

# Facturation et outils de gestion

6 Juillet 2009

# Facturation

- **Industrie**
- **Monde Académique**
- **Interne**

# Industrie

- **Prix du marché**

# National NWO-CW/UU Single Crystal Service Facility

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## PRICE LIST (as of July 2000)

Pricing in EURO's (ex V.A.T) for Profit Organizations

### 1. STANDARD PACKAGE (2500 EURO)

1. This package includes the structure determination of a molecule with up to 50 non-hydrogen atoms. Crystals should be non-twinned, not smaller than 0.01 mm<sup>3</sup> and not too air-sensitive. The structure determination includes standard data collection, data reduction (including empirical correction for absorption where appropriate) and refinement (including hydrogen atoms at calculated positions) procedures. The absolute configuration is determined when relevant. Results will be reported in the form of an extensive (PLATON/CALC) listing (experimental details, coordinates, bond-distances, bond angles, torsion angles etc.) in A4 format and one or more labelled PLATON/ORTEP and PLATON/PLUTON illustrations of the structure.

### 2. Additional non-hydrogen atoms - per atom 50 EURO

(Price includes anisotropic refinement with attached hydrogen atoms at calculated positions).

<http://www.cryst.chem.uu.nl/cscsd.html>

## 2. ADDITIONAL FEE FOR NON-STANDARD OPTIONS

1. Structure determination on a twinned crystal - 500 Euro.
2. Refinement with a (severe) disorder model - 500 Euro
3. Refinement procedure to improve the accuracy of a structure containing highly disordered solvents (with the SQUEEZE algorithm) - 500 Euro.
4. Three Day Result Service (Standard Structures Only) - 1250 Euro
5. Primary and Derived data on CD-Rom - 125 Euro
6. Write-up of the experimental, supplementary material and drawings suitable for publication - 250 Euro  
(Free-of-Charge when supplied as co-author)
7. A licence to use a copy of the detailed structure analyses program PLATON locally - 5000 Euro  
This licence (including later releases) is free of charge together with five standard structure determinations (or equivalent amount).

## GENERAL RULES

\* There will be no charge for structure determinations for which no satisfactory (i.e. crystallographic R-factor higher than 10%) results (i.e. final report) can be obtained, due to poor crystal quality (i.e. the structure determination will be aborted at an early stage, unless agreed upon otherwise).

\* The minimum charge is 2500 Euro (ex VAT). This also applies when reliable results different from those expected are obtained. (Byproduct, starting material etc.)

\* The number of atoms to be charged is based on the number of non-hydrogen atoms for which positions are determined and refined (unless agreed upon otherwise).

Note: Some crystal structures contain more than one independent copy of the same molecule along with solvent molecules of crystallization.

\* Charges for additional options will be effective only on explicit request for that option by the client.

\* Preliminary results (i.e. not necessarily refined and checked for all details) will in general be available within two weeks, after the receipt and acceptance of a sample of crystals with sufficient quality, for a standard structure determination (unless agreed upon otherwise).

\* All data and results will be treated confidentially and not made known/available to third parties unless agreed upon otherwise.

\* The client has the obligation to inform us about special precautions required for the storage, handling and disposal of the sample supplied.

\* The client is free to publish the results of the structure determination. However, we can accept 'scientific responsibility' for published crystallographic results only as a co-author of the publication and after verification of the relevant experimental and discussion sections of the paper.

## Crystal Structure Analysis Facility

The Crystal Structure Analysis Facility of The University of Sydney provides a single crystal X-ray diffraction structure determination and analysis service to both internal and external clients.

The facility is located on the first floor of the School of Chemistry and is currently equipped with two diffractometers; a Rigaku AFC7R diffractometer employing Cu radiation generated with a direct drive rotating anode, and a Bruker-AXS SMART 1000 CCD equipped diffractometer using Mo radiation generated from a sealed tube.

Supporting equipment includes SGI O2, Indigo Extreme and Indy workstations and several pentium PCs. Low temperature data collections down to 100 Kelvin are routinely undertaken with an Oxford Cryosystems Cryostream liquid nitrogen low temperature data collection system. Collections to 25 Kelvin can now be undertaken with the installation of an OxfordCryosystems HeliX system. There are currently only 6 such systems installed in laboratories world wide.

Software used includes SIR, SHELX, XSELL, teXsan, PLATON, WINGX and XTAL.

Experimental details, tables and images are distributed by email. Structure analyses and contributions to publications are provided on request, and high quality images can be provided in a variety of formats.

The facility operates on a subsidised cost recovery basis for Australian academic and government customers, and on a full cost recovery basis for others. The charge structure assumes an average data set collection time of 5 days on the AFC7R and 1 day on the SMART 1000. The charge accumulates for each 1 or 5 day collection 'unit'; please note that the units are rounded upwards. The current charges are :

\* Academic or Government:

A\$ 120 for each collection unit

100 A\$ ~ 57 €

\* Other:

A\$ 700 for each collection unit

The charge applies regardless of the outcome and a 10% surcharge is applied to data sets collected at low temperatures. The charge assumes that the crystallographers name will appear on the author list of a consequential publication of the structure. Alternatively a further A\$ 300 is charged if the crystallographers name is not to appear on the publication author list. Crystal examinations that do not result in a full data set collection, either because the unit cell clearly indicates that the structure has been previously reported or because a unit cell could not be obtained, will cost A\$ 50 an hour for Australian academic or government customers and A\$ 150 an hour for others. The charge for data collections that involve the use of the HeliX will additionally include the cost of helium gas consumed during the collection. A cylinder of high purity helium lasts approximately 17 hours.

Please note that as of 1/7/00 the charge also includes a 10% Goods and Services Tax (GST).



Indian Institute of Technology, Madras, Chennai – 600 036

Rate for Measurements using various facilities.

With effect from Apr-01-2007.

S.No.	Facility	DST Recommended Charges (in Rupees) *		
		Industries (Large scale, medium & SSI)	National Labs	Educational Institutions
1	UV-VIS-NIR spectrometer per spectrum per sample	300/-	180/-	60/-
2	FT-IR spectrometer per spectrum per sample	500/-	300/-	100/-
3	Fluorescence spectrometer	Rs. 750/-per measurement. (ie. Per excitation or emission)	Rs.450/- per measurement (ie. Per excitation or emission)	Rs.150/- per measurement (ie. Per excitation or emission)
4	ICP-OES for analysis per sample including standardization for first element	1000/- For every additional element 200/-; Sample Digestion charges extra	600/- For every additional element 120/- ; Sample Digestion charges extra	200/- For every additional element Rs.40/-; Sample Digestion charges extra
5	FT-NMR spectrometer For each half an hour or less, charges for solvents extra	1000/-	600/-	200/-
6	ESR spectrometer per sample (RT),	500/- For VT 1000/- per hour or part there of	300/- For VT 600/- per hour or part there of	100/- For VT 200/- per hour or part there of
7	Mossbauer spectrometer per hour of instrument time	1000/- with a minimum of 1000/- per sample	600/- with a minimum of 600/- per sample	200/- with a minimum of 200/- per sample
8	X-Ray Fluorescence spectrometer Per sample including standardization and estimation for first element	1500/- For subsequent elements in the same system: 200/-	900/- For subsequent elements in the same system: 120/-	300/- For subsequent elements in the same system: 40/-
9	Single crystal X-Ray Diffractometer For structure determination charges are extra. (Pl. contact the operator)	1000/- per hour with a minimum of 8000/- per crystal (for collection of X-ray data including sample handling)	600/- per hour with a minimum of 4800/- per crystal (for collection of X- ray data including sample handling)	200/- per hour with a minimum of 1600/- per crystal (for collection of X- ray data including sample handling)

1000 INR ~ 15€

# Industrie

- **Négociations**
- **Forfait**
- **Proximité**

# Monde Académique

- **Collaboration avec participation aux publications**
- **Coût de fonctionnement**

# Facturation au niveau national ?

- **Impossible : raisons historiques, différents contrats, marché globalisé, etc...**
- **Problèmes induits :**
  - **Financement : Système des ANR : facturation interne.**
  - **Développements de centres nouveaux ou petits.**

# Facturation Interne

Que facture-t-on ?

- **Fonctionnement**
- **Fonctionnement + Investissement**
- **Fonctionnement + Investissement + Main d'œuvre**

# Facturation Interne

Que facture-t-on ?

- Fonctionnement
- Fonctionnement + Investissement
- Fonctionnement + Investissement + Main d'œuvre

→ Choix politique local

# Fonctionnement

$$\text{Coût de fct} = \frac{\text{Budget de fonctionnement}}{\text{Nbre de structure moyen annuel}}$$

# Investissement

$$\text{Coût de l'invst} = \frac{\text{Montant investi} / 10}{\text{Nbre de structure moyen annuel}}$$



# Main d'œuvre

Comment évaluer cette part ?

Notre métier s'y prête mal car nous ne sommes pas habitués à décompter nos heures.

Le forfait est la formule la plus adaptée.

Autrement, on peut estimer le temps annuel dévolu au temps de résolution puis convertir en masse salariale.

$$\text{Coût de M. O.} = \frac{\text{Masse salariale}}{\text{Nbre de structure moyen annuel}}$$

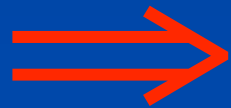
# Mise en œuvre d'une facturation qui ait du sens

## ■ Budgets de fonctionnement et d'investissement

- Si autonomie, ils sont disponibles, sinon il faut faire une comptabilité interne bien tenue.

## ■ Statistiques de production :

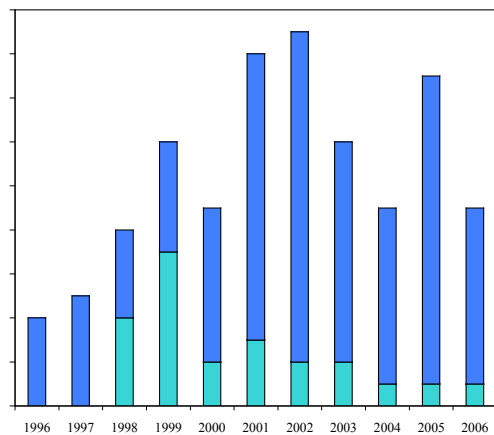
- Il faut du recul sur plusieurs années pour définir un nombre de structure moyen annuel et une incertitude.
- Il faut une comptabilité de production en ordre.



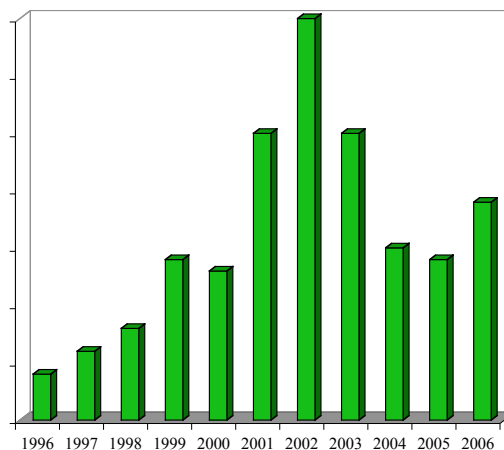
**On rejoint implicitement la mise en place d'une démarche qualité.**

# Autres outils de gestion

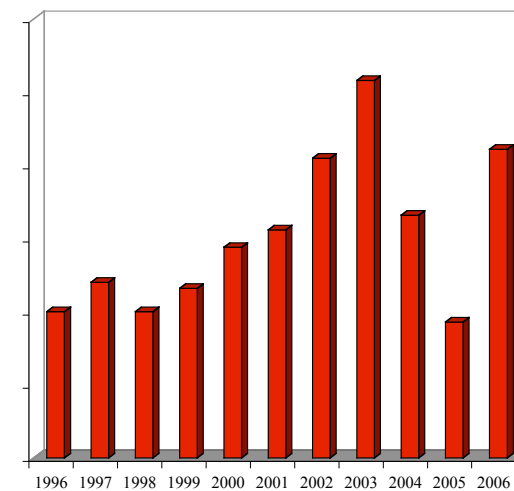
■ nombre de publication de chimie  
■ Nombre de publication de cristallographie



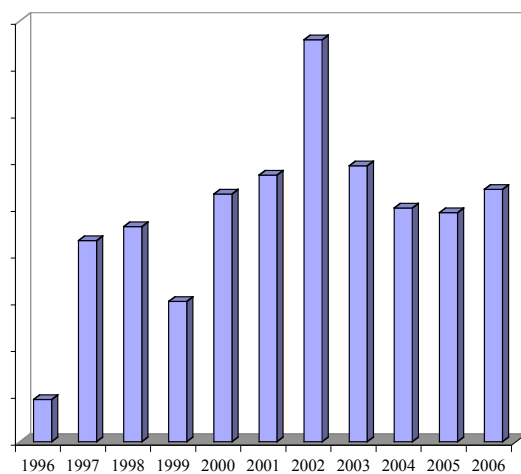
Nombre de structures déposées (CIF)



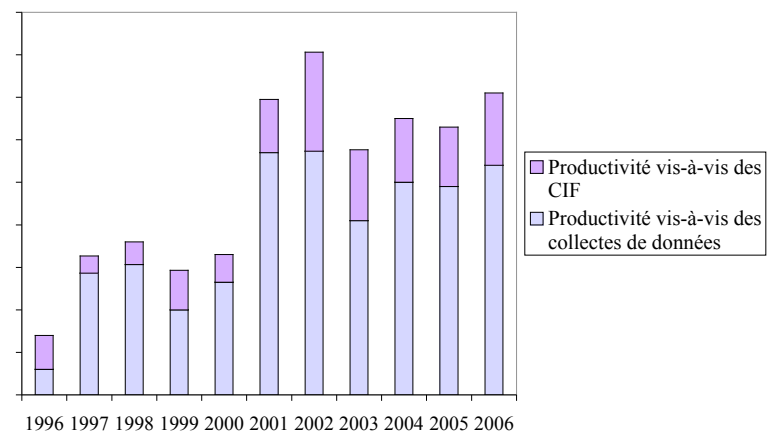
Nombre de CIF par publication



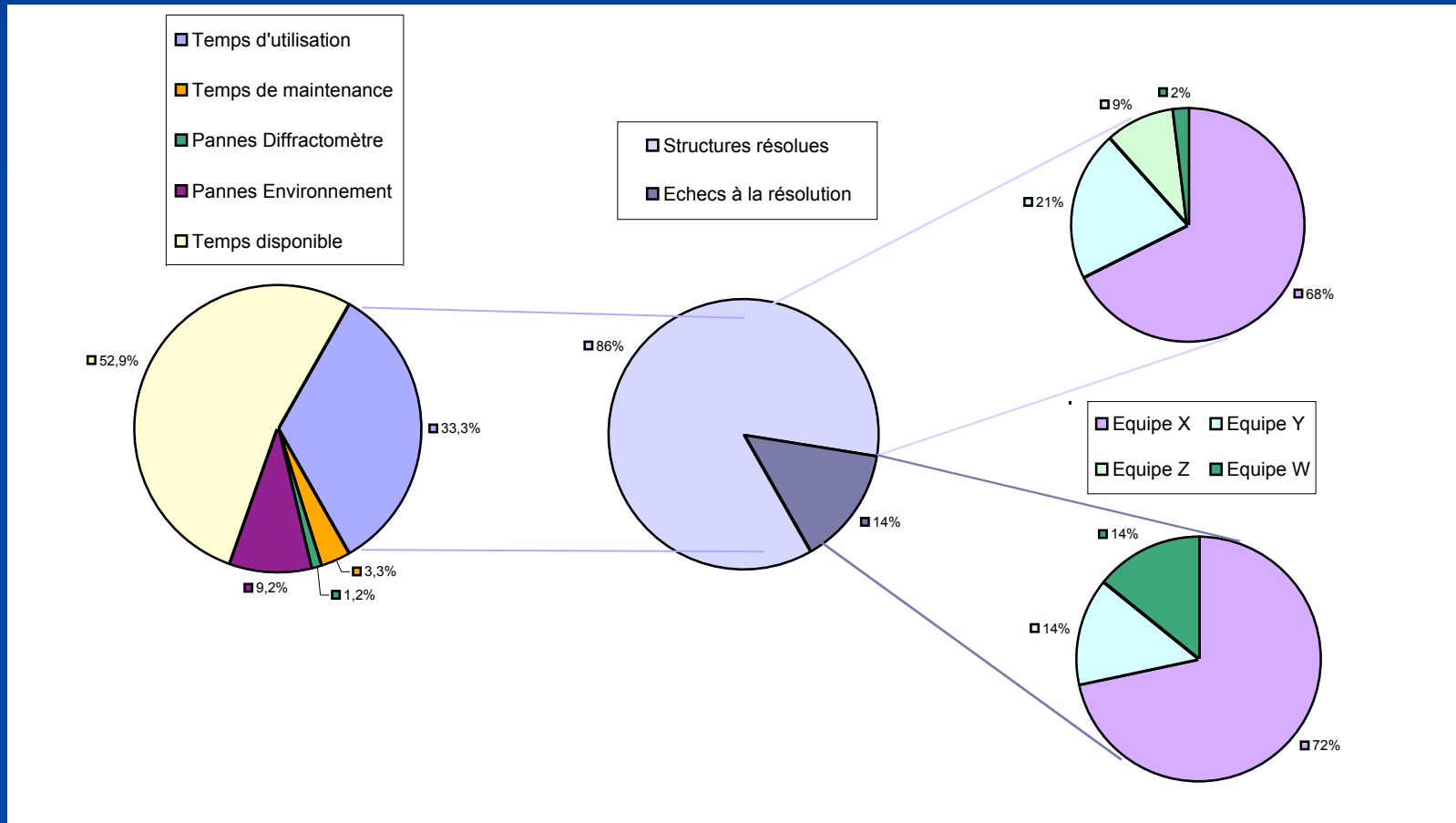
Nombre d'acquisition de données



Productivité globale



# Autres outils de gestion (suite)



# Définitions de nouveaux outils

- **Méthodes et Modèles de Gestion Quantitatifs**
- **Formation permanente au niveau du réseau**