Estonian Higher Education Accreditation Center

Evaluation of Estonian Research in Physical, Inorganic and Analytical Chemistry

Institutes evaluated:

Institutes of Chemical Physics and Physical Chemistry,
University of Tartu
Institute of Chemistry,
Tallinn Technical University
Laboratory of Chemical Physics,
National Institute of Chemical Physics and Biophysics
Faculty of Chemistry,
Tallinn Technical University

Visit dates:

11 February- 18 February, 2001

Expert team:

Prof. Pekka Pyykkö (Team chairman)
Department of Chemistry
University of Helsinki
P.O.B. 55 (A.I. Virtasen aukio 1)
FIN-00014 Helsinki, Finland

Prof. Jorma Hölsä
Laboratory of Inorganic Chemistry
Department of Chemistry
University of Turku
FIN-20014 Turku, Finland
E-mail: jholsa@utu.fi

Prof. Irene Montenegro
Department of Chemistry
University of Minho
Largo do Paco

4700-320 Braga, Portugal
E-mail: montenegro@quimica.uminho.pt

Prof. **Jarl B. Rosenholm**
Department of Physical Chemistry
Åbo Akademi University
Porthansgatan 3-5
FIN-20500 Åbo, Finland

Contents

1. THE EVALUATION PROCEDURE

The evaluation team consisted of Professors Jorma Hölsä (University of Turku, Finland), Irene Montenegro (University of Minho, Portugal), Pekka Pyykkö (University of Helsinki, Finland) and Jarl B. Rosenholm (Åbo Akademi University, Finland).

The evaluation was commissioned by the Estonian Higher Education Accreditation Center (EHEAC). The evaluation was carried out by examining the documents, sent to the experts, and by site visits in Estonia on 11-18 February, 2001. Further printed material was obtained during the visits.

The self-evaluation reports were of reasonable quality, one comment being duplication of the same material for several persons or groups. The Team were briefed by Dr. Tiit Laasberg upon arrival on Sunday, 11 February.

The main ground for ranking the research activities were to be the scientific achievements at international level.

The more detailed criteria specified by the EHEAC were:

1. **The novelty of the results of research and development,**
2. **The quality of research and development,**
3. **The strategy and perspective of research,**
4. **The competence of research groups and their capability for development,**
5. **Success in applying for funds and grants,**
6. **National and international cooperation,**
7. **The implementation opportunities for the research results and their importance to the Estonian society,**
8. **The correspondence of research and development to the international level.**

The Team decided to lump together these criteria to the following three:

1. **Competence, novelty and quality of present research,**
2. **Strategy, perspectives and implementation opportunities,**
3. **Quantitative data (funding, collaborations, publication statistics, academic degrees produced).**

Note that our point 1 mainly refers to past, well-documented achievements and includes the Government's points 1, 2, 4 and 8. Point 2 refers more to the future and includes the Government's points 3 and 7. Finally, point 3 includes the previous points 5 and 6.

Each of points 1-3 was graded in the suggested scale:

E = Excellent (väga hea)
G = Good (hea)
S = Satisfactory (rahuldav)
U = Unsatisfactory (mitterahuldav).
In a more fine-grained scale, also used by a previous group, E/G is higher than G/E.

2. INSTITUTES OF CHEMICAL PHYSICS AND PHYSICAL CHEMISTRY, UNIVERSITY OF TARTU

The evaluation Team visited the Department of Chemistry, University of Tartu, on Monday, 12 February. The Institutes of Physical Chemistry and

Chemical Physics gave presentations and some laboratories were briefly visited.

As a general impression, the Team were struck by a strong *esprit de corps* and an apparently good inner cohesion. The premises were partially renovated, partially shabby. The scientists were reasonably happy with their Library, computer facilities, and instrumentation and enjoyed many international collaborations.

Two days could easily have been spent at this site.

Granted the good inner cohesion, the formal splitting of the Department of Chemistry into three Institutes (Chemical Physics, Organic Chemistry, Physical Chemistry) appears somewhat artificial. The Laboratory or Chairs had a more clearly defined role. A united Department of Chemistry would do the job.

2.1. Institute of Physical Chemistry

The history of the Institute is related to electrochemistry, including various applications. Names of importance for the Institute include G.F. Parrot (nature of galvanism), M. Jacobi (Daniel´s battery), V. Past (corrosion and H_2-O_2 fuel cells) as well as R. Pullerits and Palm (bismuth solid drop electrode). In recent years the focus has been laid on interfacial electrochemistry under the leadership of J. Tamm and E. Lust, including reaction kinetics.

A more distant but popular topic is the introduction of environmental chemistry on the agenda by T. Tenno, focussing on wastewater monitoring with biosensors and sludge activation.

Chair of Physical Chemistry: Professor: E. Lust (7 PhD + 4 MSc students)
Associate professors: H. Keis and J. Ehrlich

Chair of Inorganic Chemistry Professor: J. Tamm (3 PhD + 1 MSc)
Associate professors (2)

Chair of Colloid and Environmental Chemistry: Professor: T. Tenno (6 PhD + 5 MSc)
Lecturers (2)
Senior researchers: (4, named)

Education and training **PhD (16, named)**
MSc (10, named)

As indicated in the short historical overview, the Institute of Physical Chemistry has gained its present scientific outline through the appointment of its professors in the 1990´ies holding the chairs indicated above. The main research fields of the professors are planned to be maintained during the ten-year period of 1996-2005. However, a thrust is laid on the acquirement and modernisation of the research instrumentation. No special plan for the education is presented.

The research group has a very solid understanding of the possibilities of electrochemical technology and the research seems to be well focussed. However, as compared to the chemical physics research groups the aims were narrower.

Enn LUST (born 1956)

Lust has been trained mainly at the University of Tartu. He has visited (duration not given) the Frumkin Institute of Electrochemistry, Academy of Sciences, USSR (1989), Laboratory of Interfacial Electrochemistry, Academy of Sciences, France (1995) and Institute of Physical Chemistry, Uppsala, Sweden (1996). He has held all his professional positions at the University of Tartu.

His current research program is on the influence of electrochemical nature and crystallographic structure of the phase boundary on the characteristics of adsorption processes and on the kinetics of various reactions. The most important outcome of the research is the construction of double layer supercapacitors which outperform the traditional faradaic supercapacitors. In the first hand it is the speed of charging and discharging and secondly it is the working at low temperatures. The supercapacitors are on the commercialisation stage in the USA.

Jüri TAMM (born 1937)

Tamm has been trained mainly at the University of Tartu. He has visited (duration not given) Moscow University (1973 and 1978), Leningrad University, St. Petersburg (1981) and Oxford University (1995). He has held all his professional positions at the University of Tartu.

His current research interest is in electrocatalysis especially hydrogen evolution reaction on nickel, cobalt and alloys as well as in electropolymerization and analytical properties of conducting polymers. His research on the conducting polymers in the presence of anionic dopants, relating to their mobility in the polymer structure was of key

interest. From semi-empirical quantum calculations conclusions as to the conformation of the polymer chains were drawn. By the use of chiral dopants it was expected that the induction of helical structures to the polymers could bring special features. As a goal the construction of a fully polymeric battery was set. K. Tammeveski described, *e.g.* about the construction of a fuel cell which may be used for the production of peroxide. T. Silk described the construction of biosensors where the bioactive element was changed by immobilizing the oxidoreductace (oxygen sensing) or other enzymes on the sensor. Another interesting field of research is the development of plastic injection moulding tools using electroforming.

Toomas TENNO (born 1940)

Tenno has been trained mainly at the University of Tartu. He has held all his professional positions at the University of Tartu. The position was the first one dedicated to environmental chemistry in the former Soviet Union.

His main fields of research are in biosensors for environmental measurements, modelling of processes in enzyme and microbial biosensors and constructing of sensors and microsensors for oxygen determination in several media, reduction of oxygen on several electrode materials, determination of superoxide in biological fluids, activated sludge processes in wastewater biotreatment and determination of nutrient removal efficiency of treatment plants. There had been a very clear commercial focus on manufacturing sensors for the oxygen reduction in particular as biosensoring, *e.g.* for analysis of the biodegradability of phenolic compounds in industrial wastewaters. The oxygen permeability studies were focused on dermatology. Two sensor systems were on the commercialisation stage, one had been patented during the Soviet era.

On the international level scientific collaboration has been listed with Oxford University, University of Milan, Moscow State University, University of California, Technical University of Denmark, University of Barcelona, Helsinki University of Technology, University of Liverpool and University of Lund. Five projects financed through foreign funds have also been listed. The senior researchers at the Institute have hosted or co-hosted 4 national and international conferences. Additionally they have served at two advisory boards for international conferences and acted as a guest editor for a conference volume in Electrochimica Acta.

Aside of the collaboration in use of equipment there has been a national collaboration with the Institute of Physics and Applied Mathematics, University of Tartu.

2.2. Institute of Chemical Physics

The Institute of Chemical Physics (ICP) was founded in 1993 by reorganisation and restructuring of the Department of Analytical Chemistry, Department of Organic Chemistry, Laboratory of Chemical Kinetics and Catalysis, Laboratory of Acid-Base Equilibria and Laboratory of Bioorganic Chemistry. One of the major tasks and functions of the ICP is teaching analytical chemistry, bioorganic chemistry as well as theoretical and computational chemistry.

Staff and structure

Chair of Analytical Chemistry Professor: I. Koppel (9 PhD + 8 MSc)
Assoc. professors: P. Burk, U. Mölder, J. Pentsuk, I. Leito
Lecturer: L. Paama
Senior researcher: M. Danilkin
Researchers (6)

Chair of Bioorganic Chemistry Professor: J. Järv (7 PhD + 4 MSc)
Assoc. professor (0.5): A. Rinken
Senior researchers: A. Uri, A. Rinken (0.5)
Researchers (2)

Chair of Theoretical Chemistry Professor: M. Karelson (5 PhD + 1 MSc)
Senior researcher: U. Maran
Researchers (6)

Chair of Chemical Physics: vacant
Support Technical staff (10)

There are 22 doctoral students enrolled which supercedes the number of master students (13).

The collective strategy of research at ICP includes the experimental and theoretical study of the reactivity and properties of chemical compounds and materials. This goal is reached by the application of different analytical (FT-NMR, FT-ICR, HPLC, AAS, AES, Thermoluminescence spectroscopy, *etc*.) and theoretical models for the study of the independence between properties (functions) and structure of molecules and materials. As described in detail the strategy of research is very clear and ambitious with distinct priorities, indeed.

Although there are plans for the foundation of Institutes with substantially overlapping functions they seem to be built on extra (EU and national) funding expectations. The most recent plan is the foundation of an Institute of Technology. It is to be hoped that the number of these time consuming operations should be kept at a minimum level.

From the report and from the presentations given it seems that the research groups are the leading ones in Estonia with a high international standing, as experienced by the quite extensive and manyfold international collaboration. Also the exploitation of the results commercially seems to be well organised and viable.

Ilmar KOPPEL (born 1940)

Koppel was graduated as PhD from University of Tartu, and as DSc at the Academy of Sciences, USSR. He is a member of the Estonian Academy of Sciences. He has made long term research visits to a number of foreign laboratories including University of California, Irvine (1974-1975, 1981-1982, 1989-1990, 1993), University of British Columbia (1978-1979), Uppsala University (1991, 1995-1996), University of Nice (1993-1994), CSIC Madrid (1994, 1998), University of Erlangen (1995-1996, 1997), University of Marburg (1995-1996), University of Freiburg (1995-1996, 1998), University of Barcelona (1995-1996), and Kyushu University (1999). He has held all his formal positions at the University of Tartu.

His major research areas are in different aspects of the acid-base concept in the gas phase as well as in solvents, leading to the design and synthesis of superacids and superbases. For this research he is applying a large number of modern instrumental techniques supported by quantum chemical calculations.

The research on super acid-super base scales, in particular in organic solvents and in the gas phase is very original and successful. It combines the development of elegant experimental procedures with advanced theoretical calculations. Also the utilisation of these results seems very promising, indeed.

The very successful fundamental and applied research on luminescent materials lead by senior researcher Danilkin deserves special attention. This group has succeeded in the commercialization of the Eu^{2+} doped CaS materials in dosimetry. Also several PhD students are enrolled in the group but, unfortunately to chemistry, from the Physics department.

Finally, the analytical chemistry research carried out by lecturer Paama is involved in the analysis of interesting materials as high T_c superconductors in co-operation with foreign research groups.

Jaak JÄRV (born 1948)

Järv was graduated as PhD and as DSc from University of Tartu, in the latter case including training at Moscow University. He has received honorary doctorates both from University of Kuopio (1991) and from Uppsala University (1996). He is also a member of the Estonian Academy of Sciences (1997). He has visited the Institute of Heteroelement Chemistry in Moscow (1975), University of Stockholm (1978-1979, 1984), University of Uppsala (1989, 1994, 1995) and Åbo Akademi University (1993, 1996). He has held all his formal positions at the University of Tartu.

His research interests are in the mechanism of ligand interaction with G-protein coupled receptors, kinetics and mechanism of enzyme catalysis, specificity and molecular recognition phenomena in enzyme catalysis and receptor binding as well as in structure-activity relationships and activity of bioactive compounds. Although sightly more distant towards bioorganic chemistry there were strong links to traditional physical chemistry. The multi-step kinetics of enzyme reactions were of particular interest.

Mati KARELSON (born 1948)

Karelson has graduated as PhD from University of Tartu in 1975. He has been awarded a "courtesy professorship in chemistry" at the University of Florida in 1992. He is the director of the Centre of Strategic Competence at the University of Tartu. He has visited the University of London (1980), University of Florida (1985-1986, 1989-1990, 1993-1996), Christian-Albrechts-Universität Kiel (1993-1996), Max Planck Institute of Astrophysics (1993-1999) and Oxford University (1997). He has held formal positions both at the University of Tartu and abroad.

His research interests are in quantum theory of condensed disordered media: Solvent effects on spectra and chemical reactivity, theoretical modelling of chemical reaction kinetics and equilibria, artificial intelligence in chemistry, quantitative structure activity/property relationships, chemical software development, molecular design of novel chemical compounds and technological processes, properties of electrolyte solutions, heterocyclic chemistry and organic conductive polymers. His research was theoretical, but oriented towards practical applications, such as artificial intelligence. The QSAR correlations include properties like toxicity, sweetness, glass transition temperature of polymers, rubber vulcanisation acceleration, *etc*. Moreover, the estimation of solvation energies, organic compounds in solution, conformations and tautomer equilibria were in the focus of the research.

The ICP has a multitude of very modern and advanced research instruments. For the analyses and structural characterization the following instruments are available: UV/vis, FT-NMR, AAS, AES, GC, HPCL.

The professors at the ICP have been active in maintaining the international co-operation including a very large number of scientific visits abroad. There is no mentioning on visits *to* the Institute, however. The international collaboration is listed under each professor. The impressive international funding infrastructure indicates that the co-operation has been successful.

A very clear and ambitious plan vas presented for the collaboration with industry, including patenting and foundation of small firms. A long-term goal of Chemistry Department is the construction of a new building, including fresh instrumentation.

3. NATIONAL INSTITUTE OF CHEMICAL PHYSICS AND BIOPHYSICS (Tallinn)

On Wednesday, 14 February, the Team visited a number of groups at the National Institute of Chemical Physics and Biophysics, both at the Rävala location downtown and at Mustamägi. This is a really unique establishment, belonging administratively under the Parliament and strongly dominated by the exceptional competence and personality of Professor Endel Lippmaa.

The National Institute of Chemical Physics and Biophysics (NICPB) was founded as the Institute of Chemical Physics and Biophysics of the Estonian Academy of Sciences 1980. The Institute was formed on the basis of the Department of Physics (now Laboratory of Chemical Physics) and the Department of Biochemistry (now Laboratory of Bioorganic Chemistry) of the Institute of Cybernetics and research group of molecular genetics (now Laboratory of Molecular Genetics) of the Institute of Physics. The Laboratory of Bioenergetics was established in 1993. Since 1998 the NICPB is a public research institution, financed from the state budget and grants, but totally independent in all research activities.

The business idea appeared to be to attract absolutely first-rate scientists by offering lower salaries than at the Universities, compensated by excellent working conditions.

This laboratory is a greatly appreciated partner internationally, functions to an extent as a domestic standard authority in certain areas, and has selected collaborations with the Universities in the areas visited by the Team.

The number of people engaged by the Institute has remained about the same over an extended period of time, being 160 people in total. However, some of the personnel are permanently employed in foreign laboratories giving an effective total of 130 persons out of which 50 have a higher academic (PhD or DSc) degree. Some 15 PhD students do their research at the Institute but are registered elsewhere.

The facilities at both sites were excellent in comparison with the other sites visited. The instrumentation was often old but very competitive due to skilled modifications and constructions made by the own personnel. It seemed *e.g.* that the Institute of Chemical Physics and Biophysics had the only advanced workshop left among the sites visited and a better library than many Institutes.

Laboratory of Chemical Physics

The Laboratory of Chemical Physics (LCP) started within the Institute of Cybernetics in 1961 under the leadership of Professor Lippmaa. The staff of the LCP includes 18 persons; 9 senior research scientists and 9 research scientists. LCP is active in several fields of physical and chemical research and several research projects are integrated with the research in other laboratories of NICPB. Thus the separation of physical, inorganic and analytical chemistry into an autonomous research topic is a somewhat ambiguous operation. The present report is connected with the chemistry related projects.

The research is obviously focussed on solid state (and) high resolution NMR for which instrumentation is provided only to LCP in Estonia. Additionally advanced instrumentation in mass spectrometry, cyclotron resonance and far IR spectroscopy are also available at the laboratory. There is also a recent interest in high performance quantum chemistry on the properties of organic and inorganic systems and calculation of chemical reactivity together with lattice dynamics of these systems.

The present research activities have been guided by target financing and ESF grants as well as by previously established co-operation with other research laboratories at Estonian Universities and with research groups outside Estonia. This will remain unchanged in the forthcoming years. With regard to chemistry the following pertinent research projects are discussed:

High field high resolution NMR spectroscopy, Principal Investigator (PI) DSc T. Pehk
High resolution solid state NMR spectroscopy, PI PhD A. Samoson
New approaches in NMR quantum computing and chemistry, PI Acad. E. Lippmaa

New methods in mass spectrometry, PI PhD J. Subbi
Physical chemistry in environmental research, PI DSc U. Kirso

Endel LIPPMAA (born 1930)

Lippmaa has graduated as PhD from the Tallinn Technical University in 1956 and as DSc from the Institute of Chemical Physics in Moscow in 1969. He has held a number of positions at the Estonian Academy of Sciences (member 1972) and has served as Minister at the Estonian Government. He has also been nominated *Doctor honoris causa* at University of Jyväskylä (1975), Tallinn Technical University (1991) and University of Tartu (1999). He is a member of the Finnish Academy of Sciences and Royal Swedish Academy of Engineering Sciences. He is also presently the chairman of the Department of Physics and Astronomy at the Tallinn Technical University.

His current research programs relate to chemical physics, radiospectroscopy and electronics, information science and quantum computing, nuclear and particle physics, biophysics and environmental science.

It was a true pleasure to enjoy the lay-out of the scientific achievements by Professor Lippmaa. It is unnecessary to point out that he has contributed to a number of scientific break-throughs in science over his long lasting career in science. It was fully clear that he was aware of all the important scientific questions dealt with at the Institute also meaning that he firmly controlled its scientific activities. His most recent extension is the purchase of an 8-processor Origin 2000 computer with modern molecular and solid state software. This system was operated with enthusiastic PhD students A. Rummel and A. Trummal. They were involved in theoretical calculations on the thermal vibration in zeolites. Since the laboratory was only a few months old, despite the very adequate software, the calculations performed were quite basic.

Tonis PEHK (born 1939)

He was engaged in rather standard high resolution ^{1}H- and ^{13}C-2D-NMR analysis of complex organic molecules. Due to the aging of the instruments, maintaining of the field caused some problems, but there seemed to be hope for an enhancement of the present 500 MHz instrument in the near future. Typical projects presented were the analysis of cholesterol-like ergosterol compounds in sea coral prostaglandins. A more advanced task was to determine the absolute mapping of the configuration of chiral enantiomers which may be used as chelating agents alike crown ethers. They were obtained through chemical oxidation. Finally he was involved in the determination and calculation of the populations of equilibrium mixtures from chromatography using different solvents. It

related further to gene schemes of compounds with very alike Brönsted acidity constants using deuterium marking at different distances from the acidic group. On the other hand his knowledge in dynamic NMR measurements for obtaining diffusion coefficients and in shift and relaxation methods for evaluating the order parameter of molecules in assemblies seemed to be slightly outdated. He reported a substantial international exchange activity and collaboration with laboratories within NICPB, IC/TTU and ICP/University of Tartu.

Ago SAMOSON (born 1955)

The impression obtained about him was very striking. He was engaged in the development of probes for solid state NMR. His designs of single and double spin rotors had reached international recognition which had opened him the access to the world's most advanced NMR laboratories. He was investigating numerous silicates and alumino-silicates, such as zeolites. Of particular interest was the influence of cations in zeolite structures and the influence of a gaseous atmosphere on Li doped zeolites. The interpretation was backed by theoretical modelling calculations. As mentioned he had a firm and fruitful collaboration with a large number of leading research groups in the world. He was clearly a leading scientist within the Institute.

Juhan SUBBI (born 1953)

His primary role had been to build and develop a time-of-flight (MALDI-TOF) mass spectrometer, including a supersonic jet injector within the evaluation period. The spectrometer was able to separate masses up to 400 000 Dalton and had been financed by the Innovation Foundation. One duplicate instrument had been sold to Finland. He had been involved in the analysis of a snake venom, *e.g.* the cleavage bonds and the enzyme specificity. Also he had characterized the dendrimers for the controlled way of introducing alcohols as an additional generation of molecules. In the future the research was directed to the physical understanding of the MALDI-process. He had also been involved in the ion cyclotron resonance measurement of the neutrino mass.

Uuve KIRSO (born 1937)

The research group was engaged in environmental analysis as a certification laboratory for the Estonian government. She had one PhD and four other scientists in the team. The methods introduced to the team were sorption analysis and HPLC analysis (with a new mass spectrometer detector) of environmental samples, such as PAH containing particles and waters. Also a claim was made for a research on colloidal sols and airborne aerosol particles, but little substance was shown. The research was, for a

good reason, of rather applied nature. Some collaboration with foreign research groups was documented.

A rich number of both national and international collaboration is listed in the report on National Institute of Chemical Physics and Biophysics. This includes the development of single and double probe spinning rotors for the solid state NMR and development of MALDI-TOF mass spectrometry. These developments have brought patents (and funding) as well as access to the most advanced instruments in the world (*e.g.* in the USA, Switzerland, Germany).

A contract from the Ministry of Agriculture of Estonia with financial support from Denmark has been obtained for the assessment of the reliability of the analytical results of official food laboratories of Estonia. The environmental research group had been licenced by the government to do environmental assessment when officially required by the government. Moreover LCP has been involved in several projects of technological development supported by the Foundation of Innovation of Estonian Technology Agency. However, no details were given on the extent of commercial contracts or services provided by the Institute.

4. INSTITUTE OF CHEMISTRY, TECHNICAL UNIVERSITY OF TALLINN

On Tuesday, 13 February, the Team visited the Institute of Chemistry, formerly belonging to the Academy of Sciences and now affiliated to the TTU. No explanation of its role or function was given by its director and the impression of a relict from Soviet times is only reinforced by reading the Annual Reports (Institute of Chemistry at Tallinn Technical University, Annual Review, 1998 and Annual Review, 1999).

The building is being taken over for postgraduate studies and other research by the TTU and some parts have been renovated.

The Teams definite impression was that this integration to the TTU should be brought to its logical conclusion and that the Institute as such has few scientific reasons to motivate its continued existence. The remaining people from the Academy should be fully integrated to the TTU, including participation of scientists in teaching. Even so, care should be taken that the 7 minute walking distance between the two premises would not be come a separating gap.

While we criticize the structure, we respect the people. The Analytical Chemistry laboratories, led by Professors M. Kaljurand and A. Öpik, respectively, were visited. We discuss them under TTU.

These premises had many Russian speaking coworkers and we note here with pleasure and respect the apparent absence of any tensions related to this factor.

5. FACULTY OF CHEMISTRY, TALLINN TECHNICAL UNIVERSITY

On Thursday, 15 February, the Team visited the Department of Basic and Applied Chemistry at Tallinn Technical University on the main campus of the TTU. An introduction to the entire Faculty of Chemistry was given by Dean A. Öpik. Clear statistical data on student streams were given.

The visit was dedicated to the Chair of Inorganic and General Chemistry (IGC) since the Chairs of Analytical and Physical Chemistry were met on Tuesday. IGC Chair is characterized by a long history, and recent renewal. The traditional line culminated with the phosphate and apatite research activity of Academician Veiderma, retired in 1997, and the new field is computational inorganic chemistry, represented by Professor Toomas Tamm, nominated in 1998. The traditional research line is now led by senior researcher Kuusik.

A stronger emphasis on teaching and applications is natural when assessing a Technical University.

Department of Basic and Applied Chemistry
Chair of Analytical Chemistry Professor: M. Kaljurand
Chair of Inorganic and General Chemistry Professor: T. Tamm
Chair of Physical Chemistry Professor:A. Öpik
Associate professor K. Lott

5.1. CHAIR OF ANALYTICAL CHEMISTRY

The Chair of Analytical Chemistry is among the oldest at Tallinn Technical University. Its predecessors can be traced back to the Laboratory of Inorganic and Analytical Chemistry (1936-1944), followed by the Chair of Inorganic Chemistry and Physical Chemistry (1940-1941 and 1944-1961). In 1961-1998 the Chair of Inorganic Chemistry and the Chair of Inorganic and Analytical Chemistry existed in parallel. In 1988 Analytical Chemistry was separated into an independent Chair. The present holder of the chair is Professor M. Kaljurand and he has a senior staff of 7 researchers.

The present research directions in analytical chemistry are twofold: 1) Investigations of the possibilities of computerised sampling methods and data processing in order to increase the measurement speed and/or the

reduction of detection limits. 2) Evaluation of environmentally friendly solvents as media for sample preparation and separation.

The future plan is to continue the investigation of the composition of complex samples found in Estonia (herb extracts and oil shale condensates), applying "green" (environmentally friendly) extracting agents and a methodology using GC, HLPC and nonaqueous CE.

The activities provided are based on a single basic research project, identified at the front page of the report, "Computerised analytical separation methods for environmental and material sciences". However, later a number of other separate research projects are identified with scattered information on the publication and education "production"as well as on the financing structure.

Mihkel KALJURAND (born 1945)

Kaljurand received the DSc from the Institute of Physical Chemistry, Moscow. He has visited NASA research center (1995-1996), and made short term visits to Stockholm, Bern and Southern Illinois Universities. He has held all his professional positions at TTU.

The research fields include the improvement and computerisation of the methods of instrumental analysis in general, capillary zone electrophoresis (A. Ebber and R. Kuldvee), thermochromatography, ionic chromatography, chemometrics (M. Kudrjasova), new methods of solid probe extractions, supercritical fluids, ionic liquids, combined methods of matter analysis, thermodynamics of organic (ternary) mixtures.

The Team were particularly impressed by the work of Dr. M. Koel on ionic liquids (molten salts) and their use as acetonitrile solutions, in capillary electrophoresis. Here the Laboratory has a breakthrough to the front of Science and it would be wise to hit hard now. Dr. Koel (with A. Orav) has also studied the use of supercritical extraction methods for the recovery of *e.g.* aroma compounds in herbs.

As a separate unit under the Chair of Analytical Chemistry there is a small research group, lead by Dr. E. Siimer, studying the thermodynamics of multi-component systems. The target group for the compilations are engineers. In addition, unpublished experimental data from the former USSR was searched for, thoroughly checked and added to the compilation. The group produces competent but scattered data at the rate of about two papers a year. The equipment is rather old and self made and consequently they hoped to obtain an advanced densitometer and later on a new calorimeter. Their support was modest and decreasing, and they had no students. The personnel were approaching retirement age or had already

passed it. We wish to emphasise the importance of thermodynamic data as a basis of physical chemistry but feel that this particular group can be gracefully retired. On the other hand, at least one research group should be maintained and supported financially within the field of chemical thermodynamics.

5.2. CHAIR OF INORGANIC AND GENERAL CHEMISTRY

The origin of the Chair of Inorganic and General Chemistry is closely related to that of the Chair of Analytical Chemistry. In 1988 Analytical Chemistry was separated into an independent Chair and the Chair of General Chemistry was joined to form the current Chair of Inorganic and General Chemistry.

The research conducted at IGC may be separated into three relatively independent research groups:
Computational Chemistry and Technology (CCT) Professor Toomas Tamm
Inorganic Chemistry and Technology (ICT) Professor Mihkel Veiderma and PhD Rein Kuusik
Detoriation and Protection of Carbonate Stone Docent Meeme Pöldme

Despite that two of the members of the evaluation team have significant competence in Materials Science the activities of Docent Meeme Pöldme were excluded from the evaluation due to financial links to the Materials Research Centre.

The staff at IGC/ICT consists of three senior researchers, one lecturer, one assistant lecturer, two engineers and a laboratory technician. Additionally 2 PhD, 1-2 MSc and 3-5 BSc students are engaged in the research.

The introduction of theoretical computing chemistry to the Faculty of Chemistry was based on the need of a modern and new topic to the research to broaden the scope. The staff at IGC/CCT consist presently of only two research scientists, one of which is joint with the Chair of organic chemistry.

Studies on inorganic chemistry and technology are related to a great extent to the Estonian mineral wealth. During the last 40 years the following topics have been focused on:

Composition, properties and processing of Estonian mineral resources
Synthesis, properties and applications of apatites
Utilisation of solid wastes of Estonian chemical and power industry
Purification of the gaseous emissions of power industry

The studies on apatites will be continued by investigation of sorption of heavy metals from waste waters and the interaction of apatites with gaseous SO_2. In the field of raw minerals and wastes the studies will be continued with investigations on natural and waste lime containing materials, on problems connected to the simulation of SO_2 capture and on composition and properties and the role of the mineral part of oil shale from different deposits. This will be executed through collaboration with other research groups in Estonia with the aim to form a Center of Excellence in Thermal Analysis.

The research at the IGC/CCT is focused on modelling of transition metal complexes, both for investigation of their structural and energetic features, as well as for the use as catalysts. The group also offers computational support for other researchers at the Faculty of Chemistry. The studies of catalytic properties of transition metal complexes will be continued. Quantum-chemical modelling of solid state systems and solid-gas interfaces is planned in order to incorporate, *e.g.* heterogeneous processes and catalysis. This requires the enlargement of the group through recruiting within Estonia or through foreign researcher exchange.

Toomas TAMM (born 1965)

Tamm was graduated as PhD (Cand.Chem.) from the University of Tartu before becoming engaged as a professor at IGC. He has made long term research visits to University of Florida and University of Helsinki.

His research interests are in the theoretical studies of solvent effects of transition metals (Ti), quantum chemical calculations on mass spectrometric fragmentation paths of dendrimers, catalytic hydrogenation of hydrocarbons and the use of metal complexes as catalysts (Sharpless reactions). Already collaboration had been initiated with other research groups. Moreover, he is interested in the design and implementation of quantum chemical computer methodology, theoretical search for new species in inorganic chemistry and studies of strong closed shell attractions between heavy element atoms in inorganic compounds. He has acted as an opponent at University of Tartu and as a referee for a journal.

He has most of his post-doctoral time spent at different laboratories abroad and has had little funding and almost no personal resources within the TTU. Since the appointment of T. Tamm was a serious and wise investment in the enlargement of the rather narrow and fading research topic of the Chair. It is quite surprising that he had not received funds for competitive equipment nor lecturing facilities (own courses at all levels) in computational chemistry. Moreover, since the National Institute of Chemical Physics and Biophysics is claiming to support all units in need in Estonia, it was immensely disappointing to note that a highly qualified

theoretician as T. Tamm had not been introduced and engaged to the very advanced facilities at the NICPB at such a short distance.

Disclaimer

Because the Chairman of the Evaluation Team (Prof. Pekka Pyykkö) has a collaboration with the group of Professor Toomas Tamm, that group was evaluated by the other three members, only.

Mihkel VEIDERMA (born 1929)

Veiderma was graduated as PhD from the Institute of Fertilizers and Insectofungicides in Moscow in 1965 and as DSc at the same Institute in 1972. He has been elected to the Estonian Academy of Sciences in 1975 and to the Finnish Academy of Sciences in 1998. He has held a number of very distinguished positions both nationally and internationally.

Rein KUUSIK (born 1941)

Kuusik has graduated as PhD from the Minsk Institute of Chemical Technology. He has been awarded a Technical Sciences award by Estonia.

His current research interests include the investigation of the composition, properties and treatment methods of (natural) mineral raw materials as well as solid fuels and environmental chemistry.

The approach of the research group of M. Veiderma and R. Kuusik was strongly technological with three general achievements during the past five year period: the investigation of the SO_2 removal from fuel gases and fuel combustion, the termal gravimetric analysis (TGA) of apatite at high temperatures (dependency on CO_2, SO_2 and F content), IR analysis of the structure of transition M-doped apatite structure and the use of apatite as sorbent for environmentally hazardous metals.

Traditionally the chemical engineering approach of the group would not be appreciated by evaluators of exact sciences. However, when compared with the depth of analyses the research carried out gets balanced. Although advanced in some respect the development of the instrumentation (TGA) and the assignment (IR), the research should merely be considered sound and systematic. A new promise for more advanced research level was suggested by a study evaluating different mechanisms of reaction for the time and temperature dependence of the SO_2 sorption on fluidized beds (A. Trikkel). Again, the overall approach was rather technological which, however, is completely justified within TTU. The research by the group of K. Tonsuaadu (including MSc M. Peld) on the

(ad/ab)sorption of transition metals including the synthesis of model apatites was very systematic, enlighting and convincing.

Due to its national interest the international research connections of the IGC/ICT have been restricted to only a few exchange of researchers. This must, however, be balanced by the domestic industrial interest.

As described above, IGC/ICT has roots in the Estonian industry through Professor Veiderma. Consequently, there is certainly no hesitation as to the industrial need and importance of the research results. Momentarily, there has been a shift of the national interest towards the exploitation of the shale oil resources, but due to environmental problems in the commercial utilization there was later increased interest in the apatite research. Some industrial projects related to the topics above were described in detail, including the personnel engaged, but the extent of the projects and the funding was not revealed. Neither is the commercialisation of the results described.

5.3. CHAIR OF PHYSICAL CHEMISTRY

The Chair of Physical Chemistry is a part of the Department of Basic and Applied Chemistry of the Faculty of Chemistry, Tallinn Technical University. The Chair of Physical Chemistry (PC) was established in 1936.

The research has been concentrated on II-VI compounds since 1968 under the leadership of Professor J. Varvas. Professor A. Öpik was elected to the Chair in 1992 and has since 1985 continued the research traditions, but has also introduced the research on the high temperature doping of conducting polymers with predetermined physico-chemical properties.

The modelling of II-VI semiconductors and conductive polymers has been carried out in collaboration with the research group of Professor O. Forsén at the Helsinki University of Technology. It is also planned to find applications of these materials mainly in the form of multilayer structures, *e.g.* as anti-corrosion coatings, environmental sensors, photovoltaic (solar) cells and actuators (artificial muscles).

Initiated by the Faculty of Chemistry and the Institute of Chemistry the Graduate School in Chemistry and Materials Science will be established in order to enhance the collaborative teaching and training of the post-graduate students. The research laboratories have recently been moved to the Institute of Chemistry premises as a part of this plan.

Andres ÖPIK (born 1947)

Öpik was graduated as PhD from Tartu University in 1980. He has held all his formal positions at the Tallinn Technical University.

His major research areas are in the chemistry, physics and technology of electronics materials. Among the topics we quote the processing of ZnS, CdTe and other II-VI semiconductors and studies of their defect structures (K. Lott, S. Bereznev), studies of polypyrrole anti-corrosion films and "artificial muscles" or actuators (K. Idla, V. Syritski), chemical synthesis of polypyrrole (J. Reut), and quartz crystal microbalance sensors (S. Bereznev).

There is quite active collaboration with both domestic and foreign research groups, including Linz University (Austria), University of Linköping (Sweden), Helsinki University of Technology (Finland), State Research Centre (Finland), University of Rennes (France), University College Cork (Ireland), IBM Research Centre (USA), University of Chemical Technology (Russia), Optical Institute All-Russia Scientific Center and Technical University of Lappeenranta (Finland).

Plans exist to find applications to the conductive polymer materials mainly in the form of multilayer structures, *e.g.* as anti-corrosion coatings, environmental sensors, photovoltaic cells and actuators (artificial muscles). This will be realised through collaboration with Estonian industry.

6. SOME GENERAL COMMENTS AND SUGGESTIONS

The long-term organizational structure of Estonian science still appears uncrystallized. There is a proliferation of parallel and partially overlapping structures. Partially this is driven by newly available, European and other, sources of financing. In the long run, a streamlining can be expected and recommended.

Establishing national, collaborative Graduate Schools in various areas is already discussed and we warmly recommend this idea. In our own experience it has worked well in Finland, where the two main goals were integration of the laboratories at national level and acceleration of the post-graduate studies at personal level.

Collaboration between scientific friends from different institutions seemed to flourish without obstacles. It was occasionally mentioned that certain types of more formal interaction would be forbidden by the rules. As an example of such a possible interaction we mention the Finnish practice of having a scientist from one institution as a "dosentti" at another institution. This is a formal connection, like the old German posts of "Privatdozent",

without salary for the individual and without scientific credit for the step-institution. Lectures, if any, are paid by hour.

A very minor comment is that in some CV's , membership in The New York Academy of Sciences or entries in various Who's Who collections were quoted. We wish to point out that the former can be bought by anyone for money and that buying the book helps one to obtain the latter distinction.

The establishment of EstELib, a national electronic library, should be considered. An embryo was already founded in Tartu. Cooperation possibilities with FinELib could be checked.

As a final reflection on general structures, University of Tartu gives the impression of an "Estonian Cambridge", while Tallinn Technical University is twice as large in undergraduate education in Chemistry. How much they should enter each other´s territory, is an open question. Our interlocutors were also sceptical of the added value of a conglomerate called University of Tallinn, combining the TTU with the Pedagogical and Arts schools.

7. FINAL CONCLUSIONS

In order to assess the quantitative output (degrees and papers) per input (funding and personnel) we studied the figures in the self-assessment reports, trying to eliminate any double counting.

Starting with production of degrees, the two units concerned are the UT (University of Tartu) and the TTU (Tallinn Technical University). Counted in MSc´s per personnel or per professor, Tartu turns out roughly twice as many degrees as Tallinn. In production of PhD´s UT still leads over TTU but by a narrower margin. On the other hand, the TTU produces twice as many BSc´s as the UT, and takes in more than twice as many first year students. Anyway, in postdraduate education UT ranks above TTU.

When counting CC publications per personnel, UT ranks twice above TTU and the NICPB more than twice above UT. Obviously the teaching load stands in inverse proportion to this productivity. Counted in number of CC papers per extra funding, UT and NICPB are comparable and the TTU has less than half of their figure. The UT is clearly the quantitatively more efficient production machine for MSc´s, PhD´s and papers, while the TTU does a good job in BSc education. These statistical aspects go to column 3.

As explained in Chapter 1, column 1 summarizes the quality of present research while column 2 evaluates the strategy and future perspectives. Both were calibrated to an international scale. Due to its first-rate standing

in fundamental superacid and superbase chemistry, QSAR, solvent effects and luminescence studies, the CP/TU was considered Excellent (E).

In intellectual brilliance and scientific insight no one can match Professor Endel Lippmaa. The scientific productivity of his Institute is also excellent and their single important discoveries should be weighted in the logarithmic quality scale. Although his people are imbued with his spirit, we placed their average at Excellent / Good (E/G).

Concerning the IGC / TTU, they are now in a transition state that hopefully can be handled and will lead to a radiant future. We see potential in both T. Tamm and A. Trikkel. They should be supported.

Our final grading becomes:

UNIT	1	2	3	Total	
TU/PC	E/G	E/G	G	G/E	J.Tamm, T.Tenno, , E.Lust
TU/CP	E	E	E	E	I.Koppel, M.Karelson, J.Järv, M.Danilkin
NICPB	E/G	E/G	E	E/G	E.Lippmaa, T.Pehk, A.Samoson, J.Subbi
IC/TTU	U	U	G/S	S	
Thermo/TTU	S	S	S	S	E.Siimer, L.Kudryatseva, H.Kirss, M.Kuus
AC/TTU	G	E/G	G/S	G	M.Kaljurand, M.Koel, A.Ebber, A.Orav, R.Kuldvee
PC/TTU	G	E/G	G	G	A.Öpik, K.Lott, S.Bereznev, K.Idla,V.Syritski
IGC/TTU	G	G	S	G	T.Tamm, M.Veiderma, R.Kuusik

1: quality of present research, 2: future perspectives, 3: quantitative production;

E: excellent, G: good, S: satisfactory, U: unsatisfactory.

Tallinn, 18 February, 2001

Pekka Pyykkö (Chairman)

Jorma Hölsä

Irene Montenegro

Jarl B. Rosenholm