Evaluation of the Research and Professional Activity of the Institutes of the Czech Academy of Sciences (CAS) for the period 2010–2014

Final Report on the Evaluation of the Institute

Name of the Institute: Institute of Inorganic Chemistry of the CAS

Fields, in which the Institute registered its teams:

Chemical sciences

Observer representing the Academy Council of the CAS: Jiri Ctyroky
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Commission No. 4: Chemical sciences
Chair: Dr Habil, Academician Christian Amatore

Date(s) of the visit of the Institute: November 30 - December 4, 2015
Programme of the visit of the Institute: see attached Minutes from the visit

Evaluated research teams:

- **Department of Syntheses**
- **Materials Chemistry Department**
- **Centre of Instrumental Techniques (CIT)**
- **Academic Materials Research Laboratory of Painted Artworks (ALMA)**

A. Evaluation of the Institute as a whole

1. Introduction

The Institute's mission is centered on its historical expertise on materials chemistry and boron chemistry topics but these traditional core research fields have now been augmented to include additional contemporary research directions in inorganic chemistry as well as related boundary branches, such as novel materials, inorganic medicinal chemistry and inorganic materials in ancient painted artworks. More recently, the Institute's research was even more diversified towards new interdisciplinary areas linked to environmental and geochemistry topics. The Institute's remarkable capacities to evolve by defining and mastering such opportunities rest on the fact that its research teams are led by established and experienced leaders with broad knowledge in inorganic materials chemistry. This provides a notable flexibility in identifying, testing and developing new research directions.

However, practical implementation of this flexibility creates a constant financial constraint on the Institute due to insufficient institutional funding (as for most Institutes evaluated by this Committee). For example, it was ca. 60% of the Institute's budget in 2015, with the remaining ca. 40% being financed through successful applications for research grants. To avoid fragmentation of research activities, the Institute and its Board have tried with certain success to equilibrate research risks with effective possibilities prone to obtain funding based on their recognized expertise. This good management provides the Institute with the ability to capitalize on successful research activities to expand into newer areas while maintaining high standards in its explorative scientific activities and thus adequately educate its students in several topical fields of modern materials and inorganic chemistry.

In terms of publications, as measured by IF or the *Nature Index* number per FTE, the Institute compares favorably with the top two CAS chemical institutes that this Committee has evaluated. This attests to its favorable research productivity.

Strengths and Opportunities

Though this is evidently implemented at different levels in each team, the research strategy of the Institute is well planned with a proper balance between pursuing its recognized areas of expertise and maintaining a reasonable level of risk. Though the

Institute concentrates on fundamental issues, it is notable that several of these have strong application potentials (new pharmaceuticals for human medicine, new bactericides, and new photocatalytic materials for air and water pollutants disposal in environment and industrial waste).

The scientific staff members are highly qualified, experienced and among the most productive when considering all CAS chemical Institutes that this Committee has evaluated. Its age distribution is favorable to ensure both a continuation of expertise and future developments.

Based on its recognition, the Institute has been able to constitute a strong network of collaborations which helps it to maintain its visibility and its good position in the international scientific community. This is evidenced by the presence of foreign scientists in most of the Institute's research teams.

Several researches developed in the Institute rely on its access to its modern instrumentation park and skilled technicians to operate the instruments (though, an important caveat is related to its financial ability to maintain the present instrumental standards).

Finally, the Committee was pleased to observe that not only the members of the Institute teach at different levels in chemical disciplines at surrounding universities and supervise undergraduate and Ph.D. students but that, in addition, it has formulated a joint doctoral program with the J.E. Purkyně University, Ústí n.L. aimed to environmental issues.

2. Weaknesses and Threats

Though the Direction of the Institute manages efficiently its personnel, some of the teams are still understaffed, mostly due to their limited amount of financial resources.

The Institute is presently benefiting from its excellent instrumental park, which is currently adequate for its researches. However, it is clear that maintaining the present instrumental standards has a financial cost that seems difficult to fulfill by the Institute alone. This assumes funding at the institutional (Czech) levels, but this may be hampered by the fact that the Czech Republic has apparently decided to concentrate on the establishment of larger infrastructures.

An additional possible threat for the future is due to the Institute is location on the campus of a private company, hence making its future liable to decision from this company rather than from CAS. However, the Commission has understood that the Institute is the owner of all the buildings that it uses as well as of the land under and around them. This certainly alleviates this danger.

4. Recommendations

The Committee has no major important recommendations to the Institute. It should be encouraged to pursue its present dynamics aimed at the modern issues in materials inorganic chemistry and its innovative avenues that present strong fundamental and applicative potentials. In this respect, the strategies towards exploration of new pharmaceuticals for human medicine, new bactericides, and new photocatalytic materials for air and water pollutants disposal in environment and industrial waste are highly appreciated.

5. Detailed evaluations

Owing to the wide panel of research interests, the detailed evaluations are performed individually in the evaluations of the different teams.

B. Evaluation of the individual teams

Evaluation of the Team: Department of Syntheses

1. Introduction

The Team has clearly evolved from traditional researches carried out in the Institute, i.e., related to the chemistry of polyhedral borane clusters. Its researches are now divided into six different areas involving: “classical” boron cluster synthesis and reactivity; application of (metalla)carborane clusters in biochemistry and biology/medicine for enzyme inhibition; extractive treatment of nuclear plant waste; polyhedral borane interaction with photons and borane applications in new light sources; modification of metal surfaces with (car)boranes for SAM’s; and theoretical/computational chemistry dealing with the problems arising mainly from the experimental works performed in the Team and sustaining them.

The Team is divided into several sub-groups focusing on the above topics, but their investigations are often interconnected, a fact that provides the team with its identity and its unity. Most of the activities are a result of very recent discoveries (i.e., made over the past ~10 years) which help the group to use their extensive knowledge of borane chemistry to penetrate into different chemical fields of chemistry and related domains where this leads to interesting entries and applications. For example, this has led the team researches to evolve towards the introduction of a new class of enzyme inhibitors or new laser materials.

Over the evaluation period, between 12–14 researchers (FTE) were involved in the research with a rather good age structure ensuring a safe continuation of the team researches in the future.

2. Strengths and Opportunities

Research of the Team is based on the long tradition of (car)borane chemistry developed in the Institute. This knowledge and the novel orientation of its research topics to modern targets have provided the team with a strong reputation in the boron-related community. This recognized position is reflected in a wide range of national and international cooperation and networking activities that were reinforced by the introduction of the team’s recent investigations. It is noteworthy, that these

collaborations are not restricted to the academic world but also include industrial partners (see below).

The Team maintains also a good involvement with universities through their teaching and theses supervisions.

The team's researches are focused on the areas where its members have an appropriately recognized expertise. This results in significant publications in leading journals, both in interdisciplinary (*Nature Commun*., *Angew. Chem*.) and good specialized journals.

Due to its substantial expertise in borane chemistry, the Team has been very successful to secure money from both national and international grant agencies. Owing to the new research directions, the Team is expected to fare well in future. Interestingly, the Team has a strong tradition in popularization of scientific issues even beyond the team research domains. For example, one of its members, Dr. Londesborough, is well-known by the public for popularizing science.

3. Weaknesses and Threats

Despite collaborations with universities, the Team has a rather low number of students involved in their research. No obvious reason seems to be able to explain this unfortunate situation.

Also, despite several results pointing to potential technological applications, the team did not acknowledge a significant funding input from industrial money involved in the Team researches.

4. Recommendations

The Team should keep its present research track and remain focused on the research angles where its members' know-how and expertise are strong, providing it with chances establish sound research collaborations.

Without limiting its participation in its present academic research networks, the Team should be more proactively looking for industrial partnerships. This would increase their funding, and most importantly, it may help to commercialize their results.

Finally, the Team should be more active in identifying the origin of its difficulty in attracting students to their research subjects, albeit the team is highly visible through its activity in science popularization.

5. Detailed evaluations

Generally, the Team investigations are focused on different outcomes of boron chemistry in which it has a strong recognized expertise. Their activities cover a wide range, from "classical" polyboron cluster research, nuclear waste treatment with carbollides, biological activity of boron clusters to materials suitable for photophysics or surface modification. Due to its discernment, the Team has been able to promote its results (and orientate its research strategy) on poly(car)borane clusters into unexpected areas of science (biochemistry, photophysics).

The "classical" boron chemistry sub-group has dealt with still not fully explored polycarboranes and has therefore identified and used some new reactivity pathways. As mentioned above, the sub-group focused on biological applications has suggested a new class of hydrophobic enzyme inhibitors which are based on unique electronic properties and size of (car)borane clusters. Work on polyborane photophysics may lead to interesting photomaterials, a field where the group investigations may be able to find some practical applications.

Owing to its expertise and proper identification of important research projects, the team publishes in very good specialized journals, mostly in inorganic chemistry, as well as even in the best multidisciplinary journals.

The Team has been active in establishing several academic collaborations, mainly in the area of biological activity of polyborane derivatives. Cooperation with other teams in the Institute seems adequate and profitably developed for mutual benefits.

Despite the correct involvement of the Team members in university teaching and scientific boards, the number of students participating in the research is not high. Only a few students (4 BSc, 2 MSc and 1 PhD over last 5 years) have finished their thesis during the evaluation period. There is an involvement in students supervising and some collaboration with small fine chemicals company (Katchem) specialized on boron chemistry. The Team is highly involved in popularizing science to the public.

Several researches performed in the Team may have some practical applications, which should be the subject of more active search for possible commercialization of these results.

Very good international reputation of the Team is based on the long tradition of boron chemistry in the Institute, which now continues into the modern era. The Institute is

one of the institutions where boron chemistry has been extensively developed since the initial discoveries. Hence the Team expertise in boron chemistry is unique in the Czech Republic and also internationally visible. Accordingly, there are several foreign researchers present in the Team. Similarly, the Team is involved in several academic collaborations, in organizing boron conferences, guest-editing special issues of boron-related journals, writing or editing monographs, etc.

The Team age distribution is good and appear appropriate to ensure maintaining the present know-how while simultaneously enhancing innovative views. Indeed, the research plans of the sub-groups of the Team seem adequate in view of the Team's expertise, involving a wide reach together with appropriate focusing on some issues. This seems to be a guarantee of its flexibility to switch its research efforts onto new goals whenever appropriate. However, in the absence of significant industrial support, there is too strong a dependence on public grant money. Although the Team has been rather successful in obtaining grants, this creates a potential difficulty to maintain the Team's unity and continue its researches.

Evaluation of the Team: Materials Chemistry Department

1. Introduction

The Materials Chemistry Department combines classical chemistry (chemistry of molecules, spectroscopy, photochemistry) and solid-state chemistry/physics with nanochemical expertise based on inorganic nanoparticles or polymer materials/nanofibres. It may then carry out a range of studies, from basic exploratory synthesis of novel materials, to development of applied methods based on these novel materials, to large scale preparations of composite materials, 2-D materials, magnetic materials, and thermoelectric materials.

The strength of the department is its focus on basic research into the synthesis of novel materials. This is a curiosity-driven basic science that often results in interesting applications. Researches range from studies of graphene and other 2-D materials, to photocatalytic and photo-responsive materials, as well to metal organic framework materials useful as active sorbents.

These researches lead to new composite materials whose functions are often based on custom-tuned photophysical properties. Thus, most of the researches are spinning around photochemistry and photophysics, synthesis/characterization of nanoparticles and nanomaterials.

An important research area is related to chemistry of singlet oxygen generated by photo-excited electrons in semiconductors, themselves produced after light irradiation of metal oxide materials such as various doped TiO_2 or other oxides, or through irradiation of molecules prone to transfer excitation energy as porphyrins or phtalocyanines. Such reactive systems are then used for depollution of harmful organic compounds (from military, environment, industrial, etc., origin leading to applications) or for disinfection (military or medical utilizations). Other fields of research are dealing with magnetic nanoparticles and materials (ceramics) for radiation protection.

The Team shows reasonable balance between basic and rather applied research. Accordingly, it has been very successful in establishing interesting collaborations which have led to interesting new materials and new applications.

The Team is the largest one of the Institute. Currently, it gathers 10 scientists, 4 technicians and 11 students (8 PhD + 3 MSc). Its age distribution is good with a strong group of researchers in the 45 to 55-year age category, promising excellent leadership in the coming years.

2. Strengths and Opportunities

The main strength of the Team inherently follows from its strong focus on the fields (photophysics-photochemistry, synthesis and characterisation of nanomaterials, application of synthetic techniques enabling scale up) where the Team has a very good expertise.

It has established collaborations with the business sector and has even led to commercial and practical applications of several researches developed in the Team. This enables the Team to secure in part its research funding.

The Team has a good access to students through teaching at universities (there is a common PhD program) and a good age balance.

The Team members publish in good chemical journals related to material, inorganic and physical topics.

3. Weaknesses and Threats

Challenges for the department are in obtaining sufficient funding for the ongoing support of the work underway, and for the expansion of the work into new areas. In the effort to support the work of the department, some collaborations have been less effective than others.

4. Recommendations

It is recommended that the focus of the department continue to be on basic research into the synthesis of new materials. This has been effective in the past, and the future of the department would be well served by this continued focus.

Additional funding from the CAS to support this basic research, in combination with the effective formation of wider collaborations (e.g., including the J. Heyrovsky Institute of Physical Chemistry) to develop novel applications, will result in a department whose international impact will continue to grow.

Finally, as the Team's nanomaterials are becoming commercialized, investigations on their effects and toxicity are highly desirable to prevent any biological/environmental issues. This may be probably performed through appropriate collaborations.

5. Detailed evaluations

The quality of the publication record of this department is quite high on an international scale. Publications have appeared in a number of high impact journals, including Langmuir, Chemistry of Materials, Inorganic Chemistry, Nanoscale, the Journal of Physical Chemistry, and the Journal of Applied Physics, in addition to important specialist journals such as Clay Science, Electrochimica Acta, and Journal of Solid State Chemistry. The great majority of the work is published in English, adding to the international impact of the work carried out in this department.

There are several high quality, enthusiastic students participating in the work of this department. Students appear to be highly motivated, and the work of the department is attractive to them. The work of this department is also of high relevance to the concerns of society, with the materials developed here having broad application in photocatalytic removal of pollutants, in the area of photo-responsive materials for application, and in the development of new thermoelectric and magnetic materials for electronic applications.

The impact of the work of this group is high on the international level. In addition, a number of projects directly benefit national concerns of the Czech Republic (active sorbents for the degradation of chemical warfare agents, for example).

This combination of international recognition and impact of the work, with applications that benefit society and applications of specific national interest, leads to a very positive view of the vitality and sustainability of the research effort of this department. Plans for future work are well outlined, and a broad effort to obtain funding for this work is underway. This department has established a good balance between direct CAS funding, and outside funding from national and international funding sources. Collaborative projects add positively to the mix of funding sources, and bode well for the future of the work of this department.

The future plans have been clearly stated and seem to be perfectly appropriate and prone to maintain the high Department status. However, owing to the Team

expertise, one would have love to see some high-risk researches. Finally, it is noted that at some instances there is a strong overlap with research plans of the Centre of Instrumental Techniques.

Evaluation of the Team: Centre of Instrumental Techniques (CIT)

1. Introduction

The Team was established in 2010 as a center for characterization and investigation of solid-state and nano-sized materials. Accordingly, it acquired mainly at the beginning of the evaluation period a number of advanced equipment facilities. From its beginning, CIT offers expertise and service in various electron microscopies, Mossbauer spectroscopy, surface and diffraction analysis and thermal analysis.

A small part of CIT, viz., the Mossbauer Spectroscopy Laboratory, is a part of the joint Laboratory of low-temperature techniques shared with Charles University (Faculty of Science, Faculty of Mathematics and Physics) and Institute of Physics of AS CR and some facilities that are located in the Rez campus. CIT is a service site for other teams in the Institute but substantial part of its working time and manpower is devoted to the, mostly expert service-like, collaborations with external partners, often from industry.

The research performed by the Center on its own, in parallel with its service-type of activities, is focused on materials with photocatalytic activity (see next paragraph) or special magnetic properties, on materials produced during possible nuclear reactor meltdown, or on mineral waste treatment. Almost all CIT research activities are spinning around its good equipment and acknowledged solid-state chemistry expertise.

The Commission noted a possible overlap of the science developed in CIT with the Material Chemistry Department concerning the field of photoactive properties of titanium oxide. However, this is a large and increasingly field that spawns several diverse topical areas, and it was apparent to the Commission that each team has found the way to develop its own research without redundancies.

Currently, the Team has 9–10 people involved in the research, several technicians and several students (BSc, MSc).

2. Strengths and Opportunities

The main strength of the Team lays in a very good characterization/measuring instrumentation for solid-state/material chemistry and physics which is sustained by a proper series of expertise.

CIT is a well established solid-state/nanoparticle center in the Czech Republic. It has established wide collaborations with industrial partners and, therefore, is mainly involved in research with strong implications to practical/industrial problems.

The CIT facilities are quite open to external partners. Its facilities for Mossbauer spectroscopy confers the center a unique position in national context. The Team has a wide international range of collaborations involving 18 foreign partners.

In agreement with its specific role in the Czech Republic, the Team has been rather successful until now to secure funding to buy and maintain its advanced equipment.

3. Weaknesses and Threats

Although the Team, overall, has a good scientific productivity, its research results are not always published in top journals devoted to materials or environment. This is certainly easily understandable owing to the applied and service characters of its researches.

However, this goes at pair with the fact that the research efficiency of the Team is somewhat dissolving into a too large number of different topics considering its size.

As it was explicitly stated by its Director during the Team presentation, its present good and expensive instrument park is progressively becoming older and will probably need some costly replacements to remain up-to-date.

4. Recommendations

If the Center wishes to maintain its present status in research, it should decide to be more focused on advanced research. Only such determination may bring results publishable in top journals and, as a consequence, is expected to bring valuable additional scientific collaborations and attract a larger number of talented students.

Although external services are part of the Center mission and necessary to rise the funds required to allow the equipment maintenance, etc., collaborations with national and international laboratories with recognized activity in basic science should become beneficial for both sides.

On the other hand, some of the results obtained up to now seem to present a high commercialization potential so the Team should consider seriously examining such issues (with collaboration with its current partners?) and possibly advancing into this direction.

5. Detailed evaluations

The high expertise of the Team coupled with its internal access to a good instrumentation park has led to very interesting research results inside the center itself and also with external partnerships among which some have led to applications of interest.

Indeed, the instrumental facilities are open to other researchers and interested parties. Although the collaborations involving CIT inside the Institute were not clearly described nor emphasized in the materials provided to the Committee, they seem to be frequent and their good levels have apparently helped these other teams to get notable results.

CIT own research results are interesting especially in the field of photocatalytic materials (though a certain overlap is noted with the Material Chemistry Department in the field of photoactive solid materials). The main strength of the Team seems to dwell in material characterization.

The Team members are involved in some teaching at universities, but the number of students who effectively participated in the research appears modest. Only a handful number of students have finished their thesis during the evaluation period, showing that the supervising and teaching activities should be increased.

The work of team is very beneficial for society as the research is timely and deals with important problems as pollution or energy matters. There is an extensive collaboration with the business sector which benefits from the Team expertise and equipment.

The expertise of the center is certainly high in national context in which it occupies a specific niche. However, the Team is less visible in international scene that obviously privileges pure research outcomes. The CIT results should be, generally, published in more reputable journals.

The age balance of the Team is reasonable and should ensure a good continuation of the research activities. Since the Team highly depends on the up-to-date status of its instrumentation, replacement and maintenance of the equipment park is expected to pose a serious financial problem if this is not handled at the level of CAS. Furthermore, the extensive dependence on external financial sources, as undoubtedly anywhere in Czech Republic, may result in problems in keeping non-permanent personnel and/or hiring new people.

Finally, the Team plans to continue research on photocatalytic materials where its position seems sensible and, therefore, acknowledged. The other future research fields seem to be reasonable provided the investigations are focused mostly to materials interesting for (future) nuclear technologies or for applications in extreme environments. These directions will suitably benefit from the Team expertise in the material characterization.

Evaluation of the Team: Academic Materials Research Laboratory of Painted Artworks (ALMA

Owing to the large number of Institutes evaluated during this campaign no real expert of the fields covered by the ALMA team was sitting in our Committee. However, though not directly active in research in these research areas, the Chair felt a sufficient expertise to handle this evaluation with adequate competence (as from his membership in the Advisory Board of the ALMA equivalent at CNRS-Louvre Museum, his organization of 2 International Symposia on these topics held in the Pittsburgh Analytical international Conference, and his membership of the Advisory Board of the Gordon Conferences devoted to Scientific Approaches to Cultural Heritage).

1. Introduction

The ALMA team is a small joint scientific laboratory of the CAS Institute (IIC) and of the Academy of Fine Arts in Prague (AFA Prague) with components located in each place. During the on-site visit, the Committee heard and evaluated the team located at IIC.

ALMA researches are devoted to the important interdisciplinary fields of cultural heritage, covering most of their aspects: conservation science, cultural heritage science and technical art history. Overall, the team comprises 3 scientists (one of them on maternity leave) at IIC, and 1 scientist, 1 technician, 1 PhD student and 2 conservators/restorers at the AFA Prague. Overall the IIC team is composed with rather young persons (2 between 45 and 55 year old).

Despite its small size, the ALMA seems to be the national leader of the area. It applies and also develops specific analytical methodologies based on a series of non-destructive micro-techniques (micro-XRD, micro-IR and micro-Raman, mobile instrumentations) to avoid the risk of false interpretations. These are mostly focused on painting pigments to analyze their properties, structures, degradation, as well as historical preparations, in particular relative to clay pigments. In this respect the ALMA team plays a key role in Czech Republic to provide important information

determining crucial decisions to be taken for cultural heritage protection and preservation.

2. Strengths and Opportunities

The team's productivity is good owing to its size (53 papers), and is properly contributing to the modern approaches developed elsewhere in the world in the field. More precisely, the small task-force of the team is not reflected in a lower quality of the researches performed but rather on their numbers. All the fields covered and the methodologies used are up-to-date and comparable to those used in France, UK, USA and Japan (such as portable XRF, portable FTIR, and portable Raman). This excellence is recognized, for example, by the past ALMA association into the EU-funded international CHARISMA network; however, this network has terminated in 2013.

The team age-distribution is adequate to predict no scientific discontinuity and possibly expansion of the team in future years.

Funding involves international cooperation and funding from the Czech SF (1 grant over the evaluated period) and from the Czech Ministry of Culture (1 grant over the evaluated period).

3. Weaknesses and Threats

As with equivalent teams elsewhere in the world, there is always an interrogation about the fact that scientific approaches to cultural heritage artefacts may have sufficient leverage to obtain access to important master pieces. Indeed, only such accesses help these teams to acquire an international visibility through providing scientific analyses that go well beyond traditional target-driven questions raised by conservators and restorers.

The team size is too small to allow high-level development of new analytical techniques, though this impression must be moderated by the evident application of the most adequate modern (portable) techniques based on critical and careful implementation of published results.

Continuous funding seems to be a high risk factor for the sustainability and development of the team.

4. Recommendations

The ALMA laboratory organizes regular biennial conferences on scientific approaches to cultural heritage and publish the corresponding material in the bilingual (Czech/English) Acta Artis Academica proceedings series. This certainly provides the team an international visibility (as documented by its involvement in the EU-network CHARISMA), but it is recommended that the team senior scientist communicates at internationally organized conferences to acquire a larger international visibility.

Date: December 29, 2015

Commission Chair: Dr Habil, Academician Christian Amatore