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# The Chemistry Preprint Server: An Experiment in Scientific Communication

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**WORKSHOP ON OAI AND PEER REVIEW JOURNALS IN EUROPE**

Geneva, 22<sup>nd</sup> March 2001

# Outline of Presentation

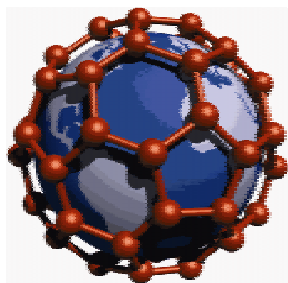
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- ◆ **Introduction to ChemWeb.com**
- ◆ **Chemistry Preprint Server**
  - ◆ Overview
  - ◆ Submission procedure
  - ◆ Browsing and searching
  - ◆ Where we are now
- ◆ **Future Directions**
- ◆ **Conclusions**
- ◆ **Questions & Discussion**

# ChemWeb.com

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- ◆ Online resource for the chemical community
- ◆ Free registration and membership
- ◆ Access to essential services and information
  - ◆ Journals, Databases, *The Alchemist* Magazine, Shopping Mall, Conference Centre, Careers Centre, Forums



# ChemWeb.com

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- ◆ Offer free services - temporary & permanent
  - ◆ Access to journals
  - ◆ AutoNom and Beilstein Abstracts
- ◆ Encourage member interaction - e.g. forums
- ◆ Exploit web technology and functionality - e.g. structure searching
- ◆ Over 250,000 members, 2.5 million page impressions per month

**Ideal host for the Chemistry Preprint Server!**

# Chemistry Preprint Server

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- ◆ Freely available and permanent web archive and distribution medium for research articles
- ◆ Scientific articles freely available for public access prior to formal review
- ◆ Preprint NOT prepublication
- ◆ The first Chemistry Preprint Server!
  - ◆ Modelled on very successful arXiv preprint server, run by LANL, for mathematics and physics



<http://preprint.chemweb.com>

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# Launch of the CPS

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- ◆ Launched 21 August 2000 at the ACS National Meeting
- ◆ 20 Preprints submitted prior to launch
- ◆ Positive response at the meeting
- ◆ Primary concerns were issues of prior publication and quality control

# CPS Procedure (1)

## ◆ Author uploads preprint:

- ◆ Article, meta-data (abstract, author details etc) & supplementary files submitted
- ◆ File types supported include PDF, MS Word, Postscript, RTF and HTML
- ◆ Author selects classification
- ◆ Automatic conversion to PDF
- ◆ Article screened by 'editor'



## ◆ Author revisions possible (version control)

- ◆ Option to redirect to online version at publisher's site following publication

# CPS Procedure (2)

## ◆ 10 Classifications:

- ◆ Analytical Chemistry
- ◆ Biochemistry
- ◆ Chemical Engineering
- ◆ Environmental Chemistry
- ◆ Inorganic Chemistry
- ◆ Macromolecular Chemistry
- ◆ Medicinal Chemistry
- ◆ Organic Chemistry
- ◆ Physical Chemistry
- ◆ Miscellaneous

## ◆ New Conference Proceedings section

- ◆ Submit pre-conference abstracts or post-conference reports



The screenshot displays the Chemistry Preprint Server (CPS) website. At the top, the logo reads "the chemistry preprint server" with navigation links for Home, Browse, Search, Submit, Help, Demo, and ChemWeb.com. Below the logo is a table titled "Browse results in CPS based on all" with columns for Classification, Total, This Month, and Today. The table lists various chemistry fields and their corresponding article counts. To the right of the table are several sidebar sections: "Communities" with a link to "What's your speciality?", "the Alchemist" with "Daily news and reviews", "last updated" showing "14 March 2001 13:46", "no. of articles" showing "164", "quick find" with links for "most viewed", "most discussed", "highest ranked", and "most recent", "quick search" with a search box and "Go" button, "[Advanced Search]", "CPS Disclaimer", and a "Log off?" button.

Classification	Total	This Month	Today
<a href="#">Analytical Chemistry</a>	17	2	0
<a href="#">Biochemistry</a>	9	0	0
<a href="#">Chemical Engineering</a>	13	3	0
<a href="#">Environmental Chemistry</a>	9	0	0
<a href="#">Inorganic Chemistry</a>	17	0	0
<a href="#">Macromolecular Chemistry</a>	6	1	0
<a href="#">Medicinal/Pharmaceutical Chemistry</a>	5	1	0
<a href="#">Miscellaneous</a>	7	0	0
<a href="#">Organic Chemistry</a>	21	1	0
<a href="#">Physical Chemistry</a>	60	19	1
<a href="#">Conference Proceedings</a>	11	2	0



# CPS Procedure (3)

- ◆ Every article is given a unique identifier
  - ◆ “Friendly URL” & Citation Reference

Please use CPS: anahens0012001 in any reference to this article

Analytical Chemistry > Crystallography

Discussion • Rank

Conference Proceedings

## ESPOIR : A Program for Solving Structures by Monte Carlo from Powder Diffraction Data

Armel Le Bail

CNRS

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Submitted on 13 December 2003/12:48

Abstract

A direct-space program (ESPOIR) for the crystal structure of small molecules, from powder diffraction data, is developed under the GNU Public License. The program allows solving the structure of the two samples distributed during the Structure Determination Powder Diffractometry Round Robin (SDPCRR): the lefthand hydrochloride and a cobalt-amine. Three calculation modes are possible, either locating up to 4 different molecule fragments starting from a set of randomly distributed atoms, or mixed approaches.



Full text

Uploaded supplement

- [esdic-7.html](#)
- [espoir-program.pdf](#)
- [espoir.txt](#)

Disclaimer

Discussion

[New thread] [Alert on entire discussion]

last updated  
13 December  
2003/12:48

viewed  
131 times

ranked  
★★★★★

Embed this content  
in a blog

CPS Disclaimer

[http://preprint.chemweb.com/  
category/YMMNNN](http://preprint.chemweb.com/category/YMMNNN)

**CPS: category/YMMNNN**



# CPS Procedure (4)

## ◆ Users can discuss & rank articles

• [Comment](#) James Boggs (28 Dec 2000 18:01:12)  
This is an innovative new work. The insights provided are useful to both experimentalists and theoreticians.  
[Reply](#) [filed on Comment](#)

Rank

Please select from the drop down menu the number of stars you think this preprint deserves.

Give rank  

## ◆ Quick and advanced searching and browsing

- ◆ Comprehensive searching across all fields
- ◆ Users can access most recent, most viewed, most discussed & highest ranked articles

### Search Preprints

Example : 'organic synthesis' and terpenoids

Restrict by field	No. of hits
All	10

Between (dates)  and

quick find  
▶ [most viewed](#)  
▶ [most discussed](#)  
▶ [highest ranked](#)  
▶ [most recent](#)

quick search

[Advanced Search](#)

# CPS Procedure (5)

- ◆ Individual user profile - email alerts:
  - ◆ Searches for key words and phrases
  - ◆ New articles added to a particular classification
  - ◆ New threads added into a discussion group

Email alerts for: Dr James Weeks

<b>Classification</b>	Conference Proceedings	[delete]
<b>Discussion</b>	All discussions in <a href="#">Formation and Colapse of Gels of Sterically Stabilised Colloidal Particles</a>	[delete]
<b>Search</b>	colloid on all	[delete]

preprint@chemwe... New article added to Analytical Chemistry Wed 07/02/01 15:..

- ◆ Recommend preprint to a friend

## Email this preprint to a friend

**Title:** ESPOIR : A Program for Solving Structures by Monte Carlo from Powder Diffraction Data  
**Authors:** Amel Le Bail

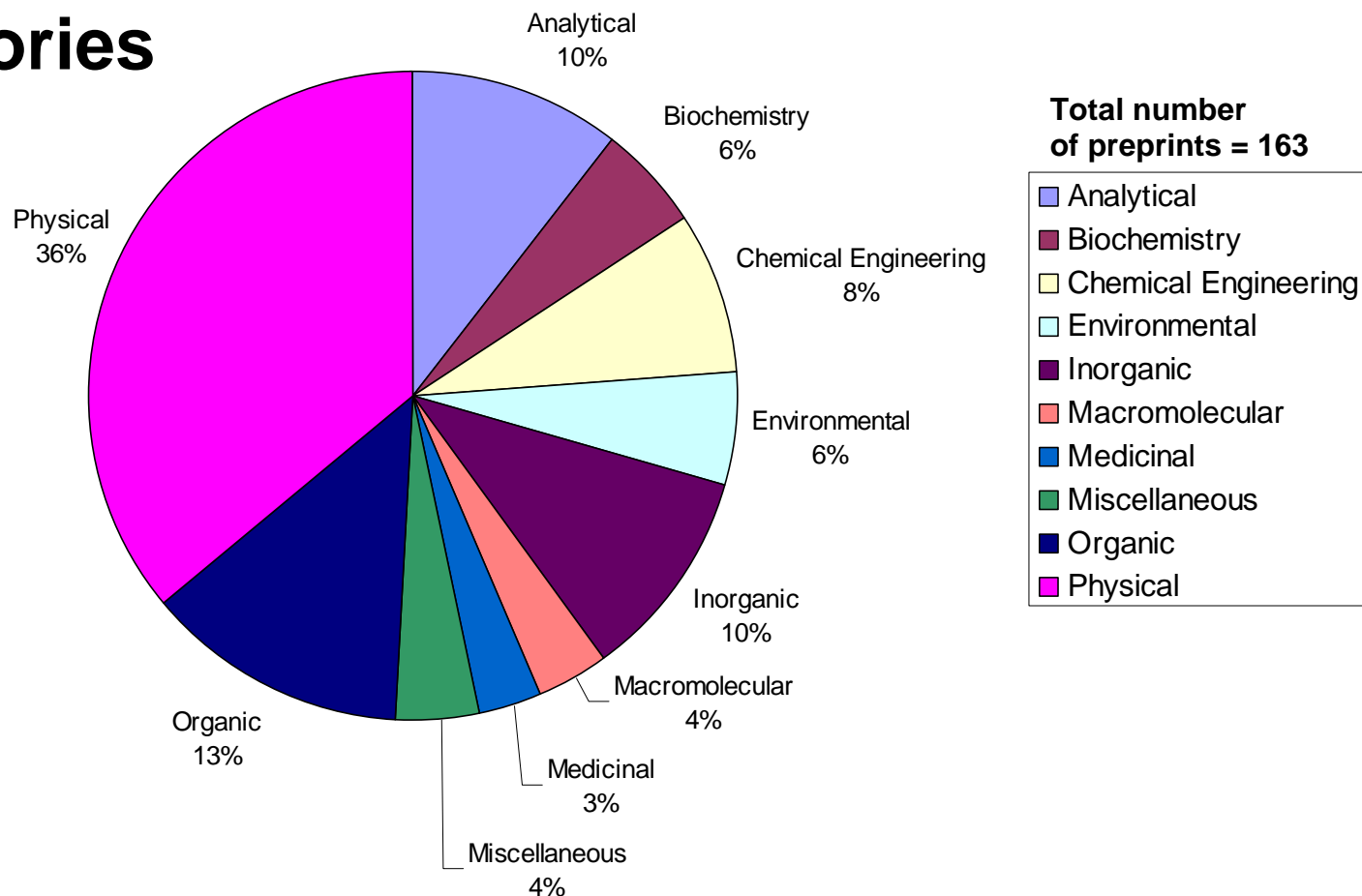
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Send Email to:

Add comment to email:

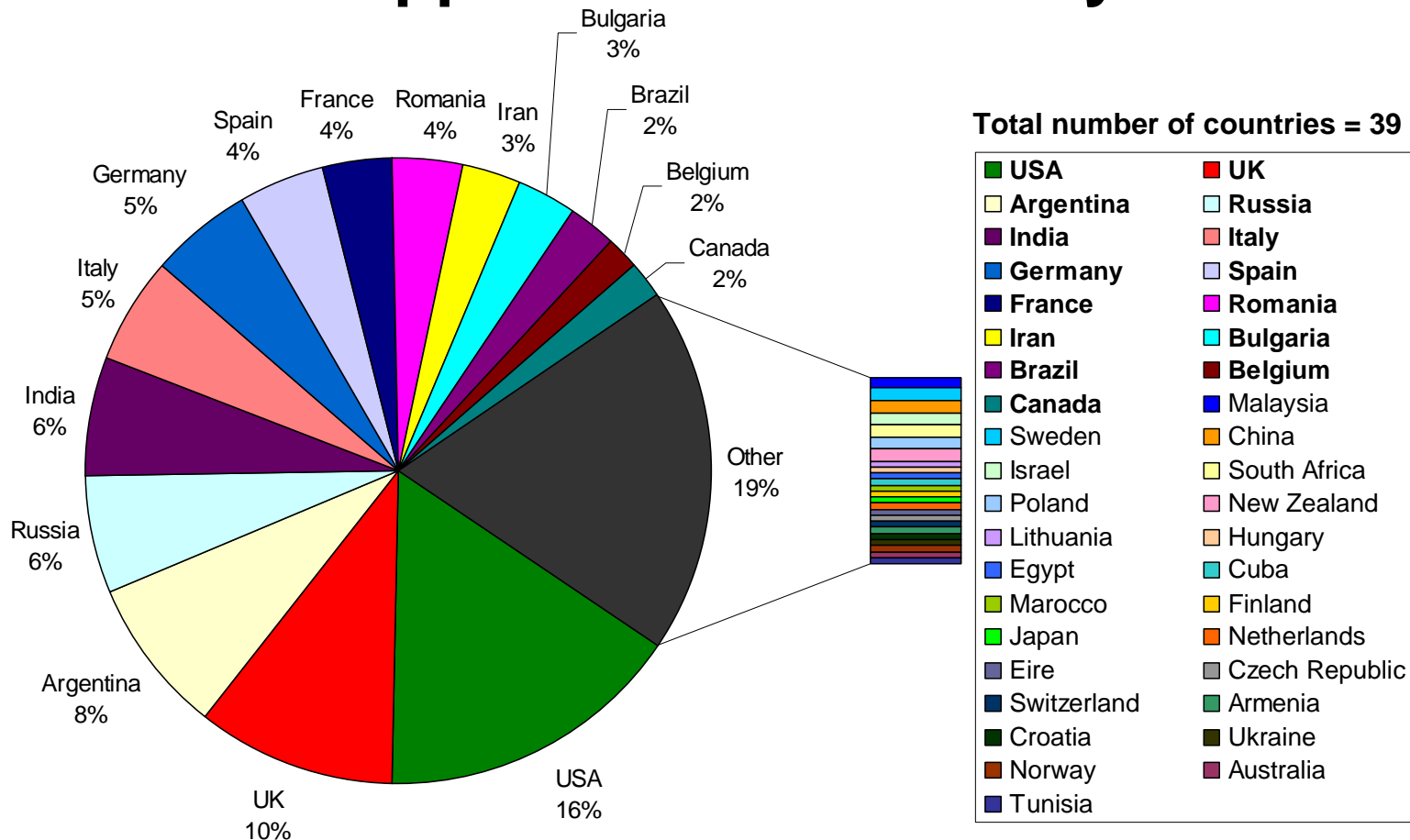
# CPS - Where We Are Now (1)

- ◆ Over 160 articles submitted in all ten categories



# CPS - Where We Are Now (2)

## ◆ World-wide appeal to the chemistry community



# CPS - Where We Are Now (3)

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- ◆ Each of the top 20 “most viewed” preprints has been viewed by more than 500 individuals
  - ◆ Top article has over 2000 viewings
- ◆ Over 100,000 page impressions per month
- ◆ Limited postings to the online discussions

# Future Directions

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## Compliance with Santa Fe Convention for Open Archives Initiative

- ◆ Implement meta-data protocols in the immediate future
- ◆ Harvest data from Los Alamos (arXiv) preprint server
- ◆ US Department of Energy initiative to develop search engine for preprints (<http://www.osti.gov/preprints/index.html>)
- ◆ **Automatic submission of preprints to journals**
  - ◆ Author selects journal (publisher-neutral) for article submission when satisfied the article is complete
- ◆ **Access the CPS on WAP and Palm devices**

# Conclusions

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- ◆ **At present, the CPS is still an experiment in scientific communication**
- ◆ **Early signs indicate a very positive response from the chemistry community**
- ◆ **Further enhancement: compliance with the Open Archives Initiative**
- ◆ **Exciting possibilities for future development, further enhancing chemistry communication**



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# Thank you for your attention!

**James.Weeks@ChemWeb.com**

**<http://preprint.chemweb.com>**



<http://preprint.chemweb.com>

