Evaluation of Estonian Research

- Analytical, Physical and Inorganic Chemistry -

Report to the Estonian Science Fund Council

by

Prof Lars Ivar Elding,
Inorganic Chemistry 1, Lund University
Prof Sture Nordholm,
Physical Chemistry, University of Göteborg
and
Prof Peter Stilbs,
Physical Chemistry, The Royal Institute of Technology, Stockholm

May 1992

The authors of this report were appointed for the purpose of this evaluation by the Swedish Natural Science Research Council.

NFR Naturvetenskapliga forskningsrådet
Swedish Natural Science Research Council

Foreword

Several Swedish organizations have been asked to take part in a general evaluation of all research performed at academic institutions in Estonia. NFR has agreed to organize the evaluation of Estonian research within the field of natural science. This report has been prepared according to an agreement between the Estonian Science Fund Council and the Swedish Natural Science Research Council (NFR).

During the spring of 1991 Estonian scientists completed reports on their research which were sent to NFR. These reports have subsequently been distributed among 14 Swedish evaluation groups. In total about 40 Swedish scientists are engaged in the evaluations. The groups are making site visits to the Estonian laboratories and institutes during 1991/92 to discuss the research performed, the plans for future activities and to get information about the working conditions, experimental facilities, financial resources etc. Each group has been instructed to produce a report assessing its particular research area.

This report concerns the sub-field of analytical, physical and inorganic chemistry and will eventually be a part of an extensive report covering all Estonian research in natural science.

The organization of the site visits is done in close cooperation with the Estonian Science Fund Council. Although difficult times prevail in Estonia all the site visits have been successful. The NFR is grateful to the Estonian Science Fund Council for its efforts to handle all practical matters in connection with these visits.

The NFR is also grateful to the Swedish scientists who with enthusiasm and great skill have taken part in the demanding evaluation work.

Finally, the Council wishes to express its sincere hope that this evaluation report will contribute to a further positive development and strengthening of Estonian science.

Carl Nordling
Secretary General

CONTENTS

INTRODUCTION

The Estonian Science Fund Council has instructed Estonian scientists in the field of Analytical, Physical and Inorganic Chemistry to prepare reports concerning their research activities during the last 5 years. These reports were completed during the spring of 1991 and dealt with the following points:

- project leader(s)
- short description of the objectives
- summary of results
- summary of resources
- scientific staff and their qualifications
- list of publications
- dissertations
- scientific meetings organized
- prognosis of the future development of the project

In most cases the reports were accompanied by reprints of scientific publications written in English and Russian.

In July 1991 the reports were sent to NFR and during the autumn the evaluators received the reports. Site visits by the evaluators to the research groups in Tallinn and Tartu were done in the period February 12-14 1992. The Estonian Science Fund Council had appointed Margus Lopp and Uno Mäeorg as organizers and contact persons for this evaluation.

ACKNOWLEDGEMENTS

The evaluators wish to express their sincere thanks to the local organizers for all assistance and kind hospitality during the site visits.

GENERAL COMMENTS ON ANALYTICAL, PHYSICAL AND INORGANIC CHEMISTRY

Estonian science if full of contrasts, e.g.

1. The country is economically poor by western standards but the academic establishment is large.

2. The equipment standard is on the average a generation behind western standards but the enthusiasm and, to some degree, also the productivity of the scientists are good.

3. The caliber of the science is in most cases behind times but in a few cases up to current western standards and in one case world leading in an important field.

4. Scientists have relatively high status but are, particularly under present circumstances, very poorly payed (well below skilled manual laborers).

The Estonian academic establishment now faces dramatic changes, e.g.

a) a large cutback in staff - perhaps as much as 50%

b) amalgamation of institutes of the Academy of Science with the universities.

Problems of Estonian science and suggested solutions

1. How to determine the appropriate size of the academic establishment?

Consider the need for university level education in western Europe, e.g. fraction of age group attending universities or equivalent institutes. The same fraction should apply in Estonia. Work out the number of university level teachers needed. Multiply by two to allow 50% research activity for each. Add 25% to allow for applied research directed towards industry and nonacademic government agencies.

2. How to keep the best academic staff through the period of cutbacks?

Terminate entire institutes and departments for reorganization. Then open up new positions for applications from Estonian staff at any institution. Use western referees in the selection of staff for the new permanent positions. Allow academic salaries to fall for an interim period of a few years. Then raise them to reasonable parity with other occupations as in western Europe.

3. How to distribute funds for equipment and research support?

By western standards, and with at least one notable exception, the laboratories would need to be completely re-equipped. The cost for such a total re-equipment plan is prohibitive even for a western country. Given the present economic difficulties in Estonia it appears that very few, it any, funds can be spared for research equipment and consumables. Even the frequently used option of doing contractual work for industry may dry up for some years. In this situation it is vital that the possibilities of continuation of good work and minor improvement in equipment and research facilities not be so low as to demoralize scientists and cause a mass exodus. The key would seem to be contacts with sympathetic European nations. At the cost of transportation a great deal of very useful equipment could be obtained from western laboratories retiring not so old equipment. This may seem less than the desired goal of working with really up-to-date equipment, but this can be arranged by collab-

orative work with a western group at least for some Estonian scientists. It is also clear that the second hand western equipment could be put to very good use in Estonia and would there find the right kind of interest, support and maintenance to remain productive for many years. The equipment could also come in sufficient quantities to reach nearly every competent end user. EEC joint projects may also in a few cases provide a select few groups with the most modern equipment.

4. How to improve publication practices?

In the future, all work of academic scientists intended for publication should be directed towards western journals or eastern journals using referees and appearing in English translation. This a vital step to improve productivity and allow for internal selfregulation of Estonian science.

EVALUATION OF RESEARCH GROUPS

Cand. Chem. Sc. Arno Kuusk
Cand. Chem. Sc. Jaan Jöers
Department of Organic Synthesis and Technology
Estonian Academy of Sciences
Tallinn

Synthesis and Development of the Technology of Surfactants on the Basis of Fat and Protein Wastes. Surfactants of Biological Interest

Principal Activities

The group, consisting of 8 senior scientists and 13 assistant staff coworkers, works on the development of routes for the combined conversion of waste fats and proteins from the fish industry into polyfunctional surfactants of technical, medical or cosmetic interest. One aspect of the work is environmental - try to turn polluting wastes into useful (and hopefully environmentally non-harmful) products - another one is local - the lack of currency to buy surfactants or their associated manufacturing technology and raw materials.

The work has so far been focussed on organo-synthetic and technical aspects. Some of the procedures developed are quite interesting. Physico-chemical studies of some surfactants have recently been been made, as well as attempts to use predictive computer modelling of structure-property relationships of surfactants.

Evaluation

11 national (former Soviet) and 4 foreign patents were listed by the group. A number of clever and feasible synthetic paths have been suggested and tested, and a technically competitive procedure has evidently been developed into a full-scale plant process in the country.

With regard to science, the general impression is that the group is far too large and has a very low international visibility. There are no publications in international journals whatsoever, and the bulk of the published work is in the form of internal reports. We also believe that the group is scientifically isolated in an unfortunate way - undoubtedly there exist similar technical procedures related to foreign food industry, for example. The level of physico-chemical knowledge in surfactant science appeared low as well.

Recommendations

Estonia will evidently turn into a market economy in the future - research of the present kind is then best made in industrial laboratories (why not form a small company associated with the present group ?) - only time will tell whether the processes developed really are economically competitive.

Professor, Dr. Sci. Endel Lippmaa
Laboratory of Chemical Physics
Institute for Chemical Physics and Biophysics
Estonian Academy of Sciences
Tallinn

Magnetic Resonance

Principal Activities

This group - or rather Institute - works over a very broad field of chemistry and physics, using different techniques related to magnetic resonance. It was actually not possible to cover them all adequately in their allotted presentation time of 2.5 hours. A few of the sub-group leaders were abroad at the time of our visit, but the work in question was lucidly presented by Lippmaa.

Lippmaa's institute is internationally very well known, and is particularly recognized for its pioneering methodological work in high-resolution solid-state NMR (Lippmaa, Kundla and Samoson), spanning basic theory, magic-angle spinning rotor design, CP/MAS-studies on Zeolite systems and high-resolution NMR on quadrupolar nuclei in the solid-state. Additional fields of study by NMR include enzyme dynamics, solid polymers, high-temperature superconductors, cellulose, liquid crystals and many other diverse problems.

More everyday and routine liquid-state NMR techniques for the structure determination of organic molecules are used by a subgroup, led by T. Pehk.

The Institute also hosts activities on Ion Cyclotron Resonance (subgroup leader: R. Pikver). This work is supported by a local quantum chemistry subgroup at the Institute, and is to a large extent made in collaboration with physical organic chemists like I.A. Koppel at Tartu University. A remarkably accurate - and possibly fundamental - study of the neutrino mass, as based on the helium-3 - tritium mass difference was recently presented by this constellation of scientists.

The combined instrumental resources of the Institute are impressive in volume and are relatively modern (a brand new milliKelvin NMR setup, manufactured by Oxford Instruments was not yet unpacked, due to the imminent relocation of the Institute to another location).

Evaluation

Lippmaa evidently is an excellent scientist, as well as director of research, having built such a well-equipped Institute. Also, he has strong links and active collaboration with internationally leading scientists in the west.

In practice, the scientific activities of the something like 20 senior scientists at the Institute correspond to those of 5-10 normal "groups", that really should have been evaluated separately. We are generally impressed, however, with the balance and quality of choice of the individual research projects, and see this as a sign of a sound scientific atmosphere at the location.

The strongest activities in the past have undoubtedly been those of high-resolution solid-state NMR - this work is excellent. The remaining work mentioned is of good to very good international standard, and is published in international journals.

Recommendations

The Institute evidently functions very well, and generally produces work of good to exceptional quality over a wide field. It should be allowed to find its own directions of research and definitely also be supported at a high level in the future. We foresee some problems, however, with the present structure - Lippmaa is now 62 years of age and may well spend more of his time on research policy and administration. He will also have to retire in a number of years - no self-evident successor was apparent to the evaluators.

The instrumentation and NMR-"know-how" of the institute generally appears to be used as a "national resource" for collaborative projects of the laboratory within and outside the country. In part, this is related to the concentration of Estonian instrumental resources at this site. While this has many good side-effects (competent personnel, efficient use of instrumentation etc.), the overall impact on the Estonian scientific society need not be optimal.

Cand. Sci. Helvi Hodrejarv
Laboratory of Environmental Analytical Chemistry
Department of Chemistry
Tallinn Technical University

Background of Heavy Metals in the Environment of Estonia - Methods and Chemical Monitoring

Principal Activities

The group consists of 5 senior scientists and 4 younger coworkers. Standard analytical methods are used to determine inorganic pollutants in the environment. Samples from plants, animals, humans, water and bottom sediments from lakes and rivers, snow etc are being analyzed with respect to their contents of heavy metals, chloride, phosphate and trace elements such as arsenic and selenium. The projects are sponsored by the Ministry of Nature Protection, the Institute of Preventive Medicine and by the Tallinn Botanical Garden. The results have been published mainly as short conference proceedings and in the proceedings of the Tallinn Technical University.

Evaluation

This is straightforward application of standard analytical techniques. The work involves no new principles, nor any development of analytical methods. The equipment of the group is partly out-of-date. The publication record in international journals and as full length papers is meagre. The chemistry content of the project is small. The scientific level of research is low. The competence of the group and the results might be valuable in the work with Estonian environmental protection.

Recommendation

Environmental monitoring has evidently high priority in Estonia. This group has a high motivation to contribute to this field. Support can hardly be justified on basic scientific grounds only. The level could possibly be raised through a better organized collaboration with toxicologists, geologists, statisticians and biologists and through increased international contacts, first of all with environmental research groups in the other Nordic countries. Perhaps attachment of the group or close collaboration with a government laboratory for environmental control would be a good solution. A moderate investment in modern analytical equipment might also help to improve the impact.

Dr. Sci. Peeter-Enn Kukk
Dr. Sci. Enn Mellikov
Cand. Chem. Andres Öpik
Optoelectronics Materials Laboratory
Department of Physical Chemistry
Tallinn Technical University

Electronic and Atomic Processes in Semiconductors. Conductive Polymers

Principal Activities

The *Optoelectronics Laboratory*, lead by Peter-Enn Kukk and Enn Mellikov, has a large scientific staff of 2 Dr Sc, 9 PhD, and 5 younger research coworkers. The main activity is synthesis and studies of semiconducting materials. Procedures for controlled formation of narrow-disperse, monocrystalline powders of compounds such as ZnS, CdSe and CdTe and their solid solutions have been developed. Thin semiconducting films are prepared by a simple sputtering technique. Point defects, doping, crystal morphology and optical and electrical properties are studied. The scientific results from the group is mostly published in Russian journals.

The *Department of Physical Chemistry* headed by A Öpik has a staff of only three scientists studying electrically conducting organic polymers, in particular polyparaphenylene doped with for instance halogens or alkali metals to be used in batteries or as semiconductor devices.

Evaluation

The *optoelectronics group* has a good competence in the manufacture and characterization of solid-state semiconductors. Both the building and the laboratories are poorly equipped. There is a lack of modern instrumentation for advanced studies of solid materials and thin films, for instance single crystal X-ray diffractometers, CVD equipment etc. The work of the group is very applied, the goal being to develop practically useful materials. The manufactured photoconductive cells have similar performance as other devices on the world market, and may find commercial use also outside Estonia in the future. With the limited resources of the group, however, it is difficult to see how it could successfully compete in this field with companies like Hamamatsu and Philips, for example.

Measured by normal academic standards the productivity from this large group is very low. The quality of the research in an international perspective is poor.

This is also the case for Andres Öpik's group which has a low scientific productivity and a focus on practical applications.

Recommendations

Both those groups should be reorganized. The present size of the optoelectronics group can not be justified on academic merit. A reduction of personnel is advisable. Perhaps part of the group could join industrial laboratories. Collaboration with companies abroad is strongly recommended.

Dr Mati Karelson
Laboratory of Chemical Kinetics and Catalysis
Tartu University

Principal activities

Dr Karelson is a physical organic and inorganic chemist if we consider the problem area in which he works, and primarily an applied quantum chemist if we consider the methods he uses. His focus is very clearly placed upon the solvent effects on molecular properties. He uses the reaction field method to study the redistribution of electron density, alteration of geometry and stabilization accompanying the entry of a gas phase molecule into a liquid solvent. Both aqueous and nonaqueous solvents are considered and particular attention has been given to electrolyte solutions. A minor experimental effort to study the effect of electroneutral solutes on the properties of strong electrolyte solutions has been based on the measurement of differential conductivity. A productive collaboration has been established with several internationally prominent scientists including M D Zerner (theory, University of Florida), A R Katritzky (experiment, University of Florida) and G H F Diercksen (theory, Munich).

Evaluation

Dr Karelson is relatively young but has chosen a very fruitful direction of his research and pursued it very competently. There is no doubt that the study of solvent effects on molecular properties by extended quantum chemical methods such as the self-consistent reaction field method has a very promising future. Dr Karelson has built a solid foundation with respect to theoretical methods and contacts with research groups in the US and Germany upon which he can be expected to build a successful scientific research program of good international standard. If he directs his publications to western or translated journals, he should have a significant impact on his field of research.

Recommendations

Dr Karelson is a promising and competent scientist in a fertile field. Thus he deserves support for his continued efforts. Most urgently, he would need to improve his computer facilities by addition of a work station, such as the IBM RS/6000, HP 700-series or an equivalent model of another manufacturer. A similar need has been noted in the case of Prof I Koppel and the purchase of two work stations of the same kind could lead to more efficient use of both. Clearly, consultations and constructive competition between these two groups with overlapping research interests could be very helpful for both.

Prof Ilmar A Koppel
Department of Analytical Chemistry
Tartu University

Experimental and Theoretical Investigation of Structural and Solvent Effects on Acid-Base Equilibria in Gas Phase and Solution

Principal Activities

Prof Koppel has a strong background in physical and organic chemistry and this is clearly reflected in his research, which has been focussed on the acidity and basicity of molecules of both organic and inorganic type. The studies have included sophisticated experimental work, such as that using ion-cyclotron resonance experiments carried out in collaboration with Dr Pikver of the Institute of Chemical Physics and Biophysics, Estonian Academy of Sciences and Prof R W Taft at The University of California at Irvine, as well as NMR spectroscopy. Moreover, theoretical calculations have been carried out using a series of semiempirical quantum chemical programs (MOPAC, AMPAC, and HAM/3) as well as the Gaussian 86/88 series of programs for ab initio calculations. Over recent years, the emphasis has been on gas phase acidity and basicity in collaboration with the Irvine group. However, considerable work has been done also in solution, both aqueous and nonaqueous (DMSO). Potentiometric titration and NMR experiments have been complemented by theoretical studies of proton affinities, solvation complexes and photoelectron spectra for the purpose of interpretation with the ultimate aim of predicting the solvent contributions to acidity and basicity. Some work has also been done on molecular affinity for Li^+.

Evaluation

Prof Koppel has set himself a target in the form of a relatively narrow but important problem of proton transfer in gas phase or solution. On the other hand, his attack on this problem has been broad. He has used a wide variety of complementary methods, very modern as well as classical experimental methods together with both empirical, semiempirical and a priori quantum chemical methods. Although he has only rarely deviated from his pursuit of the proton transfer mechanism, he has considered this mechanism in a very broad range of media and acid-base pairs of molecules. He has established most fruitful collaborations with a number of prominent groups all over the world. Prof Koppel has made very good contributions to the fields physical organic, inorganic and analytical chemistry. Some, but too few, of these contributions have been published in the English language journals. In the future we hope to see nearly all of the work appearing in the western journals. This will ensure maximal impact of the advances he is likely to continue to make.

Recommendations

The caliber of the work of Prof Koppel is high. We most strongly recommend that he is allowed to continue. His international contacts are good. It seems to us most important that he be provided with the most basic support required to supervise a new generation of students, offering them the benefits of his insights and many contacts across the world. His most pressing need for equipment is in the area of computing where he should be provided with a modern work station, e.g. an IBM RS/6000 or HP 700-series model providing 10 Mflops (Linpack) at a cost of about USD 10 000. With the aid of funds from the EEC, he might well also be able to upgrade the experimental equipment in Tartu, but continued collaboration with the Lippmaa group in Tallinn as well as with several groups abroad is a very good alternative.

Electrochemistry in Tartu

Department of Inorganic Chemistry, Tartu University

The large electrochemistry group in Tartu has made important contributions to fundamental electrochemistry, also in an international comparison. There has been a close cooperation with the Frumkin Institute in Moscow and Professor Uno Palm was an outstanding scientific leader of the Tartu group. After Palm's death in 1989 the fundamental experimental and theoretical studies of the double layer properties in various systems are continued by a research group lead by a younger coworker of Palm, PhD Enn Lust. Dr Jüri Tamm, who has previously been working with hydrogen evolution and hydrogen overvoltage at metal surfaces, has started a new project on electrically conducting polymer films as electrode surfaces, and Drs Toomas Tenno and Heldur Keis are working since long with development and manufacture of electrochemical sensors for practical purposes.

PhD Enn Lust
Laboratory of Electrochemistry
Department of Inorganic Chemistry
Tartu University

Influence of the Chemical Composition and Crystallographic Structure on the Metal/Electrolyte Phase Boundary and on the Electrochemical Kinetics of Various Practically Important Reactions

Principal Activities

Dr Enn Lust has inherited the responsibility for U Palm's work and group. The staff is now 10 persons, all working with theoretical and experimental investigations of the electric double layer, and adsorption and electrochemical processes at solid electrode surfaces in water and non-aqueous solvents.

Evaluation

Lust carries on in the previously set direction by Uno Palm with the support of Prof Damaskin at the Frumkin Institute in Moscow. Despite reasonable productivity, the evaluation group got a low opinion of the future prospects of this work. Lust is young and without teaching load, but he did not project an image of independence, enthusiasm or competence. The experimental setup in Tartu is conventional. There are no possibilities for in situ studies of the electrode/solution interface.

Recommendations

This research is important for the basic knowledge of electrochemical processes. However, the present staff and organization seems to be too large and without efficient leadership, and the experimental facilities are of low standard internationally. The committee recommends reduced support. Reduction of personnel will probably be necessary.

PhD Jüri Tamm
Laboratory of Electrochemistry
Department of Inorganic Chemistry
Tartu University

Electrosynthesis and Properties of Analytically Active Conducting Polymer Films

Principal Activities

This is a new project, which Dr Tamm started in 1990. Since the beginning of 1991, a group of 5 persons are involved, and at present the group consists of 8 persons, 6 of them PhD:s. The objectives is to develop optimum synthetic conditions for films of polypyrrole, polythiophene, and polyaniline with electrochemical activity for determination of ions or molecular compounds. Such electrodes are known to have low internal resistance and rapid response.

In his report, Dr Tamm gives a general description of the previous activities of the electrochemistry group. The main part of his publication list is work performed by other members of the group on for instance bismuth electrodes. For natural reasons, the present project on polymer films has not yet resulted in definite conclusions or scientific publications.

Evaluation

Dr Tamm is a competent electrochemist, as shown by his previous work on hydrogen evolution on nickel, cobalt, and iron surfaces. He has a long experience in this field. However, the committee is concerned about the size and plans for the new project. A group of 8 or 9 persons, most of them PhD:s is an unrealistic investment in an exploratory study with a still very uncertain prognosis.

Recommendations

The personnel in this project should be reduced. Economic support should be cut back correspondingly. At the present stage, a project leader together with one senior and mightbe one or two younger coworkers will be sufficient to pursue this project efficiently. Increased funding should not be considered until more definite results are presented. Instrumental equipment for the research seems to be appropriate and needs no new investments.

PhD Toomas Tenno
PhD Heldur Keis
Working group on Electroanalysis
Department of Inorganic Chemistry
Tartu University

Electroanalytical Methods and Complex Systems for Testing Oxygen Content, pH and Polluting Components of Environment

Principal Activities

In addition to the two responsible chemists, this group consists of 7 co-workers, some of them young. The main objective of the work is development of electrochemical methods and sensors for environmental and industrial applications. The work is mainly financed by contracts with different institutions ordering electroanalytical sensors. Oxygen sensors and electrodes for heavy metal analysis are produced on a semi-industrial scale. The authors have several patents, and their list of publications since 1986, in local journals though, is impressive. Both Tenno and Keis have a heavy teaching load.

Evaluation

Tenno is a very dynamic and enthusiastic leader of this group, which has produced good work. He is a highly competent inventor of new electroanalytical sensors. Keis is a very good collaborator. The team appears to be more competent than the previous funding levels from the state has allowed for. The research is applied, but certainly based on deep scientific insights. The evaluation committee was impressed by the productivity and enthusiasm characteristic of the group.

Recommendations

We recommend that this group should be given increased support needed to continue their work. The production of electrodes should be separated from the university department in a separate company.

APPENDIX

Background of evaluators

Lars Ivar Elding

Professor of Inorganic Chemistry at the University of Lund. Research interests include coordination chemistry in solid and liquid phase, chemical kinetics and reaction mechanisms of transition metal complexes, fast-reaction and high-pressure techniques for reactivity studies.

Sture Nordholm

Professor of Physical Chemistry at the University of Göteborg. His background is in theoretical physics and chemistry and his range of research interests includes statistical mechanics (theory of fluids), kinetics (energy transfer and reaction rates) and quantum chemistry (correlation effects and bonding).

Peter Stilbs

Professor of Physical Chemistry at the Royal Institute of Technology, Stockholm. His research interests are primarily in magnetic resonance, and development of methods based on magnetic field gradient NMR and nuclear spin relaxation for the investigation of structure and dynamics in surfuctant and polymer systems in solution and at water-solid interfaces.