

European Learning Grid Infrastructure

The European Learning Grid Infrastructure based on GRID technologies for supporting ubiquitous, collaborative, experiential-based, contextualised and personalised learning



## *Protocols for building an Organic Chemical Ontology*

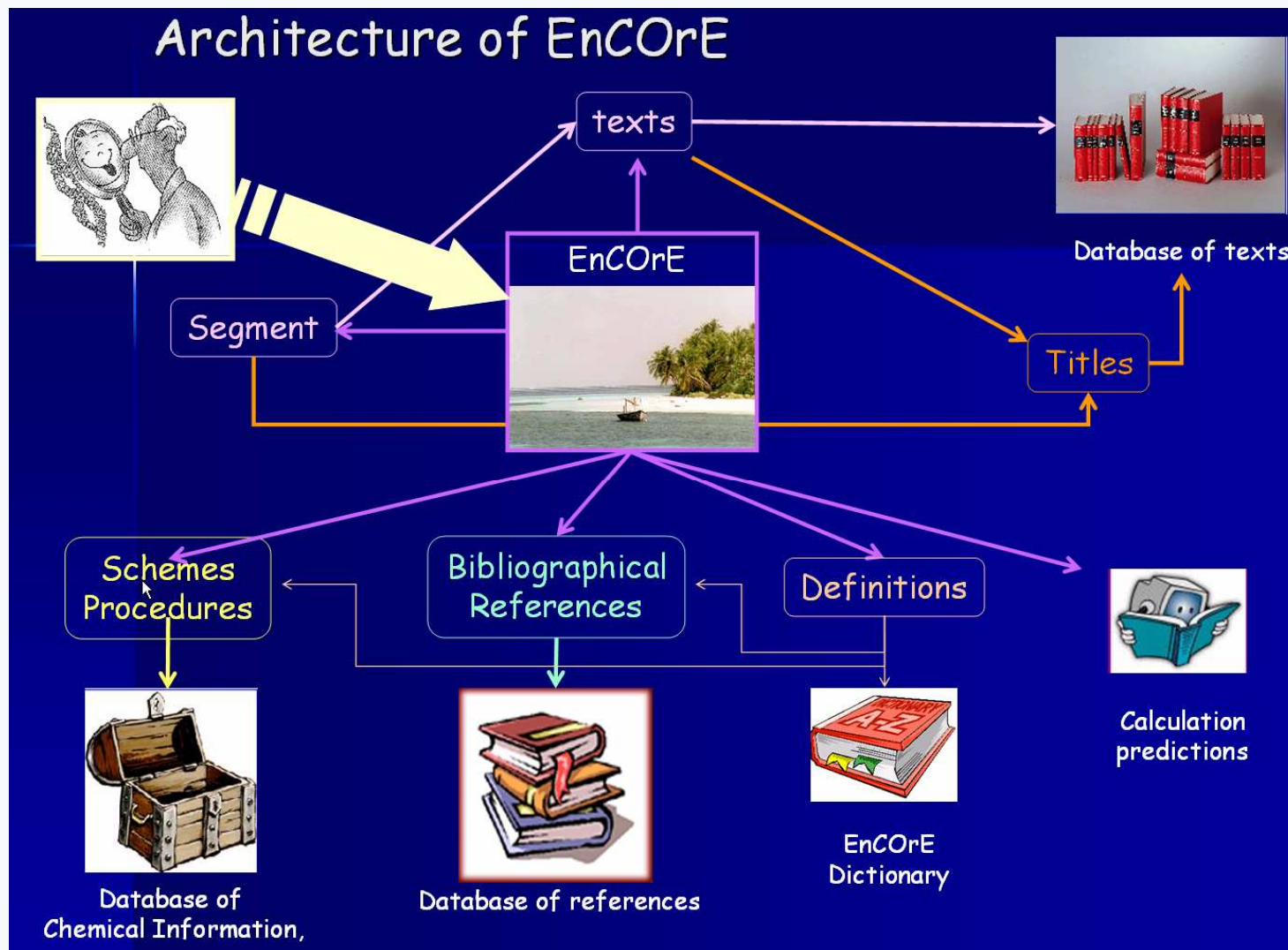
"Research is what I'm doing when I don't know what I'm doing"

Wernher Von Braun



Technology-enhanced learning and access to cultural heritage





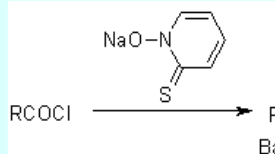
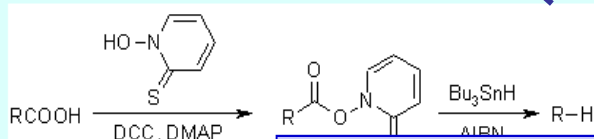
## How to proceed?

### Organic Chemistry Portal

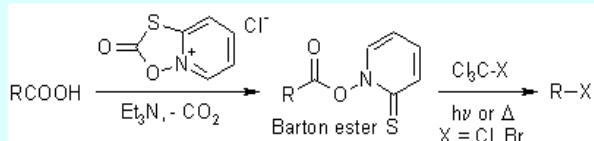
#### Name Reactions

#### Barton Decarboxylation

The radical decarboxylation of a Barton ester proceeds to the corresponding alkane after treatment with [tributyltin hydride](#) or *t*-butylmercaptan:



An alternative possibility is the formation of a Barton ester by reaction with a suitable radical trapping agent:



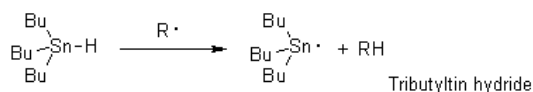
#### Mechanism

The initiation of the Barton Decarboxylation ( $\text{Bu}_3\text{Sn-H} \rightarrow \text{Bu}_3\text{Sn}\cdot$ ) is effected by [Deoxygenation](#), the driving force for the reaction itself is the formation of the

### Chemicals > Reducing Agents

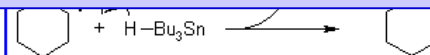
#### Tributyltin hydride (Tributylstannane) / Tin hydrides

Organotin hydrides are very good radical reducing agents due to the relatively weak, nonionic bond between tin and hydrogen ( $\text{Bu}_3\text{SnH}$  74 kcal/mol) that can cleave homolytically.

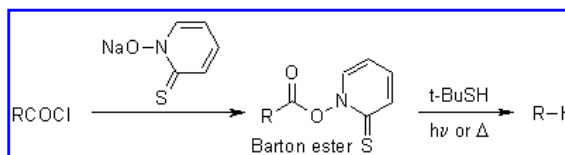


However, these compounds are plagued by their high toxicity and high fat solubility (lipophilicity). Therefore, with few exceptions, the use of tin hydrides should be avoided. The catalytic use of these reagents with a suitable second reducing

How to imagine all the different hyperlinks ?

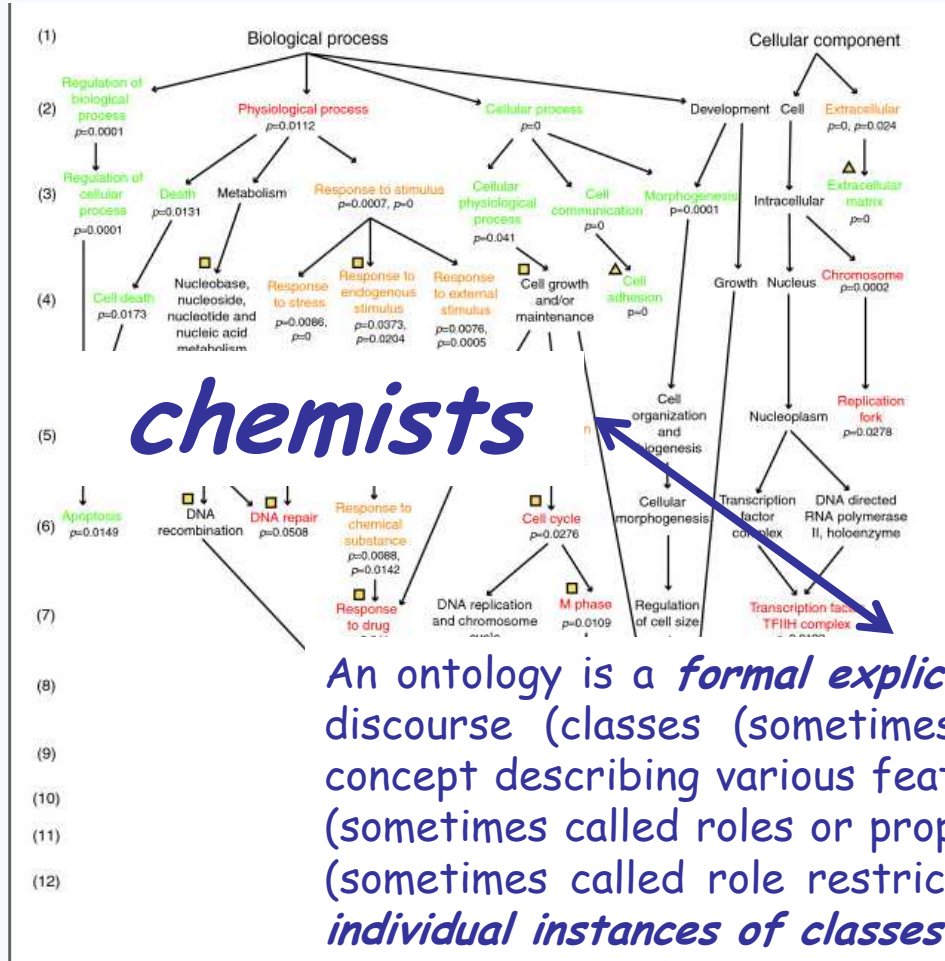


Barton-McCombie reaction



Barton decarboxylation

Additional interesting reactions that employ tin hydrides are dehalogenation and intramolecular radical cyclization.



What is an ontology?

*Ontologists*

## Drafting a protocol: first step

### Creation of a working group:

Gathering chemists of various  
technologies

How to gather so many  
persons?

Ontologists

Create a virtual community

And

Create a work through Internet

Working Group



# Services needed for Conversation & Cooperation (C&C)

The screenshot shows a FlashMeeting Memo interface in Microsoft Internet Explorer. The main window displays a video conference with five participants: a large video of 'monica' and four smaller thumbnails for 'catherine colaux', 'philippe', 'laurenco', and 'krief'. The interface includes a 'JOIN QUEUE (0)' button, a 'VOTING' section with 'Yes', 'Abstain', and 'No' options, and an 'EMOTICONS' section. A chat window on the right shows a list of messages with timestamps and names. A timeline at the bottom shows a sequence of events for 'krief', 'laurenco', and 'Tom Visser'.

Time	Sender
30:55	monica
32:05	catherine colaux
32:37	catherine colaux
33:43	monica
35:04	catherine colaux
35:24	krief
36:06	catherine colaux
36:14	laurenco
37:35	krief
38:14	catherine colaux
39:06	monica
40:03	laurenco
40:55	krief

Option	Count
Yes	0
Abstain	0
No	0

Participant	Event Type	Approximate Time
krief	Message	35:24
laurenco	Message	36:14
Tom Visser	Message	37:35

- 👤 Discussion between chemists in presence of experts in Knowledge engineering (the "ontologist")
- 👤 Integration of the concepts in the ontology, by the "ontologist".
- 👤 Explanations of the "ontologist" on his choices and his manipulations in Protégé.



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# Drafting a protocol: preparation of a Collaboration Session (CS)



- Booking a weekly session of 1 H 30 with all the different participants



- Sending documents to the diffusion list in order to prepare the session and the agenda of the session

**Préparation session\_ EnCORe02**

To: EnCORe Group - okceetris@limm.fr  
 From: Catherine Colaux  
 CC: 2 files Excel  
 Date: 26 janvier 2006  
 FlashMeeting Link: <http://flash.kmi.open.ac.uk>

Participants : Catherine Colaux, Claude Laurencio Visser, Philippe Lemoisson Stefano Cerri et Pascale

Object : fifth collaborative session on the establishment of a glossary of terms for the session.

**1 Proposition :**

**Journal officiel du 22 septembre 2005**  
 NOR : CTX2050662K  
**Termes généraux de la chimie**  
 (liste de termes, expressions et définitions adoptés)

**1. blindage, a.m.**  
 Domaine : Chimie Chimie physique.  
 Définition : Effet d'écran résultant d'un affaiblissement local d'un champ magnétique externe, dû à la présence d'électrons circulant autour d'un noyau atomique, lorsqu'il est exposé à un faible champ magnétique.  
 Note : Cet effet est à la base des méthodes de résonance magnétique nucléaire appliquées à l'étude des molécules comportant au moins un noyau atomique de spin non nul.  
 Équivalent étranger : shielding.

**2. blindage, s.m.**  
 Domaine : Chimie Chimie physique.  
 Définition : Effet d'écran résultant d'un affaiblissement local d'un champ électrique exercé vers l'extérieur par une entité chargée (noyau atomique, ion ou assemblage moléculaire), dû à la présence d'électrons ou d'ions de

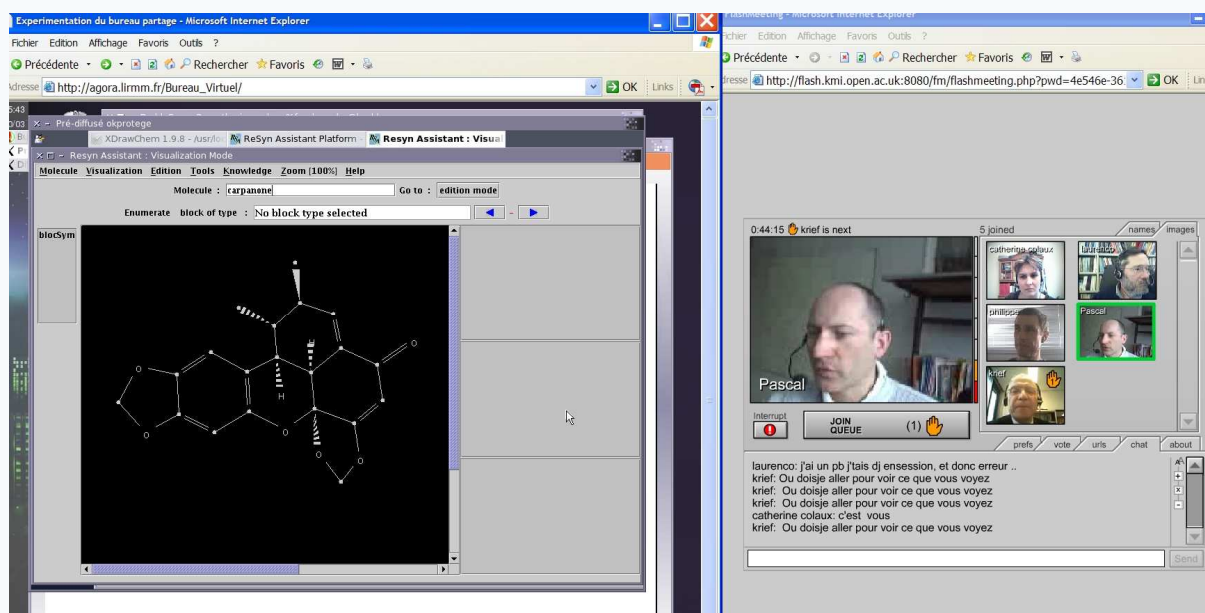
GENERAL CONCEPTS.xls		
1		
2	1	acide/base
3	2	addition
4	3	Aromaticity
5	4	atome
6	5	Bonds
7	6	Catalyst
8	7	catalyst
9	8	chemistry
10	9	Competitive reactions
11	10	compound
12	11	Configuration
13	12	Conformation
14	13	halogenation
15	14	Electronegativity

**Beilstein Data Structure**



## Drafting a protocol: the 'settings' for C&C

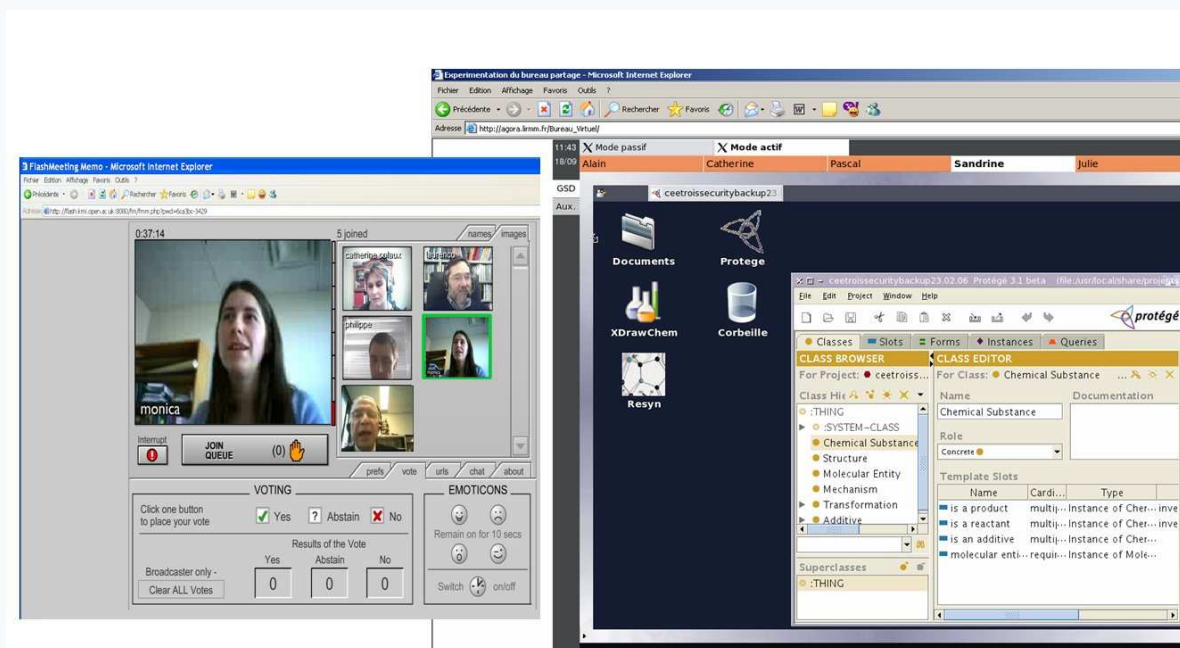
- Working through (GSD + FM) at the construction of the ontology
  - The chemists start the discussion, in the presence of ontology's expert, about the selected field, they extract from it the most adequate terms and their relations.



The screenshot displays a shared desktop environment with two main windows:

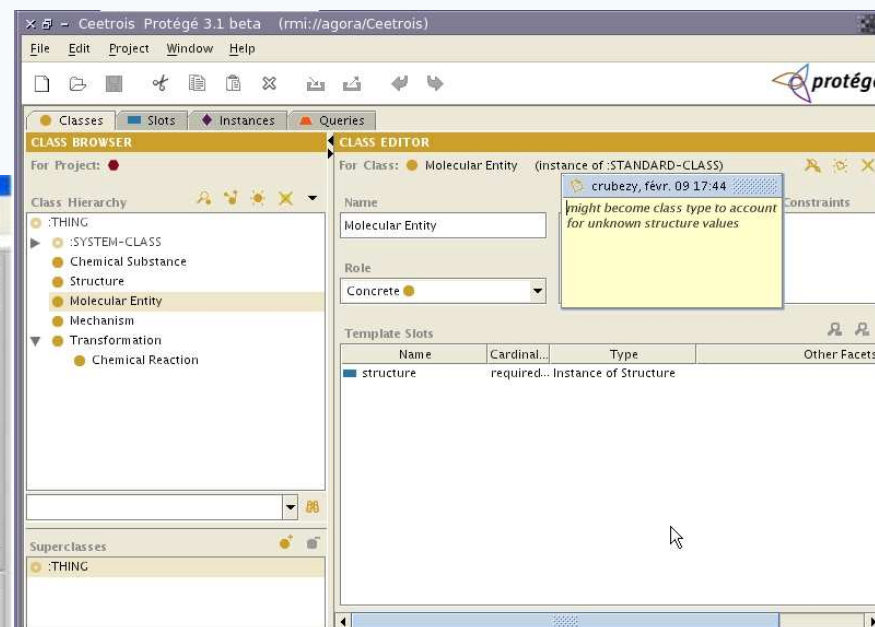
- Left Window (Resyn Assistant):** A software interface for chemical structure visualization. The title bar reads "Resyn Assistant : Visual". The main window shows a complex chemical structure on a black background. The interface includes a menu bar (Molecule, Visualization, Edition, Tools, Knowledge, Zoom, Help) and a toolbar with buttons for "Enumerate" and "block of type". The status bar indicates "No block type selected".
- Right Window (Flash Meeting):** A video conference window titled "Flash Meeting". It shows a grid of video feeds for participants: Pascal, Catherine Colaux, Philippe, and Krief. A "JOIN QUEUE (1)" button is visible. The chat area at the bottom contains the following messages:
  - laurencio: j'ai un pb j'tais dj ensession, et donc erreur ..
  - krief: Ou doise aller pour voir ce que vous voyez
  - krief: Ou doise aller pour voir ce que vous voyez
  - krief: Ou doise aller pour voir ce que vous voyez
  - catherine colaux: c'est vous
  - krief: Ou doise aller pour voir ce que vous voyez

- Each time that a concept is identified and considered to be important by the chemists, the ontologist, on the spot, integrates it in ontology, in a synchronous way, by using the shared desktop and validates in the same time the relevance of the classes, properties or restrictions.



## Drafting a protocol: conversations

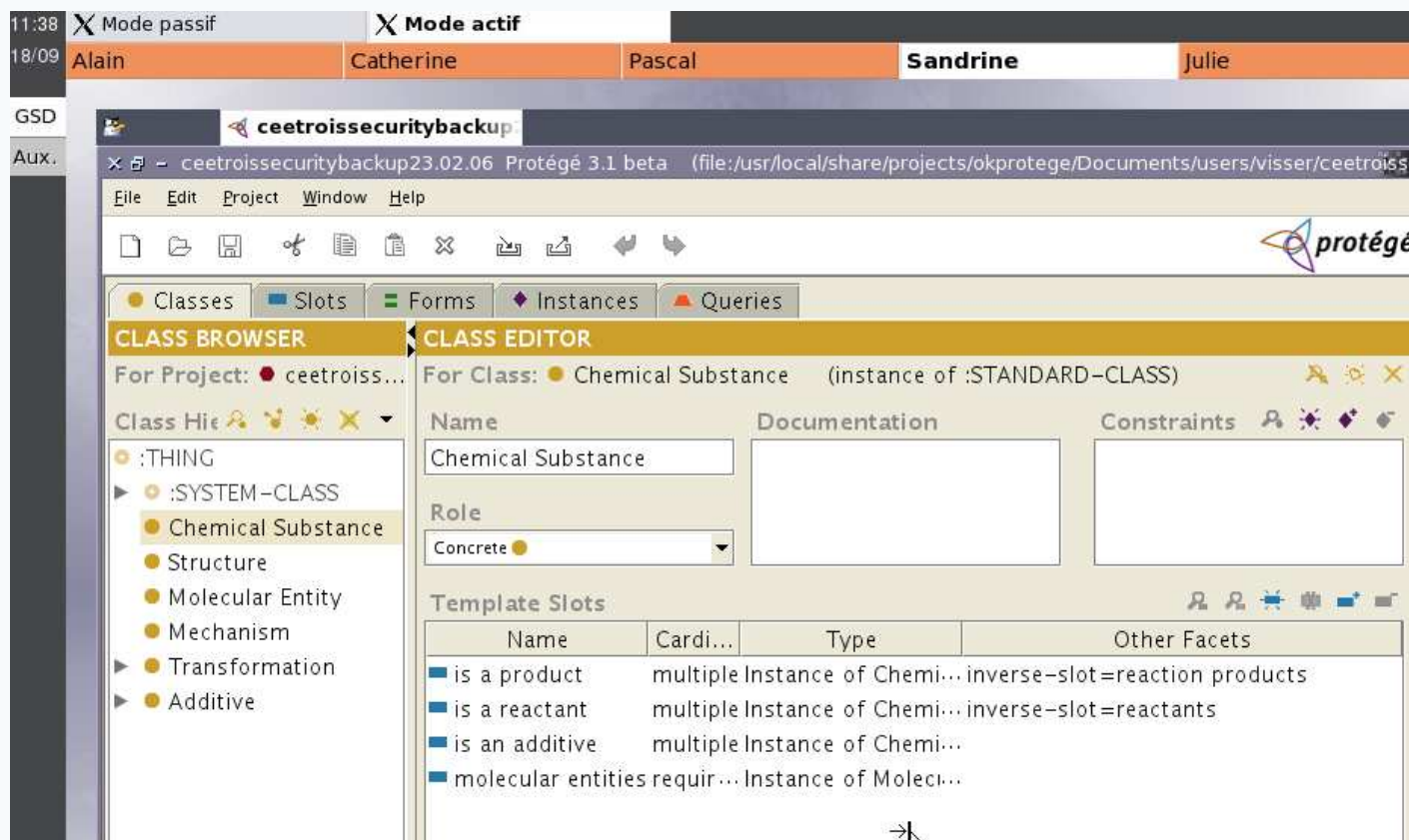
- The ontologist takes the time to explain to the chemist the reasons of his choices and how to implement it in Protégé. He also answers the questions and even in few cases revises his initial choice.



## *Drafting a protocol: keeping track of the collaboration*

- ✓ Booking each week a session of 2h with the different participants
- ✓ Sending documents to the diffusion list in order to prepare the session
- ✓ Sending agenda of the session
- ✓ Working through (GSD + FM) at the construction of the ontology
- ✓ Writing a report about the session and planning future work
- ✓ Acceptation of the report by the group and working on the next session

# Assessment of the first trial



The screenshot shows the Protégé 3.1 beta interface. The main window is titled 'ceetroissecuritybackup' and shows a 'CLASS EDITOR' for the class 'Chemical Substance'. The interface includes a 'CLASS BROWSER' on the left, a 'CLASS EDITOR' on the right, and a 'Template Slots' table at the bottom.

**CLASS BROWSER**

- :THING
  - :SYSTEM-CLASS
    - Chemical Substance
    - Structure
    - Molecular Entity
    - Mechanism
    - Transformation
    - Additive

**CLASS EDITOR**

For Class: Chemical Substance (instance of :STANDARD-CLASS)

Name: Chemical Substance

Role: Concrete

**Template Slots**

Name	Cardi...	Type	Other Facets
is a product	multiple	Instance of Chemi...	inverse-slot=reaction products
is a reactant	multiple	Instance of Chemi...	inverse-slot=reactants
is an additive	multiple	Instance of Chemi...	
molecular entities requir...		Instance of Molec...	

The assessment of this set of experiments is quite weak... Why?



## Assessment of the first trial

The facility to connect people through Internet induced us in error for gathering all these persons during the **SAME MEETING**

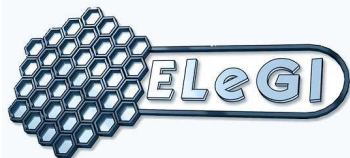
- No *precise determination of the goals*
- No *definition of the terms and their relations previously to the session.*
- Long discussion that was not without interest for Ontologist.

Working through Internet is not a simple transposition of the traditional way of working!!!!

- Opportunity to analyze errors or communication,
- Opportunity to define the protocols of collaboration,
- Opportunity to analyze errors.

## *How to improve this first protocol?*

- Thinking differently....
  - Taking advantage of the power and the facility offer by the GRID to the virtual community by
    - Cutting the work in different sessions
    - selecting the right person for the right session.
  - Selecting the tools in relation which each collaboration session.
  - Taking advantage of the recording for archiving and reporting



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## *Selection of the specific field*

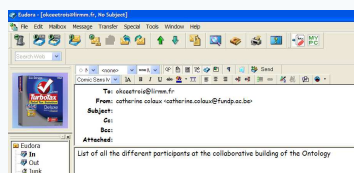
- Selection of a more **technical field** : The stirrer
- Goal? Answer to the following questions: "what is the more relevant equipment to use for an identified purpose?", "why this equipment is recommended for ?" or "where to buy it?"
- Integration of the "ontology of stirring laboratory equipment" to the "ontology of laboratory equipment" and the "ontology of organic reactions"

## 1. Study of the field to be treated

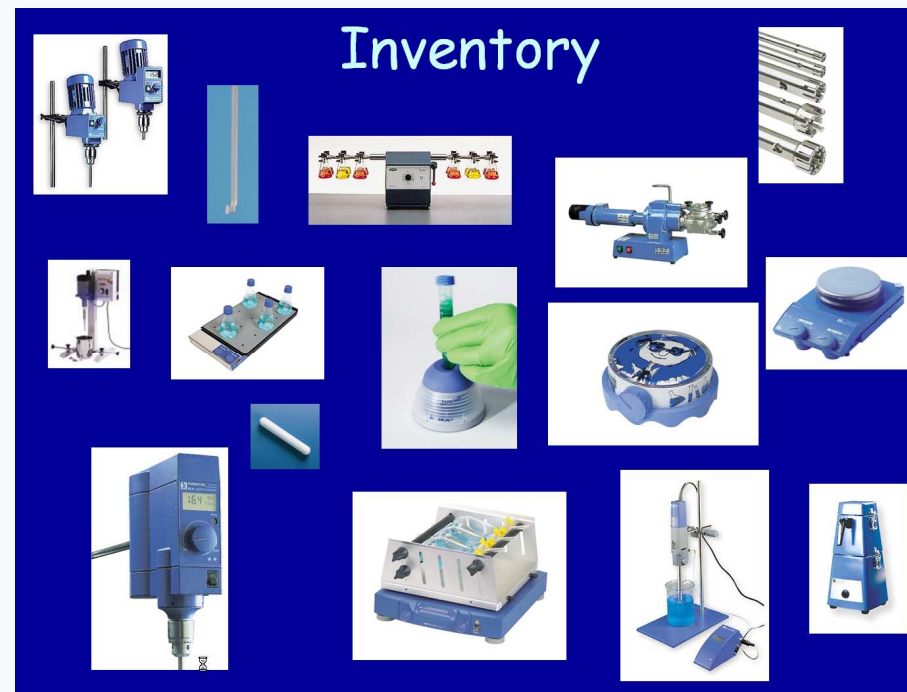
Implies Chemists

Listing of all the concepts and the terms of the delimited field to define them.

### Tools



The simple one-click video conference!  
It works in a web browser running the Flash 7 plugin!



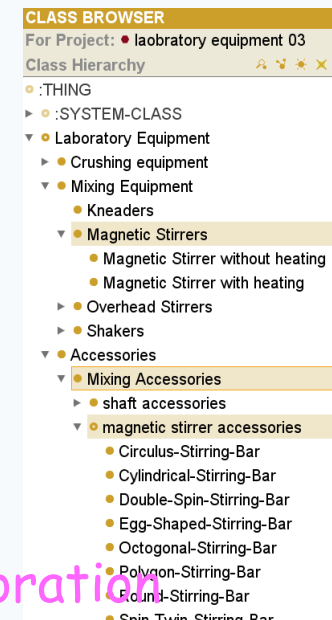
Asynchronous collaboration + Synchronous collaboration

## 2. First trail in the construction of the ontology

Construction of the first trial of the ontology by chemists who have learned protégé collaboratively with the ontologist

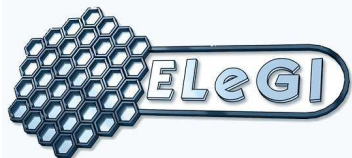
### Tools

Implies Chemists skilled in ontology building with ontologists



Asynchronous collaboration + Synchronous collaboration





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## ontology of the stirring laboratory equipments



### 3. Testing period of the first outline

Presentation to chemists in a working session using the GSD in order to validate the organization of the concepts. Detection of missing concepts, inconsistencies...

Implies all the Chemists

#### Tools



Synchronous collaboration

The screenshot shows a video conference in progress. The main window displays a video feed of a man named 'krief'. To the right, a gallery shows other participants: 'catherine colaux', 'laurence', 'philippe', and 'Pascal'. Below the gallery, there are controls for 'Interrupt', 'LEAVE QUEUE', and a hand icon with '1(1)'. The Protégé ontology editor is open in the foreground, showing a class hierarchy for 'Laboratory equipment budget' and a 'CLASS EDITOR' for 'Mixing system'. The 'CLASS EDITOR' has fields for 'Name' (Mixing system), 'Role' (Abstract), and 'Template Slots' (a table with columns for Name, Cardinality, and Type). The table contains two rows: 'Action Associated to Equipment' (multiple, Instance of type of action) and 'Equipment recommended for' (multiple, Instance of Reaction Features).

## 4. Evolution of the first version of the ontology

Integration of the remarks in the ontology.

Implies Chemists skilled in ontology building with ontologists

### Tools



Asynchronous collaboration + Synchronous collaboration

## 5. Validation of the ontology by ontologists:

Validation by ontologists of the organization.

### Tools

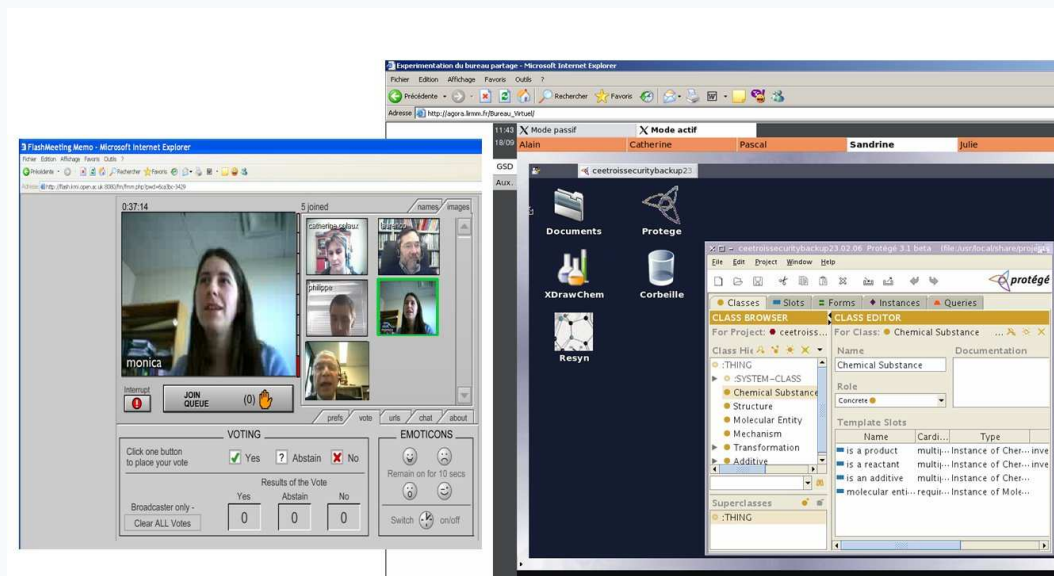


The Grid Shared Desktop Experience (GSD Beta)  
 GSD access  
 GSD Administrative  
 Audio-Video conference

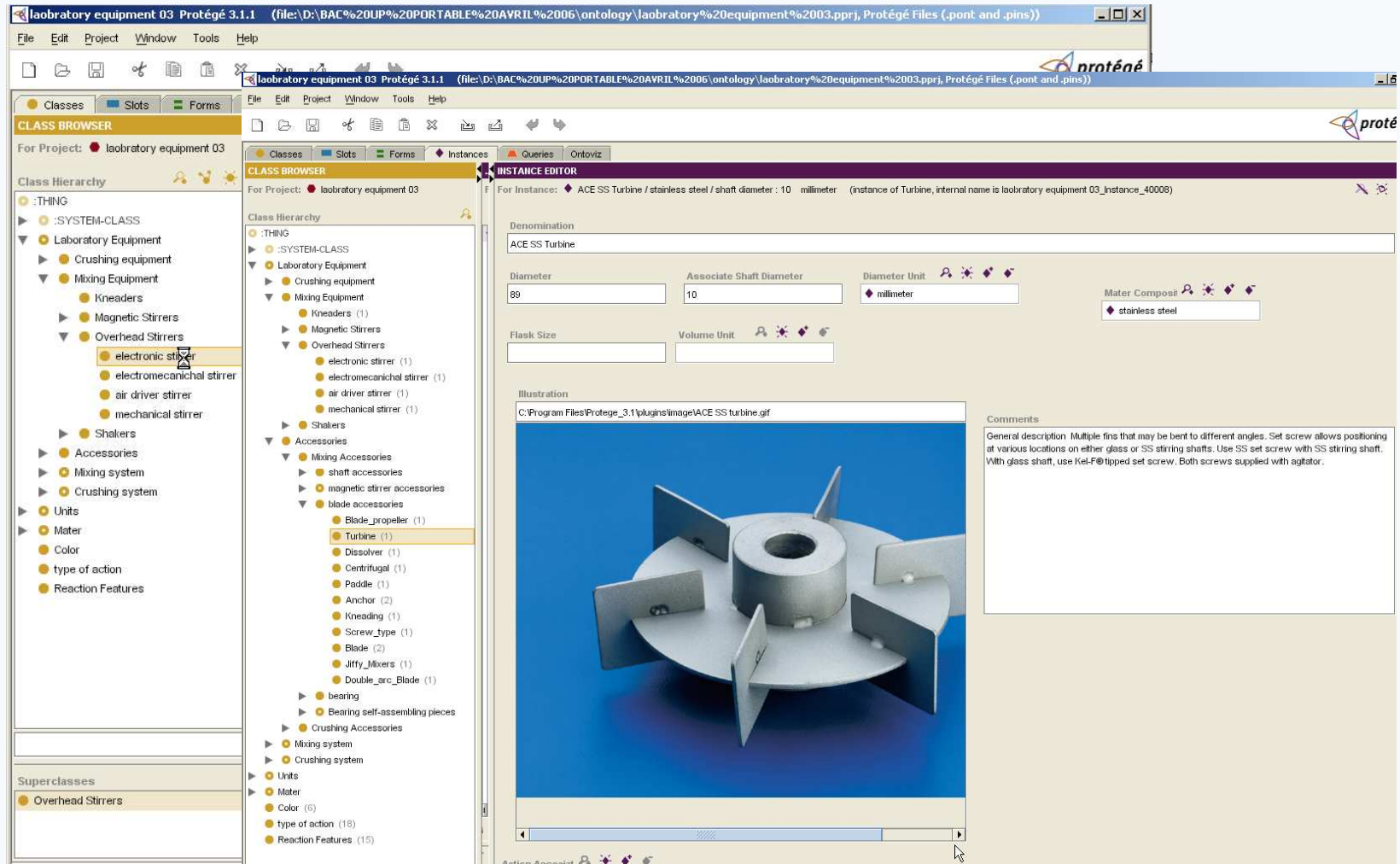


The simple one-click video conference!  
 It works in a web browser running the Flash 7 plugin!

Implies Chemists skilled in ontology building with ontologists



Asynchronous collaboration + Synchronous collaboration



The screenshot displays the Protégé 3.1.1 ontology editor. The main window is titled "laboratory equipment 03 Protégé 3.1.1". The interface is divided into several panes:

- Class Browser (Left):** Shows a class hierarchy for "laboratory equipment 03". The hierarchy includes:
  - :THING
  - :SYSTEM-CLASS
  - Laboratory Equipment
    - Crushing equipment
    - Mixing Equipment
      - Kneaders
      - Magnetic Stirrers
      - Overhead Stirrers
        - electronic stirrer
        - electromechanical stirrer
        - air driver stirrer
        - mechanical stirrer
      - Shakers
    - Accessories
      - Mixing Accessories
      - shaft accessories
      - magnetic stirrer accessories
      - blade accessories
        - Blade\_propeller (1)
        - Turbine (1)
        - Dissolver (1)
        - Centrifugal (1)
        - Paddle (1)
        - Anchor (2)
        - Kneading (1)
        - Screw\_type (1)
        - Blade (2)
        - Jiffy\_Mixers (1)
        - Double\_arc\_Blade (1)
    - bearing
    - Bearing self-assembling pieces
    - Crushing Accessories
    - Mixing system
    - Crushing system
    - Units
    - Mater
      - Color (6)
      - type of action (18)
      - Reaction Features (15)
- Superclasses: Overhead Stirrers

- Instance Editor (Right):** Shows details for the instance "ACE SS Turbine / stainless steel / shaft diameter : 10 millimeter".
- Denomination: ACE SS Turbine
- Diameter: 89
- Associate Shaft Diameter: 10
- Diameter Unit: millimeter
- Mater Compositi: stainless steel
- Flask Size: [empty]
- Volume Unit: [empty]
- Illustration: C:\Program Files\Protege\_3.1\plugins\image\ACE SS turbine.gif
- Comments: General description Multiple fins that may be bent to different angles. Set screw allows positioning at various locations on either glass or SS stirring shafts. Use SS set screw with SS stirring shaft. With glass shaft, use Kel-F® tipped set screw. Both screws supplied with agitator.

“Learning ontology building”  
and  
“building an ontology”  
are  
two distinct goals.



### Which are the differences between a traditional working session and distant collaboration within a Virtual Community ?

#### Advantages :

- ☺ You can record the conversation and use it to archive the discussions, write a report,
- ☺ You can work with different persons from different countries at the same time without any problems linked to travels,
- ☺ In case of GRID architecture, you don't need to download software on your computer and therefore avoid all the problems linked to their management,
- ☺ You can easily benefit from a tailored tutorial,

## *Conclusions after the update of the protocol*

Which are the differences between a traditional working session and distant collaboration within a Virtual Community ?

### Disadvantages :

- ☹ No meeting could be initiated on the spot, you have to book the session to ensure that all the participants will be available at this time (taking into account the time difference between Europe and the rest of the world),
- ☹ It requires much more organization, more work before the meeting. You have to prepare the session by sending documents, etc. in order to be ready to discuss at the first seconds of the session... the value of the time is no more the same through Internet.
- ☹ You need a moderator to centre the discussion in "heterogeneous" collaboration session, make beneficial of the session.

### Wishes :

- 👤 Opportunity to record the conversation simultaneously to the manipulation on the GSD.
- 👤 Possibility to invite someone to work on the GSD with least of constrain (only username and password....)

These requirements have been integrated into the design of a unified Common Virtual Environment:

- management of Users, Groups and Roles;
- single (and secure) sign-on for the whole C&C infrastructure;
- synchronized recording of the parallel conversational processes.