



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

Section des Unités de recherche

Report from the visiting committee

Research unit :

Institut Parisien de Chimie Moléculaire - UMR 7611

University Pierre et Marie Curie



February 2008



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de recherche

*Le Directeur*

**Jean-Jacques Aubert**

february 2008



# Report from the visiting committee

## The research unit :

Name of the research unit : Institut Parisien de Chimie Moléculaire

Requested label : UMR

N° in case of renewal : 7611

Head of the research unit : Mr Max MALACRIA

## University or school :

Université Pierre et Marie Curie - Paris 6

## Other institutions and research organization:

CNRS

## Date(s) of the visit :

From January 28<sup>th</sup> to 30<sup>th</sup> of 2008

# Members of the visiting committee



## Chairman of the committee

Pr. Antonio TOGNI, Laboratorium für Anorganische Chemie - ETH Zürich

## Other committee members

Dr. Valérie GABELICA, Université de Liège - Belgique

Dr. Didier BOURISSOU, Université Paul Sabatier - Toulouse

Pr. Claude PIGUET, Department of Inorganic Chemistry, University of Geneva

Mrs Michèle BERTRAND, Université Paul Cézanne Aix-Marseille 3

Pr. Paul DYSON, Ecole Polytechnique Fédérale de Lausanne

Dr. Lahcene OUAHAB, Université de Rennes 1

Dr. Dario BASSANI, Université des Sciences et Technologies Bordeaux

Pr. Carmen NAJERA, Université d'Alicante

Pr. Reinhard BRUCKNER, Institut für organische Chemie und Biochemie, Albert-Ludwigs-Universität Freiburg

Pr. Yannick LANDAIS, Université Sciences et technologie Bordeaux 1

Pr. André CHARRETTE, Université de Montréal

Pr. Florence DJEDAINI-PILARD (membre du comité national du CNRS), Université d'Amiens

## CNU, CoNRS représentants

Pr. Philippe KALCK (membre du CNU), Ecole Nationale Supérieure des Ingénieurs en Arts Chimiques et Technologiques - Toulouse

Pr. André VIOUX (membre du comité national du CNRS), Université des Sciences et Technique du Languedoc Montpellier 2

## Observers



## AERES scientific representative:

Mr Régis RÉAU

## University or school representative:

N. Lacome, Responsable du Directoire de la Recherche Université Pierre et Marie Curie-Paris 6

## Research organization representative (s) :

M-C. LASNE (DSA CNRS), CNRS

# Report from the visiting committee



## 1 • Short presentation of the research unit

- Numbers of lab members including researchers with teaching duties, full time researchers, ingeneers, PhD, students, technicians and administrative assistants : 156 (3 PREX, 4 PR1, 2 PR2, 4 PREM, 29 MCF, 1 DREM, 3 DR1, 7 DR2, 9 CR1, 2 CR2, 70 PhD, 1 PRAG, 8 ingeneers, and 13 technicians and administrative assistants)
- Numbers of HDR and of HDR who are PhD students avisors : 43 ; 20
- Numbers of PhD students who have obtained their PhD and average lenght of a PhD during the past 4 years : 81  
Numbers of PhD students currently present in the research unit : 70 ; Numbers of PhD students with fellowships : 69
- Numbers of lab members who have been granted a PEDR : 20
- Numbers of “publishing” lab members : 57/59 EC and C ; 5/5 PREM and DREM

## 2 • Preparation and execution of the visit

The visit took place on January 28-30, 2008. Prior to the visit, a detailed program has been set up by the chairman of the committee in tight collaboration with the representative of the AERES and the directors of the to date existing five UMR's (7611+7071, 7084, 7573 and 7576) constituting the Institut de Chimie Moléculaire de Paris-Centre, Organique, Inorganique et Biologique (FR 2769). The program has been sent to the involved parties in the second half of December 2007. Little adjustments had to be made during the following weeks in order to accommodate specific needs. The directors of the single UMR's have provided the committee's members with detailed reports concerning the activities of their respective UMR's during the past four years. Such reports have been available, on paper and/or in electronic form, either just before the end of 2007 or by the beginning of January 2008. These reports, while containing the essential scientific information needed for the evaluation, have not been specifically conceived for the evaluation.

The committee spent three days in Paris visiting the UMR's mentioned above. The visit started on Monday, January 28, and was focused on UMR-7611 for the full day with all committee's members attending. After an introductory presentation by a representative of the Université Pierre et Marie Curie (UPMC), the director of the UMR provided an overview of the scientific activities which were then detailed by the leaders of the in part newly composed research teams. The committee had the opportunity to ask questions, both after each talk and during a poster session during lunch time. All discussions took place in an open and pleasant atmosphere.

The committee also met with the Conseils de Laboratoire of both UMR's 7611 and 7071, before concluding with a plenary session during which first elements of the present report have been discussed.

The former UMR's 7071 and 7613 have been visited on Tuesday, January 29, by only part of the committee and the visit has been structured in much the same way as on the previous day. However, the chairman of the committee attended only the last part of the presentations.



### 3 • Overall appreciation of the activity of the research unit, of its links with local, national and international partners

The UMR 7611 is relatively large and shall be newly composed by eleven research teams. In terms of a size comparison, this corresponds to a small-to-average-size department at universities in many other countries, with the important difference that this UMR is focussing its research activities in the area of synthetic chemistry to a large extent. This confers the UMR a sufficiently large critical mass to be able to mark a prominent presence on both national and international levels. The UMR is performing innovative research in several areas of interest to synthetic organic chemistry, bioorganic chemistry, and molecular materials. The work of this UMR is characterized by a high level of collaborative networking, within the unit, with research groups at other institutions in Paris, but also with partners both in France and abroad, at universities and in industry. As one could expect from such a large operation, the awareness of the international community for the single research teams within the UMR is variable. Overall, however, this UMR surely belongs to the very best in France, being able to compete with the world leaders, in terms of both productivity and quality in the chosen areas. A more detailed appreciation of the research activities is given below in the form of specific evaluations concerning the single research teams, one by one.

### 4 • Specific appreciation team by team and/or project by project

- Team: “Chimie Organique de Synthèse”

This is the largest team in UMR 7611 and is well recognized by the international community for its leading contributions to organometallic and free-radical chemistry. The team is well organized and its charismatic leader is surrounded and supported by bright younger personalities. Over the last four years, the group has maintained its human potential, departures being more or less compensated by the recruitment of promising young researchers.

The constant flow of PhD students (14 theses defended, 16 theses under way) and post-doctoral researchers observed during the last contract period and the declared director's policy for the future are good auspices for the continuity of scientific performance and the achievement of new projects. In terms of publications, for the period 2004 to 2007, 35 of the 60 recorded papers have been published in chemistry journals whose impact factors range from good to very high. This is an attestation as to the quality of the conducted researches, both in terms of originality and creativity. Contributions to book chapters (11) must be added to the overall productivity assessment.

Three main topics are being developed, among which the synthesis of complex skeletons via organometallic- and radical-domino reactions are prominent.

Cobalt-catalyzed cycloisomerizations is a long-standing research area. Alkynylboronates are novel and promising partners for the preparation of macrocycles or conductive polymeric materials through cyclotrimerization and subsequent Pd-mediated coupling reactions. Au- and Pt-catalyzed cycloisomerization of enynes, ene-ynamides, and more specifically the behaviour of yne-allenes in these processes is a challenging topic. The contribution of this group also occupies a recognized position in the field.

In the area of radical domino reactions, the temporary introduction of silicon-containing unsaturated tethers enables the construction of elaborated polycyclic sub-structures. The use of ynamides and N-cyanamides as radical acceptors is particularly innovative. There is no doubt that the development of new radical cascades, based on the latter and leading to biologically active compounds, will be followed with great interest by both academic and industrial researchers. The use of heteroelements as radical leaving groups and as source of chirality has been investigated in the recent past. New processes involving sulfur-centered and phosphorus-centered radicals look very promising from both fundamental and synthetic point of views. Concerning synthetic methodology, special attention will be given during the next four years to “Green Chemistry” and to the use of non toxic reagents, such as for instance the use of metals such as Cu, Fe, Ti and Sm in redox reactions.



A new topic has emerged recently from collaborative projects conducted with the "PolyOxoMetallates" (POM) team. The project is ambitious since it includes catalysis and biological applications. Preliminary results obtained with POM inclusion of lanthanides that can be used as recyclable Lewis acid catalysts have demonstrated high chemoselectivities in Mannich or Mukaiyama reactions. The preparation of POMs hybrids where the organic moiety is covalently linked to tin has been achieved. The use of a chiral organic conjugate, opens perspectives with regard to the separation of POMs enantiomers and to the synthesis of chiral organometallic hybrid catalysts.

The three main axes are supported by a recently created small unit of computational chemistry performing theoretical calculations of reaction pathways and molecular modelling. Thus, an understanding of the intimate mechanism of Co-mediated cyclotrimerization depending on the nature of the partner (alkyne or alkene) and of the ligand has recently been achieved. The interaction with theoretical chemists extends the fields of expertise of the team and will in all likelihood stimulate creativity. The whole team is well integrated in international networks and in collaborative research projects with renowned leaders in the above mentioned areas of research. The different members of the team are involved in 3 different ANR programs. The equilibrium between fundamental and applied chemistry is ensured by contracts with companies such as Sanofi-Aventis, Servier, Rhodia, Pierre Fabre, etc. In addition, the UMR director is at the same time director of the "Institut Fédératif de Paris Centre". The involvement of the different members of the laboratory in the "Ecole Doctorale de Chimie Moléculaire" and in various teaching responsibilities favours the interaction between teaching and research on the UPMC campus. Thereby, the next research structure will occupy a strategic position and should be able to attract the best PhD students. In conclusion, this team produces innovative and high standard research. Its contributions are highly recognized by the international community. The team ranks among the best research groups in the field of organic synthesis via organometallic and free radical processes.

- **Strong points:** Excellent research, good management.
- **What needs to be improved:** While the quality of the papers published over the period under scrutiny ranks from high to excellent, considering the number of permanent researchers and PhD students, the productivity may be improved. Concerning the projects, a good balance should be found between time-consuming natural product synthesis and the development of new methodologies with strong impact.
- **Recommendations :** Because the research performed so far is of high quality and very coherent, the only recommendation the committee came up with is to continue on the very same line.

- **2) Team : "Synthèses Sélectives et Organometalliques"**

This team results from merging two research groups specialized in stoichiometric reactions of organozinc derivatives and in Pd-catalyzed reactions, respectively.

The first group « Main Group Organometallic Chemistry » is composed of four permanent positions (1 Professeur, 2 Maîtres de Conférence, 1 Chargé de Recherche). Over the last 4 years, 2 post-doctoral fellows, 2 PhD students and 8 undergraduate students have been working on the different research topics.

The main achievements concern (i) the diastereoselective reaction of allenylzinc derivatives with homochiral *N*-sulfinylimines and the synthetic application of the resulting propargylic aziridines, and (ii) intramolecular carbozincation reactions affording an original entry to  $\beta$ -prolines. Future research will seek to develop new routes to organozinc derivatives (intermolecular carbozincation, hydrozincation and transfer of organic residues from radical precursors). The group has acquired a very good expertise in the preparation and application of organozinc derivatives, and its productivity is satisfactory (14 over the last 4 years).

The second group « Innovative Catalytic Transformations for Organic Synthesis » is also composed of four permanent positions (1 Professeur, 2 Chargés de Recherche, 1 Maître de Conférence). Over the last 4 years, it has involved 1 post-doctoral fellow and 10 PhD students (including 4 in collaboration). Its productivity is modest (11 over the last 4 years).



The main achievements concern the methodological and synthetic developments of Pd-catalyzed allylic alkylation reactions. The intramolecular version affords a straightforward access to pyrrolidones and  $\gamma$ -lactones. The possibility of combining Pd-catalyzed alkylation and Ru-catalyzed cross-metathesis has also been demonstrated. In parallel,  $\alpha$ -sulfinyl carbanions and sulfenate anions have proven valuable partners in Pd-catalyzed allylic alkylations and arylations. Lastly, new chiral dithioether ligands have been developed and the experimental comparison of dithioethers and diphosphines has been initiated. The group is well-recognized for its expertise in Pd catalysis and domino sequences. The coherence of the research activity favors the emergence of new directions, as illustrated by the Pd-catalyzed arylation of sulfenate anions which is noteworthy. The productivity over the last 4 years is good (14 publications). In addition, the group is strongly engaged in networking at the national and European level (2 successive COST actions). Collaborations with industrial partners have also been recently settled (2 PhD co-financed by the CNRS).

- **Strong points** : Good degree of originality and coherence, good productivity in terms of publications, for both groups.
- **What needs to be improved** : Poor dissemination activity and external networking of the first group. The variety of organometallic compounds investigated and synthetic transformations thereof is narrow compared to that of competing groups worldwide and should be improved. Productivity may also be improved by the merging of the two groups. The committee also encourages this team to report their work in the general chemistry journals with the highest impact.
- **Recommendations** : The visiting committee considers the merging of the two groups very positively and encourages them to take advantage of their complementarity to engage in common research projects. In this context, the variety of organometallic compounds should be extended further including their synthetic applications. The first group is also strongly encouraged to develop external networking.

- **3) Team : "Glycochimie organique, biologique et supramoléculaire"**

For the past four years this team was constituted by six researchers and teaching-researchers with permanent position (1 PU, 2DR-CNRS and 3 MCU). This figure will be reduced to five for the next four years period (1PU, 1PU émérite, 1DR-CNRS and 2 MCU).

Overall, the quality of the research performed in this team is excellent and can be considered to belong to the top 20% in the field of carbohydrate chemistry. Further strengths of the team are as follows. The originality of the approach and the ideas, such as the synthesis of novel monosaccharide mimics or the oligosaccharides synthesis, is evident and this team is involved in national and international networks. The research coherence and its cumulative character, focused on a single, well-defined area, are outstanding. The quality, the number and the nature of the publications are excellent. For the past four years, the number and the nature of the invited lectures given by team members are impressive. Moreover, several PhD theses have been concluded.

- **Strong points** : High quality and originality of the research performed.
- **What needs to be improved** : The absence of patents deriving from the work of the team and the very low number of partnerships with private companies are an indication of the strong emphasis on fundamental aspect of carbohydrate chemistry.
- **Recommendations** : Although there is a relatively good fit between the scientific goals described in the project and the size of the team, it would be important to define specific research aspects where to focus the initial and most important efforts of the team. The long-term viability is good and the integration into the UMR 7611 is a good opportunity to optimize the access to equipments and above all to increase the interactions with the other teams such as the "Chimie organique de synthèse" or "chimie supramoléculaire" teams. The committee recommends a strong awareness for these aspects.



- **4) Team : "Hétérocycles"**

This new team is the result of one of the most significant restructuring following the creation of the new "Institut Parisien de Chimie Moléculaire". Thus, the "Heterocycles" team shall collect following "old" groups :

- Two groups of the previous UMR 7611, working on the synthesis of nitrogen compounds using chiral auxiliaries, with emphasis on the construction of 4-, 5- and 6-membered ring heterocycles and alkaloids synthesis. These teams have published overall 19 articles and got a single invitation to an international conference. Ten seminars at universities have been also presented.
- One group interested in chromium and tungsten carbenes as well as functionalization of pyridines who published 13 papers and presented 7 seminars and communications during the past period.
- A fourth group working on organometallic chemistry (mainly organo-copper and palladium) who published over 14 papers and presented 6 seminars at universities.

Thus, the new "Heterocycle" team will be one of the largest in the UMR, composed by one professor, one CNRS research director, three "chargé de recherché (CNRS), six "Maitre de conferences" and one technician.

The productivity is satisfactory although a majority of the papers are published in journals with modest impact factors. The research program proposed for the next four years is mainly a continuation of the past projects. The degree of innovation of the research proposed varies from one group to another. With the exception of the study on NHC ligands for Pd-catalyzed processes and the chemistry of allyl and allenylcopper reagents, the planned methodologies convey little novelty. There are few joint projects between the four groups, however suggesting little overlap and cohesion. Moreover, while the association of the first three groups is natural, as they use similar synthons, strategies and tools, the presence of the fourth team is less obvious. It does not appear rational, considering the creation of a specific team devoted to organometallic chemistry and developing zinc and palladium chemistry. Little support to the whole project by the organometallic team further indicates this lack of unity. From a perspective point of view, the team is composed by young researchers who will have to catch opportunities to develop innovative programs in a not too distant future.

- **Strong points** : Research in the field of catalysis (NHC ligands etc.) is interesting.
- **What needs to be improved** : There is a lack of unity between sub-groups in this team. One can also note little innovation in the future projects in the specific area of alkaloids synthesis.
- **Recommendations** : Considering the number of permanent researchers in the team, new methodologies with a certain degree of risk should be envisioned for the future. The establishment of a coherent medium- or long- term research plan should be a priority for this team to promote cohesion between the younger members and to catalyze innovative research projects with potential for higher international visibility.

- **5) Team : "Polyoxométallates"**

The POMs team is currently one of world leader in the field of polyoxometalates (POM's). The team has published 65 papers, a significant number of which in high standard journals. The distribution of published outputs over the members is quite good. Furthermore, 25 invited presentations at international meetings and 12 PhD thesis, among which 6 are already completed, are worth mentioning. The team has also a large number of international and national collaborations and takes part in international networks. It has an excellent and well established expertise in the synthesis of polyoxometallates. The team is now moving beyond the synthetic aspects towards exploiting the specific properties of POMs, as well as their functionalization in view of their use as inorganic ligands for supramolecular chemistry and for the development of new research directions in the areas of molecular materials, reactivity and molecular electronics. The project reflects a very good approach as well as coherence in the character of the conducted research. This team is managing the X-ray center and the NMR facilities, common to the whole institute and beyond.

Some important scientific results achieved in the last four-year period should be mentioned here: (1) Nitrogen transfer in the series of organoimido complexes, (2) hybrid organic/inorganic complexes for potential applications in biology and molecular electronics, (3) a single molecule magnet based on Mn complexes.



The team has to cope with important personal changes, currently and in the near future. One professor will retire next April 2008 and is expected to obtain an emeritus position to continue his research in the same team. One associate professor (MCF) moved to another university and another MCF has decided to create his own group within the new Institute. So the group will include 2 PR, 1 DR, 2 MCF and one technician and is expected to recruit soon one MCF and one AI. An emeritus professor will also join. Therefore, taking into account the available personnel and facilities and in view of what has been achieved and the plans for the future, the long-term viability of this group should work.

- **Strong points** : Synthesis, prominence of members, numbers and nature of published papers and invited lectures.
- **What needs to be improved** : The researchers in charge of common technical facilities, such as NMR spectroscopy and X-ray diffraction, should focus more on research and leave the services to engineers and technicians.
- **Recommendations** : discussions and interactions with the new group "Chimie Supramoléculaire " have to be encouraged in order to ensure the viability of this thematic area, eventually leading to a strong and fruitful impact.

- **6) Team : "Chimie Supramoléculaire"**

The emergence of a new research group filling a local void in the field of supramolecular chemistry has been proposed. The future team will be initially composed of two permanent researchers and will build on existing collaborations between the inorganic and organic chemistry groups to rapidly develop novel research directions. These exploit the advanced synthetic knowledge of the current groups to propose systems in which organic-inorganic interactions are explored for applications in biology and magnetic materials. The team leader possesses considerable experience in this area and has already built a solid reputation thanks to very promising results in the area of enzyme recognition and stabilization of inorganic POM assemblies. The proposed work will, if successful, present significant opportunities for generating high impact science. Given the current size of the team, the pursuit of all envisaged research aspects will be difficult or, in the worst case, detrimental to productivity. Priorities should be rapidly identified based on appropriate risk-taking and the establishment of a clear and original research identity for the future team. The latter point is particularly important with regards to existing research within the proposed institute.

- **Strong points** : The originality and interdisciplinary character of the research presents high potential for strong collaborative work.
- **What needs to be improved** : The proposed project does not yet possess a global research strategy, which would be useful to identify and prioritize research directions, avoid fragmentation of effort, and efficiently target funding opportunities.
- **Recommendations** : The position and viability of the future team is contingent on the support of the institute to rapidly making available human resources, particularly students and post-doctoral fellows, to carry out the proposed research projects. Continued collaborations with the inorganic and organic chemistry groups are encouraged.

- **7) Team : "Matériaux Magnétiques Moléculaires et Absorption X"**

Over the period 2004-2008, the team consisted of 4 full time researchers, 2 teachers, 1 engineer and 2 technicians. The academic productivity was rather high and well distributed over the team members: 80 articles in peer reviewed journals, partly of high impact factor; 19 invited lectures at international conferences (5 additional ones at national conferences), 28 invited talks at foreign Universities (4 additional ones in France), 24 oral communications at international and 12 at national conferences; 6 PhD theses were defended and 3 more are in progress. The team was involved in 4 national and 3 international programs (UPMC, ANR, CNRS, French ministry), 2 national (CNRS) and 2 international network (EU; Magmanet network gathers the European forefront research in molecular magnetism). The team was involved in teaching, thematic workshops and popular scientific conferences.



The major achievements were the synthesis and characterization of two single chain magnets (respectively the third and fourth examples in the literature), the report of the first photomagnetic high spin molecule, the enantioselective crystallisation of an optically active molecular magnet, and the experimental evidence of photoinduced magnetic properties in two different systems.

The strengths of the team lie (1) in the expertise in molecular materials where magnetism is coupled with another property (especially chirality and photoinduced electron transfer); (2) in highly developed skills in coupling different characterisation techniques (X-ray diffraction, X-ray absorption spectroscopy, micro-Raman spectroscopy, magnetic circular dichroism, paramagnetic NMR etc.).

In conclusion the team has gotten an excellent national and international visibility in the field of magnetic molecular materials, in relation to the originality of its research and the expertise of its members (including promising young talents), which should warrant long term viability in this context.

- **Strong points:** Among the best teams in the field of molecular magnetism worldwide. Expertise in a variety of characterization methods.
- **What needs to be improved:** The team is part of a relatively small and closed community studying molecular magnetism. The awareness of the broader scientific community for the significance of the fundamental aspects of the research carried out could be improved.
- **Recommendations:** The research carried out by this team is very fundamental in character. However, the ability of the team to implement experimental results on molecular systems towards the development of devices should possibly be improved.

- **8) Team : "Architecture Moléculaire : Auto-Assemblage, Reconnaissance, Chiralité"**

This team is constituted by 5 staff (permanent) members: 2 directeurs de recherche, 2 maîtres de conférence, 1 ingénieur de recherche.

The team is active in the general fields of coordination and organometallic chemistry. Its scientific production during the 2004-2007 period is considerable in terms of both quantity and of the scientific level of the targeted journals. The focus of the research interests on synthetic and structural aspects ensures some coherence and a minimal covering of the different topics addressed by the team. Potential applications and physicochemical properties are accessible thanks to external collaborations.

Except for the stabilization of some exotic organic/organometallic intermediates and for the design of aesthetically appealing bidimensional chiral coordination networks, the selected scientific challenges are not always clear. The rationalization of the driving forces controlling the assemblies in solution or during their transfer into the solid phase is not at the level required for obtaining a strong impact in supramolecular chemistry. Since recognized specialists in this field are currently emerging in the same UMR with the creation of a novel group in supramolecular chemistry, the ARC research team could greatly benefit from close contacts and collaborations with this new entity.

- **Strong points:** High publication output
- **What needs to be improved:** The rather vaguely defined, long-term scientific goals need some improvement, in order for the research carried by the team to gain a more specific identity.
- **Recommendations:** Since weak non-covalent interactions represent the cornerstones of a large part of the research projects proposed by this group for the next period, we recommend some brainstorming on the development of a rational approach for implementing the physical origins of these interactions in the chemical projects. A close collaboration between the ARC group and the emerging group in supramolecular chemistry is also strongly recommended in order to create the required critical mass for improving potential impact and visibility of this team.



### 9) Team : "Chimie Organique et Organométallique"

This team of 5 permanent researchers is well known for and maintains highly developed skill in the functionalisation of chromium(arene)tricarbonyl and cationic manganese(arene)tricarbonyl complexes for the preparation of organometallic dipoles, precursors for applications in NLO, as well as substituents in nucleosides chemistry. More recently, the lithiation of functionalized benzene derivatives allowed to perform efficient carbon-carbon coupling reactions catalysed by palladium that were not previously accessible. Furthermore, the team has pursued the synthesis of Iron porphyrin complexes and envisages their use in catalytic oxidation reaction with dioxygen as the primary oxidant. The level of publications is satisfactory with some contributions in high impact journals.

- **Strong points:** High research coherence, long standing expertise in a well defined area.
- **What needs to be improved:** the research project on the porphyrines presents some routine character.
- **Recommendations :** the lithiation of various arenes coordinated to the  $[\text{Mn}(\text{CO})_3]^+$  fragment appears to be eminently promising and it is recommended to further develop this specific topic. If the novel generation of epoxidation catalysts is promising, then the project could be developed; otherwise, it is strongly suggested to be careful with a too classical approach.

### 10) Team : "Nanostructures et Semi-Conducteurs Organiques"

This team's trans-disciplinary research is oriented towards elucidating complex structure-activity relationships linking molecular structure and electronic properties at the nano-scale. In particular, the arrangement of molecules and molecular architectures into two-dimensional lattices is probed using STM and STS techniques at the solid-liquid interface. The team, composed of two permanent researchers and one engineer, published twenty articles in peer-reviewed journals over the last four years. The main thrust of the work is oriented towards the adsorption of organic molecules, typically extended aromatic structures or cyclic thioalkanes, with additional efforts devoted to the development of donor-acceptor edifices for non-linear optics or solar energy conversion.

The team conducts work that is in a highly competitive and rapidly evolving field due to the substantial socio-economic benefits associated with the development of organic electronics and opto-electronic materials. The team leader enjoys a leadership position on the national level, and comfortable exposure at the international level. Whereas the overall level of the work is of good to excellent quality, it is disparate in originality. Advances in the applicability and / or understanding of two-dimensional adsorbates are likely to require a combination of advanced instrumental techniques and the use of original molecular structures associated with the testing and development of theoretical models. While the azanaphthylenes could fit into the latter category, this is not the case of some of the other systems under consideration. Similarly, a plethora of covalent fullerene-based donor-acceptor assemblies have already been investigated, and the rational for persevering in this direction remains unclear. Other work, such as the utilization of organic crystals, or the investigation of molecular packing on surfaces, is much more original and should eventually receive considerable international awareness.

The level of productivity of the group is surely acceptable, but could be improved without great difficulty. It is disclosed in journals and conferences that are good for the field, attesting to the quality of the work. Its more original aspects can potentially impact the field and offer assurance for the long-term viability of the team's goals.

- **Strong points:** The team's balance between fundamental and applied research is positively reflected in its dense national and international network of collaborations. It is well poised to take a strong international position in the area and can potentially offer high-profile research opportunities.
- **What needs to be improved:** Though of high quality, the number of publications is average considering the size of the team. This point could be rapidly improved without significant additional effort and guarantee increased international visibility.
- **Recommendations:** The team can strongly benefit from the presence of experienced inorganic and organic chemists within the proposed institute to develop and study extremely original systems. The team's remote location must not be an impediment for the establishment of these fruitful collaborations.



- 11) Team : "Spectrometrie de masse"

This team (1 PREX, 2 MCF, 1 CR1, 4 IE) is a local and national leader concerning the development and application of mass spectrometry as analytical tools for organic, bio-organic and bio-inorganic molecular systems. The strongest points of the team are (1) the excellent balance between fundamental and applied research, (2) the strong interconnections between research and teaching activities with a very good record of PhD theses, (3) the instrumental platform that was developed during the last four years, and (4) the prominence and charisma of the team leader, who maintains strong relationships with industrial laboratories, thus generating benefits for the whole team in terms of funding and training.

The publication output is very good, with 65 publications equally distributed between fundamentals and applications of mass spectrometry. Fundamental research developed in-house includes (1) studies on desorption/ionization mechanisms, (2) the determination of acidity/basicity of biomolecule building blocks, (3) studies on noncovalent complexes, and (4) studies of gas-phase catalysis of organic reactions and biomolecule fragmentation. Although the position of the team in the first three topics is not that of an international leader, the continuation of this research activity is important for the training of students, because it helps designing and adapting mass spectrometry methodologies to new analytes. The recently implemented Penning ionization method is likely to lead to important and original applications in the near future. Fundamental studies of gas-phase catalysis and reactivity induced by metals is the most original and promising aspect of the current research, and can be considered a trademark of the UPMC mass spectrometry team.

The relocation of the team in the proposed Institut Parisien de Chimie Moléculaire is reasonable and will guarantee a visibility and identity of the team for the next four years. The challenge for the long term development of the team will be the succession of the team leader within four years. The committee recommends the recruitment of an external, experienced leader in the field of mass spectrometry who should be capable of maintaining the existing network of industrial collaborations, sustaining the instrumental platform, and enhancing the international reputation of the team.

- **Strong points:** Balance between fundamental and applied research, industrial collaborations, instrumental platform, prominence of the director, number of publication and PhD theses.
- **What needs to be improved:** Publication strategy focusing on clarity and impact needs improvement. Lack of emphasis and concentration of efforts on the most promising and original research aspects.
- **Recommendations:** recruitment of an external leader for the long-term viability of the research team and of the mass spectrometry platform.

## 5 • Appreciation of resources and of the life of the research unit

One very important point that needs to be stressed above all concerns the laboratory space, both in terms of surface area and quality. An estimation of the laboratory surface available to the unit and a comparison with the corresponding situation of similar internationally recognized teams leads to the conclusion that a space increase by a factor of two would not be exaggerated, in the contrary, it would be most appropriate. This research unit deserves a compliment for being able to perform so well, as a whole, under such adverse conditions, conditions that do not fulfill current international standards. The committee, while having some understanding for the situation due to the problem of the *désamiantage*, emphasizes in all clarity that an improvement of the space situation should be given the highest priority and dealt with utmost urgency. A solution to the space problem would guarantee a higher level of laboratory safety, a better and more efficient use of the laboratory equipment, but it would also increase the motivation and identification of the co-workers at all levels, as well as the attractiveness of those laboratories for best qualified researchers.

The committee gained the impression that the above mentioned organizational changes, the UMR went through recently, have been well received by a majority of the staff members. Some took them very positively and with enthusiasm, some other with a very pragmatic attitude and only a few put forward some reservations towards the changes that have occurred.



## 6 • Recommendations and advice

- **Strong points :**

Good management, charismatic leader, several teams with high international reputation, several young and very promising researchers, high scientific productivity, high quality of research.

- **What needs to be improved:**

The reciprocal fitting of the various teams is somewhat artificial. For further remarks, see the specific comments made above for every single team.

- **Recommendations :**

For detailed remarks concerning future research directions, see the specific evaluations of the single teams above.

Since parts of the UMR have been subjected to restructuring, while others have been added from a preexisting UMR, one of the most important tasks for the immediate future will be the full integration of the old groups into the new structure and organization. The committee recommends therefore a consolidating attitude in order to attain a high degree of acceptance, as soon as possible, while not losing momentum. One opportunity would be to improve the communication to and via the new Laboratory Council.

Furthermore, the committee recognizes that this UMR has the chance, as a single unit, to represent and to be uniquely associated with the field of molecular chemistry at UPMC. It is therefore very important for every member of the research unit to appreciate this chance and identify with it.

Finally, taking into consideration both the precarious situation due to laboratory space (see section 5. of this report) and the prospected enhanced integration within the federation FR 2769 (see separate report) the committee strongly recommends the creation of new facilities, in particular the construction of a new building capable of hosting all research units of the federation.



CENTRE NATIONAL  
DE LA RECHERCHE  
SCIENTIFIQUE

Département Chimie  
La directrice scientifique

Paris, le

20 Mars 2008

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Monsieur Jean-Jacques AUBERT  
Directeur de la section des unités  
Agence d'Evaluation de la Recherche  
et de l'Enseignement Supérieur  
20 rue Vivienne  
75002 PARIS

Monsieur le Directeur,

J'ai bien reçu le rapport d'évaluation de l'unité de recherche UMR7611 que nous acceptons dans sa forme et je vous en remercie.

Conformément à votre demande de transmission par voie hiérarchique, je vous adresserai la réponse du Directeur d'Unité dès qu'elle me sera parvenue.

L'avis définitif de l'AERES sera un élément important pour les décisions que nous aurons à prendre lors de la contractualisation de cette unité.

Je vous prie d'agréer, Monsieur le Directeur, l'expression de ma haute considération.

  
Gilberte CHAMBAUD