out [about](#) Combechem and take a [tour](#)

Download [talks and software](#)

Visit CombeChem [events](#)

Follow [links](#) to related projects

Access CombeChem [publications](#)

See [who](#) is involved and how to contact them

News

See the articles on [mobile phones in the bar](#) and [e-Malaria](#) on the BBC News Web Site.

[Semantic Datagrid](#) paper accepted at [6th IEEE/ACM International Workshop on Grid Computing](#).

Latest CombeChem Related E-Prints

ECS E-Prints

De Roure, D., Frey, J., Michaelides, D. and Page, K. (2006) [The Collaborative Semantic Grid](#). In *Proceedings of 2006 International Symposium on Collaborative Technologies and Systems*, pp. 411-418, Las Vegas, USA. Smari, W. W. and McQuay, W., Eds.

Miles, S. (2006) [Electronically Querying for the Provenance of Entities](#). In *Proceedings of Third International Provenance and Annotation Workshop* (in press), Chicago.

University of Southampton E-Prints

Frey, Jeremy G. (2006) [Future Lab - "Smart not Dark"](#). In, *Smart Lab: Laboratory Informatics Exchange, Jumeirah Carlton Tower, London, UK, 15-16 Feb 2006*. UK, International Quality and Productivity Center (IQPC).

Coles, Simon, Frey, Jeremy, Hursthouse, Michael, Light, Mark, Carr, Leslie, DeRoure, David, Gutteridge, Christopher, Mills, Hugo, Meacham, Ken, Surridge, Mike, Lyon, Liz, Heery, Rachel, Duke, Monica and Dav, Michael (2005) [The 'end to end' crystallographic](#)

CombeSearch

powered by Google

Search