Evaluation of Estonian Research

- Organic Chemistry -

Report to the Estonian Science Fund Council

by

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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 organic 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

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INTRODUCTION

The Estonian Science Fund Council has instructed Estonian scientists in the field of Organic 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 July 1991 the reports were sent to NFR and during the autumn we received the reports. A site visit to the relevant Estonian research institutions was done in the period March 4-5 1992. The Estonian Science Fund Council had appointed Mihkel Kaljurand and Tönu Püssa as organizers and contact persons for this evaluation.

We had also had access to several publications from most of the groups. However, some of the published material was only available in Russian language and this fact made our job more difficult and also less complete. During two days we visited nine research groups on our agenda and had the chance to present ourself, listen to the prepared reports and ask questions or to initiate discussions. We also had some short time to see the research facilities and the equipment. Our over-all impression is that we got the information we wanted and that the procedure worked well in spite of the short time available for each group. The language barrier does exist but with a little patience from all participants its effect was hopefully minimized.

In principle we used the method of evaluation of research which we apply to Swedish projects. The formation of our opinions and the vocabulary used are based on the scale used in the ordinary chemistry committee work at the Swedish Natural Science Research Council, using a five graded scale as follows:

a) Excellent projects/research are such which is research on highest international level with a major impact in international leading journals, less than 10% is within this class.
b) Very good projects/research which is research of high international class and less than 30% belongs to this category.
c) Good projects/research on high national level with some publications in international leading journals.
d) Fair projects/research on national level without international publications.
e) Poor projects/research on deficient level only.

Publication of results in international journals with a good referee system is one of the major criteria for the quality of the research. However, we are aware that the conditions and traditions in Estonia for research are different from those in Sweden.

After each group visit we compared and discussed our impressions immediately and reached the shared opinions and conclusions presented here.

ACKNOWLEDGEMENTS

We would like to thank our hosts in Estonia and in particular Drs. Mihkel Kaljurand and Tönu Püssa for taking so good care of us in Tallinn and Tartu and for their help and information of the conditions in Estonia today and we wish Estonian Scientists good luck.

GENERAL COMMENTS ON ORGANIC CHEMISTRY

This evaluation of Estonian research in organic chemistry and some closely related topics was carried out during the months of February and March 1992, a time with severe economic problems in Estonia. The evaluation group was very well received by our Estonian hosts and the groups to be evaluated both in Tallinn and Tartu. All practical arrangements were carried out to our satisfaction. This contributed to our generally positive picture of Estonia in spite of the hardship of the present times.

After having met the Estonian groups in Tallinn and Tartu we clearly were confronted with the major problem caused by the collapse of the former Soviet Union and of its research network, of which the Estonian research was a minor part. The radical change of direction of the Estonian research from supporting Soviet industry and research organizations towards new connections and links with the corresponding Western organizations must by necessity take time and will require major changes. Research motivated by international strength in a specific field or to support strong local industry must gain continued support. However, at the present time, the Estonian responsibility for the international research and development will be less important than the responsibility to fill the need of the Estonian society, higher teaching and industry.

The Estonian research structure is different from the Swedish one and heavily influenced by the former Soviet system with a strong emphasis of research at special institutions for example The Institute of Chemistry in Tallinn. In our opinion, in order to contribute to the needs of a small country, research and higher education at such institutes should be integrated with the University. If and when a reorganization of the research in organic chemistry in Estonia will take place such an integration is the most important step.

In our view the quality and relevance of the different research projects varied considerably, some of the groups would fit in with the Swedish system nicely whereas other would have problems with the funding. One major difference is the clear definition of the research project including the start and the end of a project which is usually required in Sweden. Our criticism has often to do with this latter point, each project must be well defined and have a goal and it must also be possible to end a project.

A difficult question is the organization of the research in organic chemistry. We consider it necessary for all research groups to actively participate in the higher education, either at Tartu University or at Tallinn Technical University, to transfer their knowledge and experience to the next generation of Estonian chemists.

EVALUATION OF RESEARCH GROUPS

Viktor Palm, J. Kiho, V. Nummert, I. Koppel, J. Koppel, R. Hiob, T. Tenno, M. Tamme, I. Talvik
Tartu University

Quantitative Experimental, Theoretical, Informational and Calculative-Prognosticative Approach to the Structure and Environmental Effects on the Reactivity and Formation Enthalpies of Organic Compounds

V. Palm has made major contributions to Estonian chemical sciences by educating several scientists now active in other fields of chemistry than Palm's own area. He started in physical-organic chemistry in the sixties on fundamental problems related to chemical reactivity by measuring and collecting complete and relevant data on organic reactions, a work which has resulted in an impressive number of publications and large tables of data. At present Palm's group is engaged in converting their published data into a data bank. The work, which now is carried out by mathematicians, J. Kiho and co-workers, will make this enormous material available to the active chemist in a near future. The work has over the years had strong support from the Soviet Academy of Sciences and its Estonian branch but in recent years the main support has been local.

Evaluation and recommendation

We were not convinced of the importance of the present work but we would rate the work as fair. Within the limited resources available for Estonian research and education in chemistry we consider this type of major enterprise as beyond the possible and desirable. We consider it proper to support Palm's effort to finish his data base project, but further or expanded work should be carefully evaluated and compared with other research projects.

Heiki Timotheus, Thoomas Rodima
Tartu University

Synthesis of Pheromone Compounds, Elaboration of Pheromone Materials

The group, which consists of ca 10 persons, works on a contract with Firm Flora on pheromones and more specifically on the synthesis of acetylenic, vinylic and alcohol derivatives of C_{10}-C_{18} hydrocarbons. The group takes part in the teaching at the university and supervises diploma work but their major activities has been directed towards the research centers in the Soviet Union and the Firm Flora which produces the pheromones and the necessary traps for insect control. The work apparently relies on good collaborations with environmentalists. The potentially active compounds and mixtures are field tested and used, not to kill the insects, but rather to check the populations and from that judge the proper time for massive insect control measures.

The pheromone group has had a positive influence on the organic chemistry research and teaching, their expertise has been used in various ways and their equipment has been essential for the overall activity at the chemistry department.

The need to apply the results and the specific demand for certain chemicals have limited the research activity to relatively well established and traditional reactions, compounds and procedures. The group now seeks new contacts with ecologists and companies in the west.

Evaluation and recommendation

The project is fair and most of the scientific results of the group have been published in the russian language and used in patents and thus the group is not so well recognized internationally. The group is very active in a limited field of organic synthesis using established methods but does not actively work on new asymmetric synthesis of chiral pheromones which is the scientific challenge in the field. We could not identify any particular organic chemical result of excellence. It was not obvious to us how this group, which might become a victim of the structural reform of the Estonian science, can be integrated into the research. A part of the group could hopefully contribute to higher teaching at the Tartu university and a larger part has to rely on collaboration and support from industry.

Uno Mäeorg
Tartu University

Investigation of Synthetic Methods for Biologically Active Compounds

The research group of Mäeorg is carrying out modern organic synthesis with an emphasis on pheromone synthesis. One of the main objectives of the group is to modify the Zn-Cu-couple for new applications in synthesis and as a catalyst for hydrogenation reactions. Another interesting project concerns the use of strong bases.

Mäeorg heads the department of bioorganic chemistry and is responsible for special courses on chromatography and structure determination. His research group consists of ca 7 persons. Most of the results are published in russian but Mäeorg is presently trying to change this tradition.

Evaluation and recommendation

Mäeorgs activity in organic synthesis is of good standard and the projects are good. He is quite familiar with and uses modern methods, including enantioselective ones, in his synthesis of cyclic and polycyclic pheromones. We also would like to encourage the methodology project with the activated Zn-Cu-couple which should be rewarding and continue to give good results.

Dr Mäeorg should get continued support for his research and teaching which will constitute an important part of the organic chemistry at Tartu University, in particular after the reform of the higher teaching which is under way.

Peep Christjanson, Olga Metiltskaja, Aime Suurpere, Helle Lippmaa, Kadril Siimer
Laboratory of Polymer and Food research
Tallinn Technical University

Development of Highly Reactive Cold Setting Polycondensation Resins

This research group is the only one we visited at the Technical University in Tallinn. The present activity is mainly concentrated on the synthesis and studies of phenol-aldehyde resins using very relevant raw materials from Estonia, resorcinol derivatives. Mechanisms and intermediate products are studied, the latter with NMR-methods. An important collaboration with Lippmaa's NMR-group guaranties the quality of this part of the work.

Evaluation and recommendation

We had a positive impression of this group and consider the projects as good. The research area might be of relevance for Estonian industry. The quality of the work and the methods used are good. As usual, more international publication would make the group more visible internationally and help to make new contacts. If possible, the work should concentrate on the polymers more and on the monomers less. We recommend good support for this important group for polymer research and their involvement in higher technical education in Estonia and in industrial collaboration.

Silvia Rang, Enn Siimer, Helle Kirss, Kai Kuningas, L. Kudrjavtseva, Marina Grinchak, Anne Elvelt, Anne Orav, A.-M. Müürip
Institute of Chemistry
Estonian Academy of Sciences Tallinn

Synthesis and Physico-Chemical Fundamentals of Purification of Unsaturated Hydrocarbons and Aroma Compounds

Silvia Rang is the successor of Olaf Eisen who is the founder of this research group at the Institute of Chemistry. Much of the present activity is directed towards a systematic study of all possible isomers of C_6-C_{14}-hydrocarbons and derivatives, a research objective decided in the past. The present activities are too diversified and all the projects are not acceptable. They can be dived into synthesis of hydrocarbons (3-4 persons), determination of physical data (5-6), gas chromatography (4), mass spectrometry (3) and molecular complexes (2). The work is very exact and careful, and the group was responsible for the synthesis and supply of reference compounds for the Soviet market. The synthetic and physical chemistry of the group is well integrated and the group has their own equipment for the determination of data. Recently a new GC-mass spectrometer has been installed and research on aroma compounds has become easier.

Evaluation and recommendation

In our opinion this group can serve as an example of the consequences of the breakdown of the Soviet research system. The scientific market for this relatively large group has been dominated by Soviet organizations and a structural change is necessary. We feel that the synthesis and collection of data on C_6-C_{14}-hydrocarbons should be evaluated in detail. Only the best projects should gain further support. Instead research projects related to the new GC-MS should be defined and supported and the need to support other research groups in Estonia with good GC-MS-data recognized. The policy of publication should be discussed within the group.

Ü Haldna
Institute of Chemistry
Estonian Academy of Sciences
Tallinn

Protonation of Weak Organic Bases in Strong Acidic Media

The group led by Ü Haldna is a small one (3 persons) working on a very specific problem, the protonation of weak bases in dilute sulphuric acid, combining theory and experiment. Haldna's work was originally supervised by Palm in Tartu.

Evaluation and recommendation

The present projects are poor and we are unable to identify significant research problems of importance for the Estonian research or society among Haldna's activities. We recommend a reorganization of the group and a limited support for this process.

Koit Lääts, Kaarel Siirde, Ants Erm, Heino Rang, Ilmar Kirjanen,
Igor Kudryavtsev, Elvi Muks, Avo Kogerman, Malle Schmidt
Institute of Chemistry
Estonian Academy of Sciences
Tallinn

Electrophilic Haloalkylation of Alkenes as the Basic Process for Synthesis of Biologically Active Terpenoids

This is a large group (ca 20 persons) working on a broad program originally based on prof Lääts' study of teleomerisation and electrophilic haloalkylation reactions. The project includes basic research on the haloalkylation reaction (mechanism, thermodynamic parameters) applications to synthesis of derivatives (basic alcohols, amines, aldehydes etc) various products for agricultural use and for the perfume industry as well as pheromones. The synthesis of some of the products are carried out on a pilot plant scale in commercial quantities.

Evaluation and recommendation

The organic chemistry carried out in the group is difficult but rather conventional. Some of the projects depend on good contacts with the Estonian industry and Soviet research centers which at the present situation creates problem. We recommend that the group is reduced and reorganized. The research projects to be continued are those of relevance for the Estonian industry and they should also be supported by industry. We feel that the competence of the group could be used for higher teaching at Tallinn Technical University.

Guido Rajalo, Ilmar Kirjanen
Institute of Chemistry
Estonian Academy of Sciences
Tallinn

Optimization of Chemical and Mass Transfer Processes Using Oscillating Temperature

This group works on chemical engineering problems and we have had to consult a Swedish expert for help with this evaluation which supported our first site impression. The relatively small group (five staff members) works on applied chemical kinetics and energetics for basic organic reactions. The work is both theoretical and applied. The major idea presented for us is the use of oscillation temperatures to improve efficiency.

Evaluation and recommendation

Similar work is carried out in different countries more or less successfully when applied to large scale processes. The methods used and the problems are relevant and the results good but a careful analysis is made difficult for us due to the language problem. The balance between industrial support (50%) and support from research organizations (50%) seems to be relevant. Continued support at a proper level is recommended. The expertise in the group should be used in the higher education of the next generation of Estonian chemical engineers.

Margus Lopp, Tönis Kanger
Institute of Chemistry
Estonian Academy of Sciences
Tallinn

Asymmetric Chemical Synthesis, Development and Investigation of Chirons for Medical and Natural Product Chemistry

The present work in the group has had its origin in the prostaglandin isolation and synthesis by Ü Lille. The research program is now focused on new chiral synthons applied to prostaglandin synthesis. This type of synthetic work is strongly dependent on the use of modern tools for structure elucidation and it seems as the group has been actively collaborating with Lippma's NMR-group. The equipment is modern and appropriate for the type of advanced synthesis which is carried out. A shortage of chemicals is an important problem which is shared with several of the other group.

Evaluation and recommendation

The group and the projects are good. The group actively seeks international contacts and the recent publications appear in Western journals. The group leader seems very competent and enthusiastic. We recommend strong support to this group which we identified as the most creative one. A better contact with the University is, however, recommended so that members of the group can contribute to teaching at an advanced level.

APPENDIX

Background of evaluators

Bengt Långström

Professor in Organic Chemistry at Uppsala University. His research interest is synthesis of important biomolecules and pharmaceuticals labelled with short-lived radionuclides such as ^{11}C, ^{13}N, ^{15}O, and ^{18} for use in applications within the field of life sciences and medicine. He currently holds a position as Director of Uppsala University PET Centre.

Olof Wennerström

Docent in Organic Chemistry at Chalmers University of Technology, Göteborg. His research interest concerns physical organic chemistry with emphasis on synthesis and investigations of models of certain biomolecules, host-guest chemistry, mechanistic organic photochemistry, and electrically conducting polymers.