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agence d'évaluation de la recherche  
et de l'enseignement supérieur

Section des unités de recherche

AERES report on  
the unit:

Laboratoire de Chimie

From the

Ecole Normale Supérieure de Lyon

CNRS

Université Claude Bernard, Lyon 1

May 2010



agence d'évaluation de la recherche  
et de l'enseignement supérieur

Section des Unités de recherche

# AERES report on the research unit

Laboratoire de chimie

From the

Ecole Normale Supérieure de Lyon

CNRS

Université Claude Bernard, Lyon 1

Le Président  
de l'AERES

Jean-François Dhainaut

Section des unités  
de recherche

Le Directeur

Pierre Glorieux

May 2010



# Unit

Name of the unit: Laboratoire de chimie

Requested label: UMR-5182

No. in case of renewal: 5182

Unit director: M. P. SAUTET (M. C. Andraud)

## Members of the expert committee

### Chairperson:

Mr. A. HAUSER, University Geneva, CH

### Reviewers:

Mr. E. Jakab-TOTH, Orléans, FR

Mr. A. ZECCHINA, Turin, IT

Mrs. M.-P. Teulade-FICHOUE, Paris 11, FR

Mr. A. DAVIS, Bristol, UK

Mr. J. NØRSKOV, Kongens Lyngby, DK

### Reviewer(s) nominated by the staff evaluation committees (CNU, CoNRS, CSS INSERM ...):

Mr. M. SALLÉ, Angers, FR, representative CoNRS

Mr. I. DEMACHY, Paris 11, FR, representative CNU



# Representatives present during the visit

Scientific delegate representing AERES:

Mr. P. DUMY, Grenoble

University or School representative :

Mr. C. GOUTAUDIER, Mr. J Samarut

Research organisation representative :

Mr. C. POUCHAN, representative of "Intitut de Chimie", CNRS



# Report

## 1 • Introduction

The visit took place on the 20th and 21st January 2010. The acting director, P. Sautet, and the director elect, C. Andraud, presented the evolution of the research unit over the past 5 years and the projected reorganisation, respectively. The research of each group was presented to the members of the committee orally and with a series of posters. The committee discussed and assessed the quality and long-term impact of each project based on standard indicators.

The "Ecole Normale Supérieure de Lyon" on the site of Gerland was founded in 1986. Today's Laboratory of chemistry came into existence in 2003 as amalgamation of the laboratories of "Stéréochimie et Interactions Moléculaires" and the laboratory of "Chimie Théorique". The Laboratory of chemistry is active in various fields of chemistry, going from organic to inorganic synthesis, from material science to life science, and from experimental physical chemistry to theoretical and computational chemistry. In 2008, the research group of L. Emsley was transferred to the new Centre for High-Field NMR of Lyon. This activity is reviewed by another AERES panel.

|  |             |
|--|-------------|
| N1: Number of researchers with teaching duties (Form 2.1 of the application file)  | 15          |
| N2: Number of full time researchers from research organizations (Form 2.3 of the application file)                       | 18          |
| N3: Number of other researchers (Forms 2.2 and 2.4 of the application file)  | 13<br>PostD |
| N4: Number engineers, technicians and administrative staff with a tenured position (Form 2.5 of the application file)    | 8.3         |
| N5: Number engineers, technicians and administrative staff without a tenured position (Form 2.6 of the application file) |             |
| N6: Number of Ph.D. students (Form 2.7 of the application file)  | 26          |
| N7: Number of staff members with a HDR or a similar grade  | 13          |

## 2 • Assessment of the unit

- Data on work produced:

Globally, the research performed can be considered to be high to top-level science, resulting in a continuous and high scientific productivity, national and international collaborations and a high number of funded research projects. All professors and researchers are actively publishing in peer reviewed scientific journals. In the period from 2005 to 2009, the laboratory published 308 articles in peer reviewed journals and filed 5 patents. Its members delivered 80 invited lectures and 66 oral contributions and presented 95 poster contributions at national and international conferences and seminars. The teams of the laboratory were active in 15 ANR projects, 4 European research projects and training programs, and they were involved in 2 Initial Training Networks. They organised 10 international conferences and schools. 22 PhD theses were defended at the laboratory.



- **Strengths and opportunities:**

The strength is based on a large diversity in the science comprising a variety aspects of chemistry from theoretical chemistry to organic and inorganic synthesis. Many projects are devoted to applications in various domains, such as in chemical catalysis (green chemistry), physical sciences (functional materials), as well as in biology (bio imaging via IRM and fluorescence). The planned integration of new researchers with complementary expertise from outside laboratories and the new organization in 3 teams instead of the 7 teams in the previous format, should contribute to advance multidisciplinary projects and allows to strengthen internal collaborations.

- **Weaknesses and threats:**

The joint expertise of the laboratory should be combined in a synergistic effort and focussed towards the development of internal collaborative programs with common objectives. In view of the numerous funded programmes and applied projects (catalysis, bioimaging , ...), there is a potential for more patent applications by improving transfer of knowledge to technological applications with associated industrial partners

- **Recommendations for the unit director:**

The proposed unit director, C.Andraud, has been approved by the laboratory council. Her scientific expertise and experience in management qualify her for this position and for the responsibilities that come with it. Nevertheless, care should be taken to guarantee continuity in the management, in particular with regard to the proposed reorganisation of the research teams into 3 units. With regard to this reorganisation, care should be taken to promote internal as well as transversal collaborations between the new units.

- **Production results**

(cf. [http://www.aeres-evaluation.fr/IMG/pdf/Criteres\\_Identification\\_Ensgts-Chercheurs.pdf](http://www.aeres-evaluation.fr/IMG/pdf/Criteres_Identification_Ensgts-Chercheurs.pdf))

|  |    |
|--|----|
| A1: Number of lab members among permanent researchers with or without teaching duties who are active in research (recorded in N1 and N2)     | 33 |
| A2: Number of lab members among permanent researchers with or without teaching duties who are active in research (recorded in N3, N4 and N5) |    |
| A3: Ratio of members who are active in research among staff members [A1/(N1+N2)]   | 1  |
| A4: Number of HDR granted during the past 4 years  | 1  |
| A5: Number of PhD granted during the past 4 years  | 22 |
| A6: Other relevant item in the field   |    |



### 3 • Detailed assessments:

The research work of the Laboratory of chemistry of the ENS of Lyon covers a number of topical areas such as the chemistry of coordination compounds and spin-crossover, bio-organic chemistry, catalysis, materials chemistry, and last but not least theoretical approaches to many topical problems. The quality and impact of the scientific work of the laboratory is high as shown by i) the strong publication record in high impact factor journals, ii) the large number of invited lectures, iii) 6 covers in high impact factor journals, iv) the number of prizes and distinctions (P. Sautet: silver medal CNRS 2007, Paul Pascal prize of the French academy of Science 2008; L. Emsley: silver medal CNRS 2005), v) the participation on international editorial boards of several high-ranked scientific journals, vi) the organisation of 10 International conferences and Schools.

As mentioned above, between 2005 and 2009 the laboratory published 308 articles in peer-reviewed journals, 12 of which came from collaborative efforts of teams within the laboratory. The scientists of the laboratory gave 80 invited lectures, 66 oral communications and 95 poster presentations at international conferences and seminars. With respect to the previous evaluation period the publication rate has increased by 30% and now reaches 80 per year. The high quality is exemplified by the publications in the journals with the highest impact factors: 1 in Science, 1 in Nature Materials, 12 in Angewandte Chemie, 3 in PNAS, 39 in J. Am. Chem. Soc., 4 in Phys. Rev. Lett., and 44 in J. Phys. Chem. 22 PhD theses were defended between January 2005 and June 2009.

The laboratory is very active in collaborative research at all levels, academic and industrial, national as well as international. The quality is assessed by the participation in many European and ANR programs. The academic programs have steadily increased. On the other hand the industrial contracts (Merck, Total, ...) have slowly decreased. This could be due to the current economic crisis. New contracts may be expected from the new directions, for instance related to the application of chemistry to biology

The attribution of two silver medals, the prestigious prize of the CNRS, is particularly remarkable and together with the 80 invited talks assures international visibility. The unit regularly recruits young researchers as well as experienced scientists. From 2005 to 2009, 3 "Maîtres de Conférences" and 2 "Chargés de recherche CNRS (CR) have been recruited. A substantial number of PhD students and post-docs are recruited from outside France. One Maître de Conférences was also recruited in October 2009 on a "Chaire d'Excellence" position.

The laboratory is highly efficient in acquiring external funding at a regional, national and European level. External funding represents approximately  $\frac{3}{4}$  of the budget apart from the salaries of permanent staff, the two other sources being ENS and CNRS. This allows financing of post-docs and PhD students, consumables and equipment. Since 2005, 15 ANR projects have been or are still being funded, the laboratory has participated in 4 European projects (STREPs on the applications of non-linear optics (NLO) and in vivo imaging (HEALTH) starting at the end of 2009; NoEs on catalysis (IDECAT) and molecular magnetism (MAGMANET)), and the laboratory was involved in 2 Initial Training Networks in Nanoscience (MONET, SMALL).

The laboratory is very active in collaborations at all levels, a sign of its important scientific impact. There is a strong international collaboration with the US Air force, a joint research program with Turkey, and a student exchange program with China. In addition to numerous national and regional collaborations, interactions with prestigious foreign centres, institutes or universities have been developed (FHI Berlin, Munich, Cambridge, Barcelona, KTH Sweden, Osaka etc.). In 2009, a program was launched with Saudi Arabia on Computer assisted discovery and elucidation of catalysts for Economy development of SA in partnership with IFP and CNRS (CADENCED).

In view of the comparatively large size of the laboratory, transfer of knowledge and technology seems underdeveloped. Five patents have been deposited, despite the fact that several groups work in technologically highly relevant areas such as catalysis, photonic materials, bio-sensors and environmental chemistry. This can be partially explained by the fact that, as befitting an academic institution, a large part of the research is focussed on fundamental aspects. However several projects claim technological applications as an objective and efforts should be made towards the corresponding transfer.





The laboratory of chemistry of the ENS Lyon is well managed by the director and the consulting body of the "Conseil du Laboratoire". It possesses a unique policy for the allocation of financial resources, which allows it to plan on a long-term basis but also to react quickly to changing needs. The acting director of the laboratory, P. Sautet, is heavily involved in the creation of the federative structure of the "Institut de chimie de Lyon" together with the UCB, INSA, the Université Jean-Monet de St. Etienne, CPE and the CNRS. He is the first director of the ICL. This initiative is crucial to the organisation of chemistry and its long-term development in Lyon.

There is a strong involvement in teaching since the laboratory of chemistry with its professors and "Maîtres de Conférences" represents almost all the teaching team of the chemistry department of ENS-Lyon at the bachelor and master level. Some CNRS researchers are also involved in part time teaching activity, mainly at the master level.

Today the laboratory comprises 7 independent research groups of variable size. The research projects of the seven groups are at the forefront of current research in their respective areas. The research proposals are innovative and original. The medium and long-term perspectives are very good. The project to be realised in the period 2011 - 2014 proposes to regroup the individual research groups into three thematic units, namely theory, functional materials, and chemistry for life science. This should ensure a better embedding of the smaller groups into the activities of the laboratory and thus give them a better chance for integration and collaboration, give a better visibility to actual research projects and facilitate the elaboration of research proposals for funding at a regional, national and international level. The new structure is to provide general guidelines for future recruitments and the development of experimental facilities.

#### 4. • Team-by-team analysis

**Team 1 :** Supramolecular Chemistry and Stereochemistry (CSS).

**Team-leader:** Jean-Pierre DUTASTA.

- Staff members (on the basis of the application file submitted to the AERES)

|  |   |
|--|---|
| N1: Number of researchers with teaching duties (Form 2.1 of the application file)  | 1 |
| N2: Number of full time researchers from research organizations (Form 2.3 of the application file)                       | 3 |
| N3: Number of other researchers (Form 2.2 and 2.4 of the application file)   |   |
| N4: Number engineers, technicians and administrative staff with a tenured position (Form 2.5 of the application file)    | 2 |
| N5: Number engineers, technicians and administrative staff without a tenured position (Form 2.6 of the application file) |   |
| N6: Number of Ph.D. students (Form 2.7 of the application file)  | 5 |
| N7: Number of staff members with a HDR or a similar grade  | 3 |



The CSS team is composed of 1 professor, 3 permanent researchers, 2 technicians and 5 doctoral students who pursue research in host-guest chemistry, for which the director is renowned, and also in multifunctional hybrid materials and aspects of molecular chirality. The research in the host-guest area concerns mainly the study of cryptophanes, a family of host molecules which originated in the laboratory. The cryptophanes are being exploited in sensors for gas molecules and, most interestingly, as receptors for xenon. The xenon-cryptophane complexes have potential applications in biosensing and imaging through  $^{129}\text{Xe}$  NMR, and this was investigated in collaboration with a major US laboratory (A. Pines) as well as more recently it is developed with a CEA-Saclay team. The group has also developed a second family of hosts, phosphorylated cavitands, with interesting potential, and has initiated studies on supramolecular catalysis based on the hemicryptophane systems. The research on multifunctional hybrid materials, initiated on the integration of V. Dufaud, has focused on the spatial organisation of functional groups within porous materials (a productive collaboration with another major US group, M. E. Davis) and on performing organometallic catalysis within solids. This area offers new opportunities towards the creation of industrial relationships. The molecular chirality work overlaps partly with the cryptophane project, but also includes the design of molecules with extreme chiroptical properties and a project on parity violation.

Overall the research is topical, original and relevant, and generally of very high quality. Several aspects of the work have potential for applications, notably the gas sensing and bio-imaging with cryptophanes, and the catalytic materials.

Altogether the group has produced 46 articles, 1 book and 1 book chapter, corresponding to a good rate of publication (10 papers per year). Many articles are in high impact factor journals (Chem. Rev, J. Am. Chem. Soc., Angew. Chem.), others articles in appropriate specialized journals (e.g. Sens. Actuators). Considering the rather small size of the group, the quality of the contractual relations is at a good level (IFP, incubation of Start up BIOSAFETY). A decrease of industrial contracts in the field of chiral separation is notable possibly due to the current economic crisis. Altogether the team has contributed 20 lectures, seminars and oral communications at national and international events.

The laboratory is well known among supramolecular chemists but probably does not attract the attention it deserves (for example, in terms of conference invitations). This could be due to the small size of the group in comparison to the diversity of interests, as a result of which the group tends not to publish intensively on any single topic. The 2009 Chemical Reviews article on cryptophanes constitutes a positive step, as it reminds the scientific community that these molecules are available, unique and effectively "owned" by the group.

The group is well governed. It is notable that a researcher joined the group via internal transfer, indicating that the environment in the group is attractive. The group has a very healthy population of post-docs, PhD. students and Masters Students, so there seems to be no difficulty with recruiting. The group has a good to excellent funding record and is clearly open to collaboration with others, having several important international cooperations. 3 ANR projects have been funded, one convention IFP-CNRS has been contracted, and the creation of a start up company on BIOSAFETY is projected. The group also participates in the regional network Cluster-Chimie through 2 programs. Group members are reasonably involved in teaching at different levels in the university (UCBL) and at the ENS.

Within the new structure of the laboratory, the CSS group will join "Chimie Bio-organique" to form a larger team focused on "Organic Chemistry". Plans in the supramolecular area include continuation of the gas-sensing and bio-imaging work, which clearly have great potential. The group also intends to study the molecular recognition of biologically relevant ammonium ions (including enantioselective recognition). This also has potential, although it should be remembered that bio-mimetic recognition is a mature subject and targets must be chosen with care. Research will also be undertaken on supramolecular catalysis and on catalysis by hybrid materials, including plans to incorporate host molecules. The intra-group collaboration will study not only binding by the host molecules but also the control of molecular motion (relevant to "molecular machines"). It is of interest both scientifically and to reinforce overlap between the two sub-groups. The research on fundamental aspects of chirality will continue, and could well yield very exciting results over the next few years. The proposed work is creative and carries an appropriate element of risk. There seems to be a sensible resource allocation policy.



## Conclusion:

Considering the size of the group and the degree of subdivision, the research is at a very high level. The group leader has an international reputation for his work on the chemistry of cryptophanes/cavitands. Of the three main lines of work, the first one (host-guest systems) has been very productive and has excellent potential, while the second (multifunctional hybrid materials) and third (molecular chirality) are creative and promising.

### - Strengths and opportunities

The group is rightly focusing on finding applications for their systems, and has first-rate external collaborations, which should help them achieve their goals. The team has an interesting and complementary range of interests and there is potential for further interaction through joint projects.

### - Weaknesses and threats:

The group could perhaps benefit from greater visibility, although this should not be achieved through reduction of diversity. In the future, the group will join the "Chimie Bio-organic" team in an Organic Chemistry grouping. At present there is no collaboration between these teams, so integration might not be straightforward. The retirement of J.-P. Dutasta, planned in 2013, is a key issue that has to be considered for future management.

### - Recommendations:

Although successful and highly rated this team is quite small. To assist productivity and integration, expansion should be considered. Recruitment at the DR2/CR1 level would allow planning for succession of the team leader. It is also worth noting that the "organic" grouping in the new structure is relatively small (7 permanent staff members) and could be reinforced.



Team 2 : Bio-Organic Chemistry (CBO).

Team leader: Mr Jens HASSERODT.

- Staff members (on the basis of the application file submitted to the AERES)

|  |   |
|--|---|
| N1: Number of researchers with teaching duties (Form 2.1 of the application file)  | 2 |
| N2: Number of full time researchers from research organizations (Form 2.3 of the application file)                       |   |
| N3: Number of other researchers (Form 2.2 and 2.4 of the application file)   | 2 |
| N4: Number engineers, technicians and administrative staff with a tenured position (Form 2.5 of the application file)    | 1 |
| N5: Number engineers, technicians and administrative staff without a tenured position (Form 2.6 of the application file) |   |
| N6: Number of Ph.D. students (Form 2.7 of the application file)  | 1 |
| N7: Number of staff members with a HDR or a similar grade  | 1 |

The team consists of 2 professors, 1 technician, 1 doctoral student and 2 post-docs. The research directions described in the report are diverse, ranging from the design of enzyme responsive contrast agents for magnetic resonance imaging to the manufacturing of biomimetic polymers or fluorescent probes for enzymatic detection.

The design of the enzyme responsive MRI probes is based on an entirely original concept which has never been exploited in the development of MRI contrast agents, namely the use of a switch between the low- and high-spin state of iron(II) complexes. This is clearly a high-risk project, which is further complicated by the difficulties implied by the self-immolative concept to make those complexes enzyme-responsive. Despite the important advances achieved in the last 4 years, the first molecules to produce a proof of the concept still remain to be made.

With only 14 publications, the number of publications is rather low, even taking into account the small size of the group. These papers were published in medium-to high-quality journals. The number of theses (5) for the period of 4 years is reasonably high for such a small group. In addition, 2 patents have been filed and the work has been presented in 2 invited talks, 6 oral contributions and 10 poster presentations at international and national conferences. The two patents were filed on (i) MRI agents and (ii) the fluorogenic peptidase substrate. So far they have not been licensed. With five patents in total deposited for the whole laboratory, the CBO team has a significant and important contribution in the transfer of results towards applications.



The group has recently attracted a certain number of young post-doctoral fellows and PhD students arriving from foreign universities. This ability is of quite good level. The group acquired and continue to receive substantial financial support from various sources, including ANR, the Institut National du Cancer, La Ligue contre le Cancer and the Fondation de la Recherche Médicale. These grants were mainly dedicated to the project on MRI contrast agents. More recently, the group received financing for one post doc working on the fluorescent enzymatic probes.

The group built up a collaboration network in the field of the MRI evaluation of their agents, mainly based in Lyon, with common papers published already. This "MRI consortium" obtained financial support from ANR and INCA. Some other national collaborations have been started, in particular in the field of physico-chemical characterization of the iron(II) complexes. However, it is too early to evaluate the outcome of these collaborations (no common publications yet). No important collaborations with foreign teams.

The team is organized around the two permanent staff members who are managing in an efficient manner the group of several PhD students and post docs. The external communication is reasonable with the many posters and a few oral presentations at international conferences.

A collaboration concerning modelling of substrate organized via N-Co bond inside the catalytic pocket of the HIV protease has been initiated with the theoretical chemistry team. The group is pursuing scientifically very challenging "emerging" projects.

Two researchers both have a very important teaching load (192h/year each). That should be taken into consideration in the global evaluation of their research activity.

The scientific projects proposed for the next period are better defined and more focused with respect to the work carried out in the previous period. This is a positive evolution. In the present project there are three lines to be followed up: 1) Bioactive molecules; 2) Bio- and nanotechnologies and 3) Fundamental research on unusual ligands for biological applications. The projects are of high originality. Line 1 contains two sub lines: Responsive probes for magnetic resonance imaging and N-CO interactions as a new pharmacophore, both requiring demanding synthetic capabilities. The former is important from the point of view of applications in biomedicine. The development of enzymatically activated Fe(II)-based contrast agents and their application in small animal MR imaging remains an ambitious and high-risk project. The group should focus on providing the proof of concept within the next period. Line 2 deals with biomimetic polymer backbones and the design and synthesis of fluorophores for detection of specific biological functionalities. Although creative in character, the ideas have not yet been sufficiently developed. Line 3, concerning the creation of C3-symmetric ligands, has a more fundamental character and has already given good experimental results.

- **Conclusion:**

Overall, the group has a strong skill in organic chemistry and uses its basic principles for the developments of innovative projects that hold potential for applications in diverse fields of bio-organic chemistry (drug discovery, IRM imaging). On the other hand the team had a limited scientific production. They pursued and plan to continue their work on high-risk projects based on original ideas (contrast agents based on low/high spin Fe switch). The exploitation of the solid-state fluorophore HPQ to design enzymatic probes looks very promising and could relatively rapidly result in real imaging applications (existing contact with a company specialized in small animal optical imaging).

- **Strengths and opportunities:**

The projects are highly innovative and conceptual. The practical implications in biomedicine could be large.

- **Weaknesses and threats:**

The potentialities of lines 2a and 2b have not been fully developed. The small group is at a risk to disperse itself in too many projects.



- Recommendations:

The major problems are associated with the insufficient number of students for so many lines of research. New recruitment of PhD students is recommended. The recruitment of another permanent researcher would be also very important.

Additional expertise in the field of coordination chemistry and physico-chemical characterization of the novel MR probes could be beneficial. This could be obtained either in the form of an external collaboration, or by hiring a post doc with such a background. Attention should be paid to avoid dispersion of the research subjects.

**Team 3** : Kinetics and structure (KS).

**Team leader**: Mr Wei DONG.

- Staff members (on the basis of the application file submitted to the AERES)

|  |   |
|--|---|
| N1: Number of researchers with teaching duties (Form 2.1 of the application file)  | 1 |
| N2: Number of full time researchers from research organizations (Form 2.3 of the application file)                       | 2 |
| N3: Number of other researchers (Form 2.2 and 2.4 of the application file)   |   |
| N4: Number engineers, technicians and administrative staff with a tenured position (Form 2.5 of the application file)    |   |
| N5: Number engineers, technicians and administrative staff without a tenured position (Form 2.6 of the application file) |   |
| N6: Number of Ph.D. students (Form 2.7 of the application file)  | 2 |
| N7: Number of staff members with a HDR or a similar grade  |   |

The KS team is constituted of 1 professor, 2 researchers and 2 doctoral students and pursues research in three challenging topics: porous media and fluid confined properties, soft condensed matter and reaction dynamics modeling. The team develops accurate simulations and original theoretical approaches. The combination of different theoretical models has filled some gaps in the understanding of physicochemical properties of confined fluids.

The group has produced 21 articles in high impact factor journals and the high quality of the work is attested by 10 invited talks at conferences and 9 invited seminars. The quantity of publications is good considering the small size of the group and the broad interests covered by the three topics.

The contractual relations are few but appropriate. This is consistent with the large part of the work devoted to the development of fundamental and theoretical aspects.

The group recruits PhD and post-doctoral students but their number is quite low. This is probably due to the difficulty for a team in a laboratory attached to a chemistry department to attract students having good background in physics and motivation for theory and simulations.

External financing should be enhanced in the future in view of the possibilities associated to the breakthrough made in the area of confined fluid properties.



Regarding the small size of the permanent staff, the number of collaborations is reasonable and well appropriate to the research goals pursued.

The recognized skill of the group in stochastic approaches is actually valorized through direct collaboration with IFP for the modeling of kinetics in complex fluid systems.

The involvement of the members in teaching activities corresponds to the presence of one assistant professor.

Overall, the project is based on the well-established experience of the members and well organized around confinement and porous materials (characterization, thermodynamics and adsorption properties). The items proposed in the project are relevant and challenging. The field of structure and thermodynamics studies of porous materials is developed in high-level international teams and clever choices of the systems and of collaborations should be considered. External financing should be planned and improved.

The development of reactive force fields can be a promising tool for the description of reactivity at surfaces but their ability and validity in this area remain uncertain and this should be one of the first points to be verified.

- **Conclusion:**

The group has broad interests and good external contacts. The research topics are challenging and quite well conducted. The work done in the past four years is of good quality and recognized by publications in the good journals and by some invited talks in international conferences.

- **Strengths and opportunities:**

The success of recent theoretical developments should allow the group to extend its influence and develop new partnerships.

- **Weaknesses and threats:**

The group is small and the research topics are dispersed. The group fails internal interactions and coupling to other groups in the laboratory.

- **Recommendations:**

This group should be strengthened by PhD and post-doctoral students and maybe by the recruitment of a permanent researcher able to link different groups or topics of the future team 1.



#### Team 4 : Electronic phenomena in inorganic compounds (PECI).

Team leader: Mr Serguei Borchtch.

- Staff members (on the basis of the application file submitted to the AERES)

|  |   |
|--|---|
| N1: Number of researchers with teaching duties (Form 2.1 of the application file)  | 1 |
| N2: Number of full time researchers from research organizations (Form 2.3 of the application file)                       | 3 |
| N3: Number of other researchers (Form 2.2 and 2.4 of the application file)   | 0 |
| N4: Number engineers, technicians and administrative staff with a tenured position (Form 2.5 of the application file)    | 1 |
| N5: Number engineers, technicians and administrative staff without a tenured position (Form 2.6 of the application file) |   |
| N6: Number of Ph.D. students (Form 2.7 of the application file)  | 3 |
| N7: Number of staff members with a HDR or a similar grade  | 2 |

The PECI team is composed of 3 permanent researchers/lecturers, 1 research engineer and 3 doctoral students and a number of post-doctoral researchers. The main topics of the team are spin-crossover and other magnetic phenomena in transition metal complexes with both synthetic and theoretical approaches. Molecular magnetism is a topical and competitive research area, with the aim to provide information technology with novel materials capable of storing and treating information at the molecular level. The results obtained by the PECI team, both experimentally as well as by theoretical modelling and computational methods, are relevant to the field and beyond.

The team published 54 papers in refereed international journals. Members of the team gave 3 invited lectures, 11 oral communications and 23 poster presentations at national and international meetings. 2 PhD theses were defended in the evaluation period. The publication rate is to be considered very good given the comparatively small size of the research group. Visibility at conferences could be improved.

The team participates in 3 ANR funded projects of which they have the lead in one. It has funding from 3 regional projects and from 1 COST 26 action. It has also participated in the Network of Excellence MAGMANet. For the size of the team this constitutes a very good recognition of the originality of their work.

The group is integrated in a joint research network between French and Japanese groups working on molecular magnetic materials coordinated by the University of Rennes. National collaboration with physics groups in Toulouse and Versailles ensure physical and photophysical characterisation of compounds. The collaboration with external institutions is thus appreciable. The team leader is actively recruiting young researchers. Thus 4 post-docs (3 international) and 3 PhD students (1 international) were recruited during the evaluation period. The group is well managed. The team has one assistant professor involved in teaching.





The project of the laboratory for the next period envisages the creation of a team in theoretical chemistry in which the present team is to be integrated. The current work is to be continued in the enlarged framework with resulting synergies. Research work is to be conducted in four directions: a) synthesis of spin-crossover compounds in the form of multinuclear systems and polymers, b) the theoretical description of spin-crossover compounds, c) theoretical calculation of the electronic properties of other open shell systems, d) methodological developments. One of the goals of the theoretical approach is to find answers to long-standing questions regarding the nature of cooperative effects resulting in first order phase transitions in certain spin-crossover compounds. Two young researches, one MdC the other on CR, are beginning to generate new ideas which will result in productive research.

- **Conclusion:**

The team has a very good impact on the local and international environment. The combined theoretical and synthetic approach to multi-functional molecular magnetic transition metal compounds is topical. In their elected areas the research group is internationally competitive. The team contributes to the analysis of the chemical and electronic behaviour of spin-crossover complexes and to theoretical developments with relevance and originality, as exemplified by the theoretical treatment of open-shell systems and metal-field theory.

- **Strengths and opportunities:**

The team has developed challenging research subjects and is able to describe chemistry of spin-crossover complexes comprehensively by examining all their degrees of complexity. The complementary theoretical and experimental approach can be regarded as a strong point as it results in a more rational design of compounds and systems with desired magnetic as well as photophysical properties. The high variety of spin-crossover systems, which can be synthesised, ensures great opportunities for future studies.

- **Weaknesses and threats:**

Only one person represents the very productive experimental part, and there is a gap between the expertise in synthesis and in computational approaches with regard to the physical characterisation and physical investigation of the relevant processes. This is partially bridged by national collaborations. However, integration with other groups in the laboratory is not very strong and may threaten continuity in the otherwise topical work. This may be somewhat remedied with the proposed new and more integrative structure of the laboratory. Unfortunately, there is a certain danger that in the new structure the synthetic part of the research project becomes even more isolated.

- **Recommendations:**

If the laboratory decides to continue with the fruitful synergy between experiment and theory on a longer term, the experimental part needs to be reinforced. This could be achieved by the allocation of human resources or by transversal integration with the experimental teams in physical chemistry and thoroughly anchoring the synergy in collaborations with external laboratories. Considering the future retirement of the senior staff in charge of both the experimental and the theoretical part, the team and the laboratory should be vigilant to the transfer of know-how to new staff members. In view of this, a better integration of the younger researchers and networking with other units of the laboratory are called for, as sketched in the project of the "Laboratoire de chimie" of the ENS together with the University and the CNRS.



**Team 5 :** Reactivity, Catalysis and Spectroscopy (RCS).

**Team leader:** Françoise Delbecq.

- Staff members (on the basis of the application file submitted to the AERES)

|  |   |
|--|---|
| N1: Number of researchers with teaching duties (Form 2.1 of the application file)  | 2 |
| N2: Number of full time researchers from research organizations (Form 2.3 of the application file)                       | 5 |
| N3: Number of other researchers (Form 2.2 and 2.4 of the application file)   | 3 |
| N4: Number engineers, technicians and administrative staff with a tenured position (Form 2.5 of the application file)    |   |
| N5: Number engineers, technicians and administrative staff without a tenured position (Form 2.6 of the application file) |   |
| N6: Number of Ph.D. students (Form 2.7 of the application file)  | 8 |
| N7: Number of staff members with a HDR or a similar grade  | 3 |

The RCS team is constituted of 2 professors, 7 researchers/lecturers, 8 doctoral students and post-docs. It performs high-level research in a very important (scientific, technical and economic) field (catalysis). The work in the group is highly innovative has a high quality and impact as measured by the number (103) and quality of the journals where it is published, by the number of invited talks (40) at international conferences and by the number of citations. A healthy number of PhD theses from the group were defended during the past four years, and the a member of the group received a major French award.

The team has external funding from a good number of external contracts including several national and regional contracts, one with industry, two EU Networks, two COST programs and one international contract, an a large number of national and international collaborations with top universities and institutions. The field (catalysis) is of enormous technical and economic importance, and this is going to increase with the present focus on new, sustainable energy technologies. Catalysis is at the heart of solving problems of storing the energy from sunlight as a fuel or converting biomass to fuels and chemicals. The group has good contacts to applied research and industry.

On the personnel side the group is well equipped. Better access to computer power will be essential to the future success of the group. The best international competitors will have access to larger and larger computer systems.

The direction of the projects in the group is ambitious but also realistic, given the expertise in the group.

- **Conclusion:**

The group is one of the jewels of the Laboratory and could serve as a model for other groups. It covers a large spectrum of modelling in the field of catalysis, reactivity and characterization of surfaces and interfaces. A recent interesting addition is modelling of enzymes and bio-molecules. The impact of the work through a very large number of publications and invited talks at international conferences place the group at a very high international standard. The team is recognized and well integrated in the local community, its success in external financing is important. The organization and the governance appear harmonious.



- Strengths and opportunities:

The group has a broad base of theoretical methods, and a good balance between applications of well-established methods and development of new ones. The group has several outstanding scientists and a very good net of international and national contacts.

- Weaknesses and threats:

The largest threat is not to have access to sufficient computer resources, including computer management.

- Recommendations:

More synergy with other groups would be good. At the same time it is important to maintain good internal communication to avoid fragmentation of the group. The new activity in biological catalysis must be supported strongly to develop its full potential. It is important that the next generation of (permanent) researchers is supported so that it will reach the same status as the more senior members.

**Team 6 :** Chemistry for Optics (CPO).

**Team Leader:** Mrs Chantal ANDRAUD.

- Staff members (on the basis of the application file submitted to the AERES)

|  |   |
|--|---|
| N1: Number of researchers with teaching duties (Form 2.1 of the application file)  | 1 |
| N2: Number of full time researchers from research organizations (Form 2.3 of the application file)                       | 3 |
| N3: Number of other researchers (Form 2.2 and 2.4 of the application file)   | 0 |
| N4: Number engineers, technicians and administrative staff with a tenured position (Form 2.5 of the application file)    |   |
| N5: Number engineers, technicians and administrative staff without a tenured position (Form 2.6 of the application file) |   |
| N6: Number of Ph.D. students (Form 2.7 of the application file)  | 6 |
| N7: Number of staff members with a HDR or a similar grade  | 2 |

The main topic of the CPO team is the design and synthesis of new organic molecules as well as metal complexes for applications in different fields of non-linear optics and photonics. The expertise of the team is well recognized at the national level and the international visibility has been significantly improved over the past four years. The large impact of the research is seen from the numerous collaborations established with physicists and biologists and the involvement in many projects and networks. The highlights are related to i) NLO quadratic effects with new amphiphilic dyes derived from pyridine dicarboxamides that are highly efficient for potential membrane imaging by SHG, ii) the conception a new family of highly photostable dyes for electro-optic modulation produced at gram scale, and iii) design of linear and branched oligofluorenes for optical limiting in the IR and NIR. Interfacial projects for bio-labelling using new trispicolinates lanthanides complexes for two-photon absorption are promising.



The group is currently organized around 3 senior scientists (1DR2 and 2 CR1). One Maître de Conférences has left to take a professorship position in 2007, and a CNRS researcher has been recruited in 2005 with an ATIP funding from CNRS. Also, very recently, a Maître de Conférences has been recruited on a Chaire d'Excellence position. The quite large number of post-doctoral students and PhD students (6 and 5 respectively) reveal the high dynamic of the team.

The group has published more than 47 articles, 5 proceedings, 2 book chapters and has co-edited one book. Most articles have been published in high impact factor journals (*Angew. Chem.*, *J. Am. Chem. Soc.*, *J. Phys. Chem.*). 5 PhD theses have been defended during the evaluation period 2005-2009. The team leader has a robust reputation in NLO field and is regularly invited to international conferences. Altogether, the group leader presented 19 lectures and members of the group presented numerous posters at international meetings. Two patents have been deposited (one international patent US 2006, one patent application in 2009). Further patents can be expected from the activity of the group.

The team is involved in numerous national and international programs: 2 ANR, 1 EU-STREP- on NLO materials, a collaborative European project on luminescent polymers. Two industrial programs are developed with Thales and CisBio Int. PhD fellowships and financial supports have been obtained from defence organizations (DGA: 3 PhD grants, Air Force research lab) as well as from the Region (Chemistry Cluster, CIBLE, FINOV1). In addition the team has established a strong network with several specialists of NLO (J. Zyss, et al/ENS Cachan; F. Charra/CEA-Saclay, J. M. Nunzi/Canada), which is significant of the recognition of the expertise of the group. Several international collaborations have been developed with material chemists (Malström/KTH Sweden) and experts in spectroscopy (Norway, UK, Italy) and within a cooperative program with Turkey in 2007-2008 (CNRS-TUBITAK). Collaborations with biologists are essentially centred on local and regional contacts (Grenoble, Lyon) and the FP7 Health program.

For the next four years, the project proposes several new topics in addition to pursuing the main axis based on the conception of probes for material applications (organic chromophores for protection against laser and for photonics). In particular new directions will be explored such as photodynamic therapy and bio-imaging with lanthanides. The objectives seem realistic in the medium to long term but several key issues will have to be addressed i) instability of trispicolates-lanthanides complexes at the biological concentrations ii) finding new photosensitizers displaying both efficient singlet oxygen generation and high two photon absorption.

The project is based on mastery and understanding of light/molecule/matrix interactions in various systems and in this regard is highly ambitious. On the other hand, the diversity of the interfacial projects will require establishing strong interactions with biologists. This is already done with the CisBio company but efforts should be made to reach the claimed objectives related to medicine such as imaging and treatment of Cancer, diagnostic and treatment of Alzheimer disease, Material for artificial retina.

- **Conclusion:**

High standard research by a group which is well-established in the international community; the scientific production is of very high impact and excellent visibility. There is strong involvement in different programs with the emergence of transverse programs within the team in creation

- **Strengths and opportunities:**

The research is excellent, fully in line with today's requirements of society, such as improved tools for medical diagnostics.

- **Weaknesses and threats:**

Many transverse projects are planned within the new team whose size is going to increase significantly related to previous format. A strong effort of internal communication at the level of the team will therefore be needed.

The recruitment of a Professor in physics (section 30) appears critical in order to avoid isolation, reinforce the physical and fundamental aspects of the research and globally to increase independency with regard to collaborations.



Less researchers than programmed in the activity report will finally join the team (4 vs. 7). Care must be taken not to impact on the quality of the scientific project, and priorities will have therefore to be defined.

- Recommendations:

Arrival of additional 4 researchers with complementary skills to the current team is very relevant, and definitely constitutes one of the main issues of the new structure; broadening to new horizons / frontiers is opened through integration of new expertises (Materials Science (x3 researchers) and one researcher in Photonics). The resulting ensemble opens very promising perspectives in term of applied materials, as shown by the variety of the proposed projects. Good integration of the two teams has to be a key goal for the next period.

**Team 7** : Hybrid Materials (MH).

**Team leader:** Laurent BONNEVIOT.

- Staff members (on the basis of the application file submitted to the AERES)

|  |   |
|--|---|
| N1: Number of researchers with teaching duties (Form 2.1 of the application file)  | 2 |
| N2: Number of full time researchers from research organizations (Form 2.3 of the application file)                       | 0 |
| N3: Number of other researchers (Form 2.2 and 2.4 of the application file)   | 3 |
| N4: Number engineers, technicians and administrative staff with a tenured position (Form 2.5 of the application file)    |   |
| N5: Number engineers, technicians and administrative staff without a tenured position (Form 2.6 of the application file) |   |
| N6: Number of Ph.D. students (Form 2.7 of the application file)  | 2 |
| N7: Number of staff members with a HDR or a similar grade  | 1 |

This small team of 2 permanent researchers, 1 post-doc and 2 doctoral students is performing good quality research based on interesting and promising concepts and ideas. However, the overall scientific production is not very large (13 pub), although it should be noted that the group is based on 2 professors with heavy teaching loads. Only one paper is published in a really top rank journal (Angewandte Chemie, 2005). Moreover, a leading author on this latter paper has since moved to the team SSC.

The number of invited seminars is nil. With the loss of an important actor in the field, the team is becoming dangerously small. Despite the small size, the team is however still attracting a reasonable number of post-docs and PhD/master students, so testifying a persisting vitality.

The ability to obtain external funding is good and the team is involved in a good number of external collaborations. Contractual relations are likewise fully adequate.

The departure of one permanent staff from this small team raises questions concerning organisation and governance. The merging into a larger group can help to solve the problem. Both permanent group members are very much involved in teaching activity.



In the future the team will join a larger unit, working on Functional and Photonic Materials. The team is planning to extend its research on mesoporous materials by including a new line on drug delivery. An extension of the efforts in catalysis is also foreseen. Furthermore the team will develop new materials for gas purification and capture. All these aims are topical and worthwhile, and could in the future raise the productivity beyond the modest levels of the past. All the project aims are original and can allow overcoming the difficulties of the past.

- **Conclusion:**

Despite its small size and rather low profile, the team has promising ideas and shows good creativity. The team may continue its research more successfully in the new environment.

- **Strengths and opportunities:**

Incorporation in the new Materials grouping could be very helpful, given that the team seems not to have achieved critical mass on its own. Furthermore the team has the opportunity to develop further collaborations.

- **Weaknesses and threats:**

Correlations and overlap between the group's work on heterogeneous catalysis by nanoporous materials and that of other groups involved in heterogeneous catalysis will need careful attention and management.

- **Recommendations:**

The team should increase the productivity and establish constant contacts with the other groups of the unit involved in catalysis and gas capture.

## **Team 8 : Photonic and functional materials**

The group of the four researchers who are to join the Laboratory of chemistry of the ENS are reviewed in their current structure. With regard to the Laboratory of chemistry, the arrival of several researchers from outside laboratories is programmed, in connection with the creation of team number 3 "Matériaux Fonctionnels et Photonique" within the new structure of the laboratory. More precisely, the transfer will concern four permanent researchers: a professor, a director of research CNRS, and an assistant professor from two different laboratories of the UCBL, as well as a director of research CNRS from Grenoble. Together with the teams CPO and MF, this will result in a strong, interactive research team at the Laboratoire de chimie of the ENS Lyon with good possibilities of collaboration with different units in and outside Lyon. In conclusion this is a highly relevant integrated project, offering strong scientific guarantees and promising developments of the research activity of the ENS Lyon team to new frontiers.

- **Strengths and opportunities:**

The strong reinforcement provided by the new organization resulting in team number 3 of the Laboratoire de Chimie of the ENS Lyon, appears fully justified from a scientific point of view. It will put together, at the same place, actors with ideal complementary skills, covering different aspects of molecular chemistry, materials science and photonics. The two last items will be clearly reinforced. Therefore, this operation offers a strong added value, and can be considered as exemplary, since it opens new promising perspectives in term of applied materials, related to various fields (medicine, optics and photonics and environment).

The experts have also noticed that this operation results from already existing strong collaborations between the different actors, and that the scientific projects have been built jointly on the basis of the past common experience. Therefore, the project appears very consistent and matches perfectly with the broad expertise of the group.



- **Weaknesses and threats:**

The project has initially been devised based on a higher number of permanent researchers. Attention must be paid so that this will not impact on the global quality of the project.

- **Recommendations:**

It appears critical that a position of Professor in Physics (30e section) is proposed to this group, to avoid isolation of the group.



### Laboratoire de Chimie

| Note de l'unité | Qualité scientifique et production | Rayonnement et attractivité, intégration dans l'environnement | Stratégie, gouvernance et vie du laboratoire | Appréciation du projet |
|-----------------|------------------------------------|---|--|------------------------|
| <b>A</b>        | <b>A+</b>                          | <b>A</b>  | <b>A</b>                                     | <b>A+</b>              |

Nom de l'équipe : Supramolecular Chemistry and Stereochemistry

| Note de l'unité | Qualité scientifique et production | Rayonnement et attractivité, intégration dans l'environnement | Stratégie, gouvernance et vie du laboratoire | Appréciation du projet |
|-----------------|------------------------------------|---|--|------------------------|
| <b>A</b>        | <b>A+</b>                          | <b>A</b>  | <b>A</b>                                     | <b>A+</b>              |

Nom de l'équipe : Bio-Organic Chemistry

| Note de l'unité | Qualité scientifique et production | Rayonnement et attractivité, intégration dans l'environnement | Stratégie, gouvernance et vie du laboratoire | Appréciation du projet |
|-----------------|------------------------------------|---|--|------------------------|
| <b>A</b>        | <b>B</b>                           | <b>B</b>  | <b>A</b>                                     | <b>A</b>               |

Nom de l'équipe : Kinetics and structure

| Note de l'unité | Qualité scientifique et production | Rayonnement et attractivité, intégration dans l'environnement | Stratégie, gouvernance et vie du laboratoire | Appréciation du projet |
|-----------------|------------------------------------|---|--|------------------------|
| <b>B</b>        | <b>B</b>                           | <b>B</b>  | <b>B</b>                                     | <b>A</b>               |





Nom de l'équipe : Reactivity, Catalysis and Spectroscopy

| Note de l'unité | Qualité scientifique et production | Rayonnement et attractivité, intégration dans l'environnement | Stratégie, gouvernance et vie du laboratoire | Appréciation du projet |
|-----------------|------------------------------------|---|--|------------------------|
| <b>A+</b>       | <b>A+</b>                          | <b>A+</b>   | <b>A+</b>                                    | <b>A+</b>              |

Nom de l'équipe : Chemistry for Optics

| Note de l'unité | Qualité scientifique et production | Rayonnement et attractivité, intégration dans l'environnement | Stratégie, gouvernance et vie du laboratoire | Appréciation du projet |
|-----------------|------------------------------------|---|--|------------------------|
| <b>A+</b>       | <b>A+</b>                          | <b>A+</b>   | <b>A+</b>                                    | <b>A</b>               |

Nom de l'équipe : Electronic phenomena in inorganic compounds

| Note de l'unité | Qualité scientifique et production | Rayonnement et attractivité, intégration dans l'environnement | Stratégie, gouvernance et vie du laboratoire | Appréciation du projet |
|-----------------|------------------------------------|---|--|------------------------|
| <b>A</b>        | <b>A+</b>                          | <b>A</b>  | <b>A</b>                                     | <b>A</b>               |

Nom de l'équipe : Hybrid Materials

| Note de l'unité | Qualité scientifique et production | Rayonnement et attractivité, intégration dans l'environnement | Stratégie, gouvernance et vie du laboratoire | Appréciation du projet |
|-----------------|------------------------------------|---|--|------------------------|
| <b>B</b>        | <b>B</b>                           | <b>B</b>  | <b>B</b>                                     | <b>B</b>               |



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**Le Directeur général de l'ENS de Lyon**

à

Monsieur Pierre Glorieux  
Directeur de la section  
des Unités de recherche  
AERES  
20, rue de Vivienne  
75002 – PARIS

Lyon, le 22 mars 2010

Monsieur le Directeur,

Vous m'avez transmis le rapport du Comité d'experts concernant l'évaluation de l'unité « laboratoire de Chimie » UMR 5182.

L'ENS de Lyon a apprécié la qualité de l'analyse et l'encouragement très valorisant apporté aux équipes pour poursuivre leurs activités. Elle prend bonne note des suggestions et recommandations formulées par le Comité et réaffirme son soutien à l'unité en vue de maintenir une recherche innovante et reconnue au niveau national et international.

Je vous remercie ainsi que les évaluateurs pour la qualité de leurs travaux et vous prie d'agréer, Monsieur le Directeur, l'expression de ma plus haute considération.

**Olivier FARON**

