

**Strategic Plan
Department of Chemistry
University of Tromsø
2006-2012**

Approved by the Board of the Department 31.05.2006

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1 Background

The Board of the University of Tromsø approved in their meeting on June 22 2005, Sak-45-05 a new structure for the scientific and administrative leadership at all administrative levels at the University of Tromsø. In particular, the head of the Departments would be engaged for a four-year term of office and have both scientific and administrative responsibilities. The new head of Departments could, in principle, be given broad ranging executive powers. At the Faculty of Sciences, it was decided that the head of Departments should be hired among the permanent faculty members of the department.

In their meeting on August 30 2005, the newly elected board of the Department of Chemistry decided to adopt this model by giving the head of the department extensive executive powers, with the board focusing on the core activities: strategy, budget and finances, as well as the hiring of full professors. In addition, the board has a continuous responsibility for evaluating the performance of the head of the Department and the development and activities of the Department. In order for the head of the Department to have guidelines for how to develop the Department, a well-defined strategy for the Department was needed.

During the early parts of this millennium, an increasing fraction of the University funding has been based on results produced, both with respect to teaching (the number of students passing the exam of a course, the number of Master and Ph.D. students graduated) as well as with respect to research (the number of publications and in which journals, the amount of external funding secured, and the number of Ph.D. students graduating).

As the number of chemistry students has been slowly declining for the last few years, it has become increasingly apparent for the Department of Chemistry that the only way it can stay competitive as an independent chemistry department, both with respect to teaching and with respect to research, is with a strong focus on scientific excellence. Although the department is committed to improving short term recruitment to chemistry, this is ultimately a longer-term project that will require a change of sentiment in the population as a whole, both with respect to natural sciences in general and to chemistry in particular.

It is with this background the present strategic plan has been developed. The department regrets that the need to focus on scientific excellence in the present economic situation and with the current number of chemistry students may lead to less flexible study programs for chemistry students. However, the Department will actively seek to minimize any practical disadvantages for students, and will be happy to change the focus and profile of the strategy of the Department should the number of chemistry students increase or the financial models for funding of the universities be revised.

Vision for the department

The Department of Chemistry will be a leading chemical research department, which is clearly visible at the national level with several internationally recognized research groups. The Department will foster a biological chemistry profile to enable collaborations within the University and to allow for larger project applications at the national and international levels. The Department will provide high-quality educational programs aimed at securing our high international standards of research.

Summary

The present strategic plan observes that in the current period of poor recruitment of students to chemistry, the Department must secure its position through added focus on research of high quality. The general research goals for the Department are:

1. A primary strategic goal of the Department will be to ensure that NorStruct is extended for a second five-year period (2007-2011) to secure the activity of the structural chemistry group at the current level.
2. Considering the documented scientific competence in the fields of molecular modeling through the establishment of the CTCC, and in biomolecular studies, experimentally and theoretically, through NorStruct, the Department sees it as a high priority to hire a new staff member with scientific competence in biomolecular modeling. Building on the competence available at the Department, and the long-term commitment to CTCC by the RCN, such a position will have great potential to make the Department internationally leading in biomolecular modeling.
3. The Department will work toward the establishment of a Ph.D. research school in chemistry.
4. The Inorganic chemistry and Theoretical chemistry groups should consider the establishment of joint proposals to the NANOMAT program, where the joint efforts and competence of both groups may give sufficient strength and size to be successful in attracting funding from this program.
5. The competence in the synthetic organic chemistry group as a whole is very broad and unique in a Norwegian perspective. The members of the group should therefore try to establish larger constellations around joint research projects and in this way attract substantial funding from the RCN.
6. The structural chemistry group should seek to establish a clear, local research profile and lead their own research projects in national and international collaborative efforts (in particular in EU initiatives).

The Department will provide education in chemistry of a high international standard. In order to integrate students in the chemistry program better, courses at the bachelor level will only be given every fourth semester, bringing chemistry students from the second and third year of the bachelor program together in one class.

The introductory course in chemistry KJE-1001 will be actively used to attract students to chemistry. This will be ensured through the use of highly qualified and motivated staff members as teachers on the course, as well as well-structured web pages that show the excitement of modern chemistry research.

The Department will support all initiatives that will help maintain or increase the high publication record of the Department.

The Department will in the recruitment of new staff, emphasize as much the future plans of the applicants as their scientific track record, by requiring the submission of a research plan as part of their proposal. The evaluation committee is also asked to evaluate how well the different applicants support the overall strategic goals of the department.

The technical staff is considered a common departmental resource, and the Department will actively give the

technical staff the opportunity to qualify themselves for more responsibility in research and teaching at the Department.

A primary concern for the Department and the future scientific development of the Department is the chemistry building, which is the oldest building at the University campus, and which is neither of the necessary technical standard to support modern chemistry research nor of a size to support the large activity at the Department. The Department fears that this already hinders recruitment, and that the scientific potential of the Department will be increasingly hampered in the future if the Department remains in the current physical facilities.

The Department has established an active program for upgrading the laboratory equipment at the Department.

2 Evaluations and recommendations

Norwegian chemistry research at Universities and colleges were evaluated in 1997 by an international committee at the request of the Research Council of Norway (RCN). Although this report is by now fairly old, we quote the general recommendations for the Department of Chemistry at the University of Tromsø :

- The department should largely be kept with its current profile, but the establishment of stronger connections to chemistry activities in pharmacy and medicinal chemistry should be encouraged.
- The department has a well-established, strong position in protein crystallography in Norway. This advantage at the national level should be secured.
- Instead of hiring a permanent faculty member in inorganic chemistry, prof.II positions in both organometallic and bioinorganic chemistry should be established. This would strengthen the activity in organic synthesis and support the activity in bioinorganic chemistry (now called Inorganic chemistry and materials science).
- A joint instrument center should be established, for instance in collaboration with groups in pharmacy.

Based on the international evaluation report, the nationally appointed ``Fagplanutvalget for kjemi" in 1998 made the following recommendations:

- The main activity in organic chemistry should be in the field of organic synthesis, including activities in organometallic chemistry. Collaborations with pharmacy and medicinal chemistry should be further developed.
- The activity in protein crystallography must at least be kept at its present level.
- A research activity in inorganic chemistry should be established.

The National Council for Chemistry also presented some recommendations to the national meeting for science faculties, and for Tromsø these recommendations were:

- Inorganic chemistry should be established.
- The activity in organic chemistry should be directed toward pharmacy and medicinal chemistry.
- Protein crystallography should be further strengthened.

These evaluations are all fairly old, and the Department would welcome a new international evaluation under the auspices of the RCN.

3 Primary activities at the Department: Research

The Department currently consists of four research groups. In an ideal economic situation, the Department of Chemistry has 12 faculty members, and this forms the basis for the following idealized sizes of the groups: (1) Inorganic chemistry and materials science with 2 permanent faculty member, (2) Organic chemistry with 4 permanent staff members, (3) Structural Chemistry with 4 permanent staff members (of which one position is currently vacant), and (4) Theoretical chemistry with 2 permanent faculty member (of which one position is vacant). Currently, a position in protein crystallography (structural chemistry) is in the process of being hired.

The Department has a strong national standing in Chemistry. In 2006, the RCN awarded the Department of Chemistry a Center of Excellence (Center of Theoretical and Computational Chemistry) in which the theoretical chemistry group and the group in inorganic chemistry and materials science are members. The Department is also an active partner in a Center for Research-based Innovation (MabCent) awarded by the RCN, and the structural chemistry and organic chemistry groups are participating in the center. As such, all research groups at the department are thus involved in the center of excellence or the center of research-based innovation.

The good scientific standing of the department has a longer tradition at the Department. In 2004, two of the Faculty members (Ghosh (Inorganic Chemistry) and Ruud (Theoretical Chemistry)) were awarded Outstanding Young Investigator (YFF) awards from the RCN. The Structural Chemistry group is responsible for the Norwegian Structural Biology Centre (NorStruct), which is a national platform in the Functional Genomics initiative of the RCN, and which has been evaluated in 2006 with good reviews. The continuation of the platform is expected in 2007. In organic chemistry one group has been strongly involved in the establishment of the first company started and owned by the University of Tromsø (LyTiX). The department does well with respect to the research activity in terms of scientific publications, in part due to a large number of publications in level II journals, but primarily due to a large volume of scientific papers.

3.1 Inorganic Chemistry and Materials Science

3.1.1 Present situation: research profile

The group consists of one faculty member (Abhik Ghosh), and is internationally visible. The scientific focus of the group is broadly centered on bioinorganic chemistry, and the group's research methods encompass chemical synthesis, a variety of physical techniques, and computing. The theoretical activity of the group is an integrated part of the CoE Center of Theoretical and Computational Chemistry hosted by the Department of Chemistry.

In the area of chemical synthesis, the group's efforts are focused on the synthesis of novel transition metal complexes relevant to metalloprotein active sites. Of interest are also self-assembly-based methods aimed at porphyrin synthesis and the potential application of these studies to prebiotic chemistry (the origin of life). The synthesis of fluorinated and perfluoroalkylated compounds is a third area of research. The group has synthesized large libraries of new high-valent transition metal compounds, which are contributing to many incisive spectroscopic and theoretical studies.

For routine compound characterization, the group's synthetic work depends on the same infrastructure (NMR, MS, IR, UV-Vis) as that used by the organic chemists. In addition, the group pursues a variety of spectroscopic studies aimed at a detailed understanding of transition metal electronic structure such as NMR spectroscopy of paramagnetic compounds, EPR and various pulsed EPR methods (such as ENDOR), a variety of absorption spectroscopies (absorption, fluorescence, and multiphoton), resonance Raman spectroscopy and electrochemical studies.

Core level spectroscopies (XAS, XPS, AES, etc.), where the group leader has a significant background, are increasingly being applied to high-valent transition metal complexes prepared in the laboratory. Also of interest in this connection is the problem of charge localization in mixed-valent and other dynamic solids. A major XPS study of low-barrier hydrogen bonds in solids has been the flagship effort in this area. Attempts are underway to extend this work to mixed-valent complexes, ionic solids, superconductors, and other materials.

The excellent computational facilities at the University of Tromsø have made it possible for the group to carry out theoretical research in a number of areas. While much of the computational research complements experimental studies on high-valent transition metal compounds, a major effort has also been directed toward understanding the problem of diatomic ligand discrimination by heme proteins, where a number of insights have been obtained. Benchmark *ab initio* calculations on important bioinorganic model systems are yet another direction of theoretical work pursued by the group.

3.1.2 Infrastructure

The inorganic chemistry group has, as has been the case also for the organic chemistry group, struggled to operate under the crumbling experimental infrastructure of the department. In particular, the lack of adequate access to MS is seriously hindering the group's synthetic work. With the acquisition of new MS equipment by the department and the Department of Pharmacy in 2007, this limitation will largely be eliminated.

A significant investment in small items is also needed. The bioinorganic research lab also doubles as a teaching lab for Master's and Ph.D. students, for which these smaller acquisitions will strongly improve the group's teaching abilities.

The group also consumes a considerable amount of supercomputing time from the university's and national supercomputer resources. Continued access to such resources is critical for the research conducted by the group.

3.1.3 Collaborations

The group's work on NMR of paramagnetic compounds (for which the department is well equipped) is complemented by collaborations with some of the leading pulsed EPR laboratories in the US. The group's surface science experiments (XPS, AES, etc.) are carried out largely in California, particularly in academic and industrial laboratories in the Silicon Valley. The group also carries out a variety of NMR and theoretical analysis in collaboration with major inorganic groups in the US. As of 2006, collaborative projects are underway with several University of California campuses, Stanford University, The Scripps Research Institute, the University of Arizona, the University of Notre Dame, Northwestern university, the University of Minnesota, SUNY Stony Brook, and the Massachusetts Institute of Technology.

A major collaboration is underway with the University of the Free State, South Africa, encompassing many aspects of porphyrin and phthalocyanine chemistry.

Attempts are being made to secure funding devoted specifically to collaborations with different countries (Japan's JSPS program being a good example), as was done in the case of the group's collaboration with South Africa.

Local collaborations in Tromsø are somewhat limited, the Inorganic chemistry group being the only bioinorganic group in Tromsø. Efforts are being taken to build collaborative relationships with Biotec Pharmacon in the area of bioconjugate chemistry, and with Unilab in the area of surface analysis. Joint theoretical projects have been initiated with the theoretical chemistry group, and the group is a member of the Center of Theoretical and Computational Chemistry.

3.1.4 Future strategy

Fundamental transition metal chemistry, including synthesis, characterization, and theoretical studies, will continue to be a major thrust of the group's research efforts. However, very recently, the group has substantially broadened its activities, increasingly emphasizing organic- and metal-organic-based materials chemistry. Current upgrades in the department's small and medium-scale equipment will also permit a wide range of spectroscopic, photophysical, kinetic, and mechanistic studies. After a certain hiatus, the group plans to pursue surface science applications to chemistry and materials science with renewed vigor, but this effort will be largely based on off-site equipment.

The major new direction that the group hopes to pursue in the area of chemical synthesis is combinatorial chemistry, as applied to the synthesis of porphyrins and related macrocycles. However, this is dependent on successful acquisition of new equipment.

A strong effort has been initiated to bring to bear state-of-the-art *ab initio* methods on electronic-structural problems arising in the course of our laboratory work. Attempts will also be made to extend the group's findings on cofactor-ligand interactions to a deeper understanding of protein-cofactor-ligand interactions for heme proteins via QM/MM and QM/MD calculations.

Currently, the group lacks access to two major classes of equipment: (1) EPR and Mossbauer spectroscopy and (2) surface science techniques such as XPS, AES, static SIMS, etc. Given that several groups study heme proteins and other paramagnetic biomolecules in Tromsø, the establishment of EPR and Mossbauer spectroscopy may be an important goal for the local chemical biology community. The establishment of surface science techniques, where the group leader (Ghosh) has substantial experience, may well be a national priority and the possible involvement of the Tromsø group in this matter will be carefully explored.

Overall, the group will seek to capitalize on its key strength, namely an integrated experimental and theoretical approach to fundamental chemical problems. However, the group also suffers from significant insecurities, resulting from its small size (the group is led by just one professor) and very many different responsibilities (for instance in the maintenance of a large number of different equipment). Adding a second faculty member in the inorganic area is highly desirable.

3.2 Organic Chemistry

The group consists of four faculty members (Annette Bayer, Rolf Carlsson, Tore Lejon and John Sigurd Svendsen). The activity in organic chemistry is focused on experimental synthetic organic chemistry and directed toward the synthesis and investigation of molecules of medical interest. Within this broad field, each faculty member conducts her/his own specific research project, and as such the group can be considered a pluralistic monolith with a broad and fairly complete competence in the field. The research conducted by the faculty members partly overlap, manifested through intra-departmental collaborations.

3.2.1 Present situation: Research profile

The group in organic chemistry does research in three main areas:

1. Development of new synthetic methods
2. Development of strategies for experimental studies of synthetic reactions
3. Synthesis of biologically active compounds

Development of new synthetic methods is a research field in which all faculty members contribute. The goal is to make new synthetic routes that can be used to make medically interesting compounds. These methods should seek to increase the spectrum of useful synthetic pathways. The following topics are currently being explored: (1) Preparative use of halogenated vinylic ketones; (2) donor-substituted vinylketones as building blocks in synthesis; (3) asymmetric synthesis using chiral aziridines; (4) development of metal-free catalysis

of asymmetric reactions; (5) development of new catalysts for asymmetric hydrogenation and hydroformylation and (6) development of new methods for library synthesis on solid phase.

The goals in the *development of strategies for experimental studies of synthetic reactions* is: (1) Establish methods for solving problems encountered in experimental organic synthetic chemistry using multivariate mathematical and statistical models on synthetic reactions, (2) use this methodology to develop new and optimal synthetic reactions.

In the field of *synthesis of biologically active molecules* the group has a large research project devoted to lytic peptides with antibiotic or anticancer effects. The medicinal chemistry of lytic peptides is pursued by utilization of novel solid-phase methods, elucidation of quantitative structure-activity relationships and molecular modeling concerning stability of enzymatic degradation. This work has also contributed to university-industry technology transfer and commercialization in a separate company.

3.2.2 Research facilities and equipment

The group currently has access to a 400 MHz NMR spectrometer as well as a recently installed 600 MHz spectrometer. There have been significant investments in equipment needed by the group in 2006/2007, and with a new IR spectrometer, a double glove box, a solvent-purification system and new hydrogenation equipment, new equipment for automated synthesis and a new mass-spectrometric laboratory, the most pressing needs of the group is very well covered. Some general improvements in low-price equipment, as well as a polarimeter and the possible need for replacing old gas chromatographers would still be needed, but the group should be well equipped by the end of 2007. The department needs to ensure that this favorable situation can be kept through continuous upgrades and replacements.

Keeping the research equipment up-to-date will be particularly important in view of the central role the group will have in the SmallStruct activity of the recently initiated Center of Research-based Innovation MabCent, where the group will have a key role in determining the structure of small molecules identified as possible medicinal compounds. This activity will also lead to the need for more laboratory and office space. The Department will try to utilize the SmallStruct activities as a means for developing a joint research infrastructure with the Department of Pharmacy on mass spectrometry.

3.2.3 Collaborations

The group has a close collaboration with a group in synthetic organic chemistry at the University of Marseille. This collaboration is maintained by an extensive agreement between the two Universities and provides the group with contacts to a large research group with 8 senior researchers. The members of the group also have several individual research collaborations, in particular in Europe. In addition to providing fora for discussing, initiating and conducting joint research projects, these collaborations provide the group with access to experimental equipment not available at the Department.

The group working on the synthesis of biologically active molecules has close collaborations with several research groups at the University of Tromsø, including the Department of Pharmacy and Department of Medical Biology.

The group also has ongoing collaborations with the University of Stavanger (also formalized in the form of letters of intent), NILU and with commercial parties in the field of environmental analysis.

3.2.4 Future strategy

Arctic resources and environment receives an increasing attention at the University and the society at large. The synthetic competence in the organic chemistry group represents an attractive partner for surrounding institutions working with environmental surveillance, by the group's ability to synthesize standards and metabolites of environmental pollutants. Access to such reference compounds will greatly benefit the

institutions working in this important field.

Arctic marine bioprospecting is another field where the group in organic chemistry is encouraged to participate. The group in organic chemistry has access (with some limitations described above) to state-of-the-art equipment for structural elucidation of new natural products. Faculty members of the group are active in MabCent, and in particular in the part related to the structural determination of small molecules (SmallStruct).

3.3 Structural Chemistry

The structural chemistry group currently consists of three faculty members (Richard Engh, Lars Kristian Hansen, and Arne Smalås). Procedures to fill a fourth position are currently underway. The research activity in the structural chemistry group ranges from structure elucidation of small organic compounds (chemical crystallography), to that of proteins and their macromolecular complexes (protein crystallography), and via biophysical and biochemical methods to dynamic structure-function relation studies of biologically active macromolecules (structural biology). Structural biology is by far the largest activity and this will be the main focus also in the future.

X-ray crystallography is the main experimental technique used for both chemical and macromolecular structure determination. The structural biology activity, however, covers the full range of techniques from cloning of genes to structure determination by crystallographic techniques, and structure-function relation studies by biophysical and biochemical methods, computational biology and bioinformatics. The structural chemistry group is currently the host of the Norwegian Structural Biology Centre (NorStruct), a national technology platform financed by the programme in functional genomics (FUGE) in the Research Council of Norway (RCN). A major part of the activity in the group is connected to NorStruct. The group is also engaged in the Center for Research-based Innovation (MabCent), with a particular responsibility for the structural determination of biological macromolecules.

3.3.1 Present situation: Research profile

Structural biology is now the main focus of the research group. The structural chemistry group has emphasized a broad competence in the field of macromolecular and structural biology. The biological chemistry approach of the research has been shown to be an important competitive merit of the group that will be further developed. Macromolecular crystallography is a key research technique employed by the group, and is used in a close interplay with a solid expertise in biophysical/biochemical methods and computational biology. The requisite molecular and cellular biology is to a large extent taken care of through external collaboration, but the group has through the employment of postdoctoral researchers in temporary positions been able to keep a certain minimum of facilities and competence in molecular biology within the department. This situation is thus vulnerable since this expertise is in particular important for protein production and mutagenesis, which are crucial for almost all research in the field.

Structure-function relation studies of biologically active macromolecules have been developed as the main research profile of the structural chemistry research group. The thematic research areas are not static, but projects related to marine biotechnology molecules involved in aquaculture species virulence, fish defense systems, fish vaccine design etc., are important research targets. Research connected to the chosen model organism, the psychrophilic and fish pathogenic bacterium, *Vibrio salmonicida*, is in particular important in this context. As an integrated part of the above-mentioned research themes, basic research in areas such as the molecular basis for cold-adaptation, protein-protein and protein-ligand interactions, and protein stability, is carried out. With the hiring of Prof. Richard Engh in the group (from August 2006), expertise in the areas of signal transduction and drug design has been added to the department. These areas should find connections both in medicine and diagnostics, and in topics relevant for example to marine biology

The research carried out in chemical crystallography is to a large extent directed toward pharmaceutically

important compounds.

3.3.2 Research facilities and infrastructure

The structural chemistry group has recently installed new diffractometer systems and X-ray generators for both chemical and macromolecular crystallography. The group is now equipped with state-of-the-art facilities for in-house crystallographic data collection. The new installment of calorimetric equipment (Differential Scanning Calorimetry (DSC) and Isothermal Titration Calorimetry (ITC)) is expected to advance biophysical aspects of the research (protein stability and protein-protein/ligand interactions) significantly. The group is also equipped with state-of-the-art instrumentation for protein purification, gel documentation systems and dynamic light scattering (DLS) experiments. An old crystallization robot system, however, will in 2007 be replaced with a modern crystallization robot, including an up-to-date imaging systems.

Only one departmental technician is connected to the group, with responsibility for data collection and the X-ray equipment. The remaining technical services for the group (protein purification, crystallization, DLS, calorimetry), are currently taken care of by the NorStruct technicians in temporary positions. A second technical position is therefore of high priority to the group.

The structural chemistry group, including NorStruct, employs offices and laboratories at two floors of the chemistry building. The group moved into a larger laboratory at the second floor in the chemistry building in late 2006. The physical laboratory space is now adequate for the activity, but some rebuilding is still necessary in the X-ray laboratory at the third floor. With the hiring new staff members and their needs to build up independent research activity, office space may be inadequate.

3.3.3 Collaborations

The Norwegian Structural Biology Centre (NorStruct) is a joint effort with research groups at the Norwegian College for Fishery Science (NFH) and the Faculty of Medicine, at the University of Tromsø, of which the structural chemistry group is particularly closely associated, and through NorStruct the group also has a large number of national collaborators from all the six universities in Norway. The group is participating in projects with two Norwegian companies in the development and commercialization of macromolecules for use in biotechnological processes. In addition to a close interplay with research activities at various synchrotron facilities in Europe, the structural chemistry group is collaborating with a range of international research institutions and individuals. The group is also a part of the Center for research-based innovation (MabCent) headed by researchers from the Norwegian College for Fishery Science (NFH).

Basic research in structural biology also requires access to expertise in chemical synthesis. The most essential protein functions subject to structure-function studies involve chemical reactions, and an understanding of the essential intermolecular interactions may require alteration of specific chemical moieties. Basic research in structure-function relationships therefore requires expertise both in chemical reactions and in the ability to synthesise ligands that mimic or trap steps along kinetic pathways, or that enable dissection of intermolecular interaction energies, etc. Synthetic modification of proteins is similarly an essential research tool. Access to chemical synthesis expertise is also essential for basic and applied research in drug-target interaction studies. This need forms the basis for collaboration within the chemistry department.

3.3.4 Future strategy

The structural chemistry group aims to continue to hold a leading national role and a high international standard in structural biology generally and macromolecular crystallography specifically. The research group will thereby continue to be an attractive collaborator for external partners, which in turn will contribute to maintenance or growth of grant funding in the future. Macromolecular crystallography will also in the future form the basis of the research activity of the group, and will be an essential aspect of the majority of the projects. This requires the maintenance of solid expertise in all aspects of macromolecular X-ray

crystallography as a major strategic goal for the group. However, when new faculty members are to be hired, the Department needs to ensure that additional and complementary techniques in structural biology are added or maintained in the research group, although not necessarily as the primary research focus of the new faculty members. Basic expertise in molecular biology techniques, as well as in various biophysical and biochemical methods must be found within the permanent staff. Similarly, computational biology methods are becoming steadily more important in structural biology as the nature of the problems to be studied becomes more complex, both as a separate field of research and as a complement to the experimental methods. The increased importance of biomolecular modeling will also be considered with respect to the establishment of the Center for Theoretical and Computational Chemistry established at the Department of Chemistry. The structural chemistry group will emphasize the need to continue to use such methods as an integrated part of the ongoing research, and ensure that expertise is held by the staff members through the recruitment in coming years.

Thematically, the structural chemistry group will in the future focus on a few but relatively broad topics. This will allow for a clearer research profile for the group and the individuals, and strengthen the competitiveness for external grants, nationally and internationally. The four research topics are:

- 1) Signal transduction pathways
- 2) DNA-modulating molecules and systems
- 3) Molecules involved in host-pathogen interactions
- 4) Environmental adaptation of molecules.

Basic research of e.g. protein-ligand and protein-protein interaction, and protein stability will continue to be important research interests within the chosen topics. Basic research in the four topics is highly relevant to applied research, as molecular structure-based engineering of small molecule drugs, biopharmaceuticals, enzymes, etc. becomes standard. Therefore, opportunities for commercialization will have increased attention from the group. This will arise both from in-house activities and via stronger interactions with commercial enterprises.

Instrumentation and competence for the structure determination of small molecules (organic and inorganic compounds) will be maintained in the group, both due to the need for such data in some of the structural biology projects within the group and to secure the position of the group as an attractive partner in external collaborations in related fields. It is also of great importance for the research groups in organic and inorganic chemistry to have this technique readily available, and the Department will also continue to offer this service externally, both through collaboration and as a fee-based service. Pure service activity is presently taken care of by a scientific staff member, but will over time be dealt with by strengthening the technical staff of the research group. In case this activity is maintained as a support-service only, the Department needs to develop an appropriate financing model for this service.

3.4 Theoretical Chemistry

The group in theoretical chemistry currently has one permanent staff member (Kenneth Ruud)---who is also acting as head of the Department and a temporary associate professor. A new faculty member will be hired in 2007. Through extensive use of temporary positions and professor II positions during the last 4-5 years, the group has been able to provide a complete bachelor, master and Ph.D. curriculum. The group was in late 2006 awarded project coordination of a Norwegian Center of Excellence in the Center of Theoretical and Computational Chemistry (CTCC). In addition to the theoretical chemistry group, the group in inorganic chemistry and materials sciences is involved, as well as researchers from the Department of Physics and Technology, and the Department of Mathematics and Statistics. The establishment of the CTCC is expected to lead to a significant increase in the activity of the group, and the CTCC is expected to have between 20 and 30 members.

3.4.1 Present situation: Research profile

The current research is focused both on the development of new computational methods as well as the application of these methods to relevant chemical problems. Current activities focus on: (1) the development of computational methodology to calculate new molecular properties, in particular involving geometric or magnetic perturbations, (2) the study of medium effects (liquids, and possibilities for extensions to solids) on molecular properties, in particular non-linear optical properties, (3) the development of new computational methodology for determining wave functions and densities using wavelets, (4) highly accurate studies of molecular properties using high-level coupled-cluster methods.

The group has contributed to three different internationally recognized computer programs that are all distributed free of charge to the scientific community (though under slightly different terms): ACESII, Dalton and Dirac, of which Dalton is tightly connected to Tromsø and currently distributed to more than 500 research groups worldwide in the latest release. The strong involvement in computer program development is central to maintaining the high international visibility of the group, though there is significant administrative overhead on the scientific staff due to the need to maintain and support these codes without any technical assistance.

3.4.2 Infrastructure

The group is currently occupying 4 offices in the top floor of the Chemistry Department. The significant increase in the activity in the group resulting from the establishment of the CTCC leads to a very critical need for more office space. The CTCC is expected to need about 15 offices in addition to access to conference facilities and lunch areas. There is little room in the Chemistry building to accommodate such an expansion, in particular considering the expected need for office space due to the activities connected to MabCent. A dialogue with the Faculty of Science and the University administration needs to be initiated quickly to resolve this problem as soon as possible. Although the group in theoretical chemistry can easily be moved, it would clearly be beneficial from the point of view of the Department of Chemistry could be established in rather close proximity to the existing activities at the Department of Chemistry.

Apart from office spaces and computer access, the group primarily depends on high performance supercomputing facilities, currently provided in reasonable amount by the University of Tromsø through their HPC program and by the NOTUR-II project run by Uninett-Sigma.

3.4.3 Collaborations

The group has a large number of international collaborations, some informal and others formalized through the participation in three different international networks (one FP6 Research and Training Network, one COST-D37 network). The group has also received support for international collaborations through the Deutsche Akademischer Austauschdienst (DAAD) with Germany, Aurora with France, and through the BiLat program with Canada, the latter which also lead to a FRINAT project approved in 2006. The group is also coordinating site for a national Strategic University Program in Quantum Chemistry, involving all the theoretical chemistry groups in Norway, as well as a partner in a national theoretical modeling network in nanotechnology financed by the NANOMAT program of the RCN. The most significant collaboration is however that of the CTCC. This project involves both the University of Tromsø and the University of Oslo. In Oslo, there are researchers involved in computational modeling from several branches of chemistry involved. In Tromsø, the group in inorganic chemistry and materials science is a partner in the CTCC in addition to the theoretical chemistry group, as well as researchers from the Department of Physics and Technology and the Department of Mathematics and Statistics.

3.4.4 Future strategy

Part of the explanation for the high productivity of the group is due to the well-established international collaboration of the group and the unique expertise of the group that is of international interest (molecular

integrals, vibrational corrections, solvent effects). The department should consider it of strategic interest to support these collaborations beyond the basic minimum funding of the group. The international networks in which the group participates also provide a valuable source of highly qualified Ph.D. students and postdocs to compensate for the at times limited supply of local students.

A central part of the strategy of the group will be focused on the implementation and development of the Center of Excellence in Theoretical and Computational Chemistry. The strategy of the center is currently in the process of being written.

3.5 General strategic goals for the Department

7. A primary strategic goal of the Department will be to ensure that NorStruct is extended for a second five-year period (2007-2011) to secure the activity of the structural chemistry group at the current level.
8. Considering the documented scientific competence in the fields of molecular modeling through the establishment of the CTCC, and in biomolecular studies, experimentally and theoretically, through NorStruct, the Department sees it as a high priority to hire a new staff member with scientific competence in biomolecular modeling. Building on the competence available at the Department, and the long-term commitment to CTCC by the RCN, such a position will have great potential to make the Department internationally leading in biomolecular modeling.
9. The Department will work toward the establishment of a Ph.D. research school in chemistry.
10. The Inorganic chemistry and Theoretical chemistry groups should consider the establishment of joint proposals to the NANOMAT program, where the joint efforts and competence of both groups may give sufficient strength and size to be successful in attracting funding from this program.
11. The competence in the synthetic organic chemistry group as a whole is very broad and unique in a Norwegian perspective. The members of the group should therefore try to establish larger constellations around joint research projects and in this way attract substantial funding from the RCN.
12. The structural chemistry group should seek to establish a clear, local research profile and lead their own research projects in national and international collaborative efforts (in particular in EU initiatives).

4 Primary activities at the Department: Education

As part of the "Kvalitetsreform" (the quality reform of higher education), the complete curriculum of the chemistry department was revised in 2003. With two exceptions, the department now offers 10 study point courses (1/3 of a semester's workload), 10 at the bachelor level and 24 at the Master level. 15 of the master level courses are also offered in slightly extended versions as Ph.D. courses. The latter does not give economic credit as a part of regular teaching.

Whereas three of the bachelor courses (KJE-1001, KJE-1002, KJE-1003) are offered as part of other bachelor programs (pharmacy, fishery science, biology, and geology) the remaining 5 courses (KJE-1004, KJE-1005, KJE-2001, KJE-2002, KJE-2003) are primarily targeted for bachelor students in chemistry, though they are also part of the curriculum for the program for educating teachers in chemistry and mathematics as well as chemistry and biology. The number of bachelor students in chemistry has in recent years been low with a declining trend, and the Department must consider whether it would be possible to offer the more specialized bachelor courses KJE-1005, KJE-2001, KJE-2002, and KJE-2003 only biennially. In order for this to be achieved, additional flexibility in the suggested curriculum for bachelor studies in chemistry must be introduced. A curriculum for studies starting in even-numbered years could be:

Spring Y-02	KJE-1005	Free	Free
Autumn Y-02	KJE-1004 ¹	Free	Free
Spring T-01	KJE-2003	KJE-2001 ²	Free
Autumn Y-01	KJE-1003	KJE-2002	BIO/FYS/MAT
Spring Y-00	KJE-1002	BIO/FYS/MAT	BIO/FYS/MAT
Autumn Y-00	KJE-1001	Ex.phil.	MAT-0001/MAT-1001

whereas a study-program beginning in an odd-numbered year could be:

Spring Y-03	KJE-2003	KJE-2001 ³	Free
Autumn Y-03	KJE-2002	Free	Free
Spring Y-02	KJE-1005	Free	Free
Autumn Y-02	KJE-1003	KJE-1004 ⁴	BIO/FYS/MAT
Spring Y-01	KJE-1002	BIO/FYS/MAT	BIO/FYS/MAT
Autumn-01	KJE-1001	Ex.phil.	MAT-0001/MAT-1001

This scheme could help ensure that the faculty members are only involved in bachelor-level teaching every second semester at the most, the level of teaching activities at the master and Ph.D. levels determined by the availability of students. A similar flexibility can be introduced in the curriculum for the study program for science teachers.

Due to the low number of students in chemistry, the Department have had few benefits from the new regulations for external examination of student exams (in practice, an external examiner is involved in evaluating all students in all courses except KJE-1001 and KJE-1002). As such, the expected reductions in the costs of evaluating exams have to a large extent not been possible to achieve at the Department.

The Department considers it worrisome that several students enrolled in the chemistry bachelor program quit after KJE-1001. Various initiatives to give these new bachelor students closer ties to the Department, through for instance mentor programs using higher-level bachelor/master students, or by providing an oracle service for the students at KJE-1001, will be supported.

In the first attempt at a revised KJE-1001 with two intermediate exams, there were significant added workloads on the teaching staff due to the high number of students on the course. Based on the evaluation both by the students and by the teaching staff, the Department has now returned to one, single exam at the end of the course. However, the students need to pass 4 obligatory tests given through the ClassFronter system. This approach is also used in KJE-1002. This appears to be a manageable way of ensuring student progress and minimizing teacher efforts. If economically possible, the department would like to use an external examiner for evaluating all student exams, also in the large courses KJE-1001, KJE-1002, and KJE-1003.

For KJE-1001 and KJE-1002, the use of ClassFronter has significantly improved the progress of the students and the workload of the teaching staff. However, the general experience of the Department is that the use of

¹ Although desirable, it may not be possible to offer KJE-1004 only biennially.

² Evaluation of KJE-2001 seems to indicate a preference among the students to postpone this course until the last semester, or at least until after MAT-1004.

³ Evaluation of KJE-2001 seems to indicate a preference among the students to postpone this course until the last semester, or at least until after MAT-1004.

⁴ Although desirable, it may not be possible to offer KJE-1004 only biennially.

online teaching services has a very high initial cost, a cost that in many cases cannot be justified with the current number of students in chemistry. Thus, whereas the Department will continue to improve and extend the use of online teaching solutions (for instance through the use of ClassFronter) for the large courses KJE-1001, KJE-1002, and KJE-1003, the Department does not consider it economically viable to try to develop such schemes for teaching in the more specialized chemistry courses.

A fairly high percentage of the bachelor students in chemistry have taken part of their studies at foreign institutions. The Department will continue to encourage such international studies as part of the bachelor student's curriculum. The Department is pleased to note that it is also attracting foreign students, and there are in general more students taking part of their studies in Tromsø than there are Norwegian students going abroad (primarily due to the low number of bachelor students locally).

An important course for the department which has high costs in terms of man-power and laboratory facilities is KJE-2003. With the revision of the bachelor program in Chemistry, the majority of the laboratory exercises have been collected in the course KJE-2003 (laboratory exercises in organic chemistry excluded). Although the course can be considered resource intensive, the Department considers this an important course for the Department and for the students in chemistry.

The Department provides the laboratory course of FSK-1000, a bachelor course in chemistry offered by the Norwegian College of Fishery Science. About 20-30 students participate in this laboratory course in the spring terms.

The department offers master and Ph.D. programs in four subjects, corresponding to the profile of the research groups: Inorganic chemistry and materials science, Organic chemistry, Structural chemistry and Theoretical chemistry.

At the master and Ph.D. levels, the amount of teaching given and the intervals between courses must to a larger extent be based on the availability of students and their plans. Attempts should be made, by the program committee for the master studies in chemistry, to develop a study plan for accepted master students that minimize the number of times a course must be given. The Department will seek to get more information from the Research Training Committee at the faculty about newly accepted Ph.D. students and their study plans, in order to further optimize the interval between each time different courses are given at the Ph.D. level.

4.1 Ph.D. training and employment

The Department of Chemistry has a fairly high need for personnel due to the need for staff to do teaching in the laboratory courses. In particular, two of the largest courses offered by the Department in terms of the number of students taking the course, KJE-1001 and KJE-1003, have extensive laboratory courses. The Department also offers the laboratory course FSK-1000 on behalf of the Norwegian College of Fishery Science, with a total of 20-30 students every spring.

The Ph.D. students at the Department provide an invaluable service in making sure that the Department can offer adequate teaching in these courses. As such the Department feels that the general rule should be that all Ph.D. students, also those financed by external funds, should be hired for a period of 4 years with 25% of their time dedicated to service functions for the Department, in particular teaching activities.

However, due to the poor recruitment of Norwegian students to chemistry at the bachelor and master levels, the Department has increasingly been forced to hire foreign students with little knowledge of Norwegian, or students trained in related disciplines such as molecular biology or physics. Whereas such hiring has distinct benefits with respect to the scientific activities at the Department, these students may not be sufficiently qualified for doing teaching in chemistry, as language may be a barrier at the introductory courses in chemistry. The Department will therefore, as part of the evaluation of the technical and administrative needs of the Department, also consider other Department support functions to be done by these students. Such

duties may include responsibility for maintaining departmental web pages, technical services, and outreach programs. The Department will establish such duties in close collaboration with each student to ensure the greatest mutual benefit for the Department and for them in their Ph.D. training programs.

The Department has experienced several instances where large and expensive experimental equipment has broken down due to old age and inadequate resources for maintenance and replacement. Ph.D. students who have been affected by such breakdowns have been granted extra time for their Ph.D. program and employment at the expense of the Department. In certain cases, delays in the progress of a Ph.D. project have occurred, and Ph.D. students have been hired in part-time positions with a full teaching load to allow for the Ph.D. project to be completed. Although this has been possible due to vacancies at the Department, this affects the freedom of the Department in its ability to replace old equipment or support other strategic efforts. At the same time, since in most cases these students have been hired for 4 years, failure to complete a Ph.D. degree has serious economic consequences for the Department, as a substantial amount of the strategic financing for research is based on the number of graduated Ph.D. students.

The Department will as a general rule not provide support for Ph.D. students beyond 4 years. As soon as delays are expected in a Ph.D. program, the supervisor(s) are required to inform the Head of the Department to discuss possible actions that may prevent delays in the progress. Only if such reports have been reported to the head of the Department *during* the Ph.D. program---and necessary measures have been taken to avoid further delays---will the Department consider hiring Ph.D. students for a period for more than 4 years on Departmental funds. The Board of the Department will monitor the effects of these guidelines, and consider possible changes at the yearly strategy meetings.

4.2 Research school in chemistry

As the Department is united behind the vision of being a nationally visible chemistry department with a clear biological chemistry profile, the Department will actively seek to establish a Ph.D. school in chemistry. The school will focus on the common chemical basis for the activities in the Department, and focus on providing the students with a training program that gives them insight into the large array of different methods that can be applied to solve problems in biological chemistry, from the isolation, identification and synthesis of biologically active compounds, through studies of their interactions with active bioinorganic sites in proteins, to theoretical studies elucidating the electronic origins of the behavior of these molecules. Topics such as structure based drug design that are inherently interdisciplinary within chemistry provide an attractive basis for recruitment.

A research school both benefits from and supports other integrating activities within the Department. Activities such as regular Department seminars and intra-departmental collaborative research strengthen interdisciplinary expertise to enhance post-graduation employment opportunities for graduates and research quality.

Although the Department will focus on the establishment of a research school in chemistry, other initiatives by individual research groups, such as the Ph.D. school in Molecular and Structural Biology---in which the structural chemistry group is already taking part---will be supported, but the Department will not take a leading role in such initiatives.

4.3 Recruitment

The Department will seek to integrate new bachelor students in the activities at the Department and contribute to contact among bachelor and master students in order to establish a good social environment for the chemistry students. The Department will also seek to make chemistry attractive by improving the quality of the introductory course in general chemistry, KJE-1001. An integral part is here to provide the chemistry students (and others who are interested) with an attractive web-site for the largest chemistry courses with

useful links to popular presentations of exciting new science in areas of relevance to these courses. The scientific staff is encouraged to keep their web pages up-to-date and containing information also of interest to the students in chemistry.

5 Primary activities at the Department: Outreach and dissemination

The number of chemistry students is in general declining. This is a worrisome development considering the central role of chemistry for future Norwegian industry in many fields, including energy, environmental technologies, pharmaceuticals, aquaculture, agriculture, and materials science. The Department will support, in the ways possible, any national and local initiatives to increase the interest and recruitment to chemistry. Faculty members with funding from large research initiatives should have a special responsibility for popularizing the results of their research.

5.1 Publications

The latest statistics (2005) for publication activities at the Faculty of Sciences at UiT indicate that the Department of Chemistry is the most scientifically productive department at the Faculty in terms of publication points, and also the most productive Chemistry Department in Norway in terms of publication point per scientific staff⁵, to some extent achieved by a very high ratio between level 1 and level 2 journals (approximately 2:1). The Department will support all activities that will secure the high scientific productivity and quality of the department. Considering the current number of students in chemistry, keeping up the high scientific quality of the Department, and the culture of doing and reporting high-quality research, will be the primary focus of the department. This will help secure the national and international awareness of the activities at the Department.

5.2 Outreach to schools

The Department has a long history of outreach activities toward schools. These activities include visits to the Department by school classes starting at the sixth grade, as well as visits outside of the university, such as Lillestrøm and Bodø. Staff members of the department participate in "Forskningsdagene" in Tromsø and is one of the larger contributors to the HPC group's "Supercomputer days" at UiT.

The Department has made a contract with Kongsbakken videregående skole, providing special activities for students at all levels in their chemistry courses. A mentor program for selected students from Tromsdalen videregående skole has also been established from the autumn of 2006. The Department will continuously evaluate the benefits of this collaboration and consider the extension of this program to other schools. The Department is glad to have been able to establish a closer connection to Vitensenteret, and hope that experiment classes, tutorials and exhibits can help demonstrate the fun of chemistry and in this way create an awareness of chemistry already at a very young age, as well as with the parents.

The department considers outreach to schools as an important way of attracting students. At the same time, it is a costly activity that can only have very long-term potential benefits. The Department will therefore have to monitor the cost of these operations and evaluate them in relation to the possible long-term benefits, as there is currently no economic incentive for these activities.

The Department will seek to attract interest from prospective students, the general and scientific community and from media through up-to-date and user-friendly web-pages. A working group will be established with the purpose of evaluating what information should be provided by the Department, the individual research groups and the individual researchers, and whether a unified profile should be adopted at the department or not. A strategy for maintaining and updating these web pages will also have to be decided.

⁵ Professors, Associate professors, researchers and postdocs

6 Primary resources at the Department: Personnel

The size of the Department has been set by the Board of the Faculty to 12 faculty members (Sak 21/00). As of 01.01.06, 9 of these positions are filled and one position is in the process of being filled. The current staff includes by March 15 2007 (the first number indicates the number of personnel hired by the University, the second by external sources):

	Inorganic	Organic	Structural	Theoretical	Department	Total
Faculty members	1/0	4/0	3/0.2	2 ⁶ /0		10/0.2
Postdocs/researchers	0/0.2	0/3	0/6	0/1		0/10.2
Engineers		3/0	1/3			4/3
Ph.D. students	0/4	0/1	1/3	1/3		2/11
Administrative leader					1	1
IT consultant					1	1
Research technician					1	1

The key to the future success of the Department is its staff members: scientific, administrative and technical. The Department will therefore continue to nurture the good social atmosphere at the Department, as this is one of the most effective ways of ensuring the high quality of the job delivered by the staff members.

6.1 Scientific staff

The scientific staff is at the core of the Department's activities. As a large part of the budget of the Department is based on the performance of the scientific staff, in terms of publications, external funding, and teaching, ensuring good working conditions for the scientific staff is the most important priority of the Department. The Department is currently in a phase where many of the faculty members who have been with the Department since its inception is retiring. The choices made with respect to the hiring of new faculty members will therefore shape the Department for many years to come and will be critically important decisions for the Department.

6.1.1 New openings, scientific staff

In the time frame of the present strategic plan, 3 openings are available/expected:

- Tor Dahl (2005, X-ray crystallography)
- Lars-Kristian Hansen (2011, X-ray crystallography)
- Rolf Carlson (2013, Organic chemistry)

The majority of the openings are therefore affecting the structural chemistry group. The group currently hosts the Norwegian Structural Biology Centre (NorStruct), and has a well-established and active collaboration with research groups at the Faculty of Medicine and the Norwegian College of Fishery Science. Two of the positions (Dahl and Hansen) are related to research and service functions on chemical crystallography. The service functions for the other research groups, in particular organic and inorganic chemistry, as well as the Department of Pharmacy, are important activities and should be secured. However, it is not clear that the activity needs to be connected to an ongoing research program, and it is suggested that the bulk of this function should be secured through a highly skilled technician. In this case, the cost of such services for non-departmental research groups must be established and negotiated.

In order to maintain and further develop the strong position in structural biology of the group, one of the

⁶ One associate professor in a temporary position.

other open positions will also be devoted to the structural biology activity of the group. A third faculty position in structural biology should also be centered on protein crystallography, but will be expected to add competence in one or more of the following fields: biophysical methods, spectroscopic techniques applied on macromolecules (including protein NMR) or computational biology. Although not the primary research area, basic molecular biology knowledge should be covered by one of the four faculty members in structural chemistry.

The Department considers the minimum number of faculty members in a research group to be two. The Department will therefore has as an overall target that the sizes of the groups are in accordance with that outlined in Chapter 3 (2/4/4/2). However, in case the current and future economic situation does not allow for all positions to be filled, the Department will have to consider whether the overall profile and strength of the Department is best secured through a temporary reduction in size of either the structural chemistry or the organic chemistry groups. This decision is of such high strategic importance to the Department that a decision on this matter needs to be made by the board of the Department.

The considerations given in the above guidelines, forms the basis for the strategy for replacing faculty members at the Department.

Priority is given to establish a second position in inorganic chemistry and materials science. Since there is little opportunity within the regular departmental budget to obtain new expensive experimental equipment, the Department will either have to secure the necessary infrastructure for a more extensive activity in inorganic (metallo-organic) chemistry from the University centrally, or through special incentive financing from the RCN.

If such funding cannot be secured, the research profile of the faculty member hired should be chosen such that internationally high-level research is possible with existing infrastructure. In case a new faculty member is hired in inorganic chemistry, it is suggested that the group changes its name to "Inorganic chemistry". The department sees no opportunities to further extend the activities in materials science, and this would not strengthen the profile of the department.

The establishment of the CTCC is in principle for a period of 10 years, with the last 5 years pending an evaluation by the RCN after approximately 3,5 years. As part of the contract with the RCN, the leader of the CTCC, prof.Kenneth Ruud (theoretical chemistry) will be paid in full by the CTCC, freeing salary funds at the Department for the duration of the CTCC. Considering the expected longevity of the CTCC, as well as the competence of the Department in theoretical chemistry and in biomolecular chemistry, the Department considers it to be strategically important to hire a new faculty member in biomolecular modeling, who can build on the expertise in the two groups at the Department to create an internationally recognized group in biomolecular modeling.

The Department has a high, national---and to some extent also international---standard of research and visibility. Still, the Department cannot in general be expected to be competitive for highly qualified, well established personnel. As such, the department will as a general rule seek to attract highly qualified young researchers, and new faculty positions will in general be announced as associate professor positions. Only in rare circumstance will new faculty positions be announced as a full professor position, or as both associate and full professor to be decided depending on the qualifications of the person hired. The Board of the Department must make the decision to announce a position as full/associate professor in their yearly evaluation of the strategic plan. These decisions have to be made such that the requirements imposed by NOKUT for the ratio of full professors to associate professors is fulfilled (there has to be at least 50% full professors). However, the department would like to secure this ratio by qualifying the internal faculty members for full professor positions by personal promotions.

On this basis, the Department has the following plan for the hiring of new faculty members for the period of this strategic plan:

- An associate professor in structural chemistry/biology will be hired in 2007.
- Associate professor in biomolecular modeling. The position should be announced as soon as possible

in 2007, and be expected to act as a scientific link between the CTCC and NorStruct.

- Associate professor in inorganic chemistry (2011/2012). The position will be in the field of metalloorganic and/or bioinorganic chemistry. The person hired will have to be familiar with the research facilities offered by the Department. The Department does not at this stage see any opportunity to initiate activities requiring the investment in major new equipment. Efforts should be made to hire a person who has research activity that would have potential for collaboration with other areas of experimental activity at the Department in addition to within the inorganic chemistry group. Specific directions (toward organic or structural chemistry) should be considered by the board of the Department before the position is announced.

The latter position will in reality be transferred from structural chemistry, resulting in a reduction from four to three faculty positions. However, when this becomes relevant, the overall situation and profile of the structural chemistry group and the Department as a whole must be evaluated before a reduction in group size is effectuated. Possible future openings in organic chemistry will have to be evaluated in relation to the actual situation in structural and/or inorganic chemistry. This position will also have to be considered in view of the status of the CTCC and its future funding (e.g. from the University) as the period of this center comes to an end.

6.1.2 Strategies for hiring new faculty members

The primary criterion for hiring new faculty members should be scientific quality. As such, new positions should be announced with a fairly broad field of research interests. To ensure complementarities in the scientific staff, it is suggested that the international scientific evaluation committee is asked to evaluate also the candidates in view of the profile and strategy of the Department. In case of candidates of approximately equal qualifications, priority will be given to candidates with a research profile that suits the strategy of the Department---that is, with a biological chemistry profile. However, the preference of a biological chemistry profile should not overshadow the evaluation of the scientific quality of the candidates. A 10-page research plan should be required for applications for permanent faculty positions, and be an integral part of the evaluation of the applicants. This will then also serve as a useful starting document for faculty members when applying to the RCN for external funding.

In order to attract the most highly skilled international researchers for permanent faculty positions, the international visibility of our research groups is the most important marketing tool. Activities in the research groups promoting international visibility will be supported by the department. The department will, for exceptionally well qualified candidates, actively seek to secure attractive start-up packages for new personnel from the Faculty and the University. For all new personnel hired, the Department will seek to enable a rapid start-up of the research activity of the newly hired personnel by giving high priority to these activities when applying for Ph.D. and postdoc positions from the pool of such positions at the University.

The Department acknowledges the very skew gender profile of its faculty members. In accordance with general regulations, the Department will encourage and support female applicants for faculty positions. The Department will actively seek to support female faculty members in qualifying for the title and position of full professor.

6.1.3 Sabbaticals

The University of Tromsø has historically put much emphasis on giving their scientific personnel sufficient opportunities for scientific development and focus on research through frequent sabbaticals. With the restricted support for travel expenses in connection with sabbaticals from the RCN, the Department needs to more clearly define to what extent the frequency of sabbaticals can be maintained. The Faculty of Science strongly encourages faculty members to include expenses for sabbaticals as part of research proposals to the Norwegian Research Council. To what extent the University of Tromsø, and the Faculty of Science will support such expenses in the future is currently not clear.

As a general rule, in line with the focus on scientific excellence, the Department encourages frequent

sabbaticals in combination with stays at foreign research institutions, and will give faculty members the opportunity to take a full year sabbatical every fifth year (or half a year sabbatical every 2,5 years) if financing can be secured from external sources or from the Faculty or from the University.

In case the faculty members primarily do teaching at the bachelor level only once every year, the Department sees it as a general rule not as a high priority to support faculty members with the added costs of stays abroad during periods without teaching. However, the Department will consider such support as part of the possible incentives and rewards for excellence in scientific or educational work.

6.2 Technical staff

The Department will consider the possibility of a less rigid association of the technical staff to specific research groups, and rather that the technical and administrative staff all should be considered departmental assets. In this manner it *may* be possible to run the Department with only 4 engineers in the future, though it is important that the size of the technical staff is sufficient to ensure that the scientific staff can focus on the core activities of research and teaching. However, such a decision will have to be based on the expected need for technical assistance on expensive scientific equipment, as well as the activities in the experimental groups. The future of the position in chemical crystallography as well as the expected economic future of the Department must also be considered in the evaluation of the possibilities to have 5 engineers at the Department.

If economically feasible, the second engineer position in structural chemistry should be filled as soon as possible, in particular if the responsibilities of in-kind contributions to NorStruct are expected to continue. Assuming that the Department does build down the research activity in chemical crystallography, one engineer position must be held by a person competent in X-ray crystallography. The competence of any new engineers hired will also have to be considered in view of possible new activities in the field of inorganic chemistry. However, the Department may also consider the possibility of hiring a faculty member whose teaching obligations are transferred to an obligation to provide services in small-molecule crystallography.

In a time of increased focus on scientific quality and production, the focus of the scientific staff should be on the core activities of research and education, and the Department will have a keen eye on providing training for our technical staff such that they can contribute to the core activities in research and education, including advanced use of the Department's expensive scientific equipment. The current competence of the technical staff in chemistry is a very strong asset for the department, allowing the technical staff members to participate significantly and with large responsibility in teaching as well as in research projects. The technical staff should be encouraged to train themselves through taking part of courses within or outside the department on advanced use of scientific equipment.

7 Primary resources at the Department: Infrastructure

The Department of Chemistry is localized in the C-block of the Science Building at the University Campus in Breivika. Apart from a "study room" for science students on the second floor, the remaining parts of the 1st, 2nd, and 3rd floor are at the disposal of the Department of Chemistry. In addition, the department's stockrooms are localized on the ground floor of the C-block. Laboratories for the basic chemistry courses are now in "Forskningsparken".

7.1 Building

The Science building is the oldest building at the University Campus, and has not been the subject of any major renovation since its original construction in 1979. The premises for the Department of Chemistry do therefore not meet modern standards neither for teaching nor for research. In particular, the laboratory facilities for research purposes are not well-functioning for modern requirements. Most serious is the lack of adequate ventilation in virtually all laboratories. This is a serious risk to health, in addition to restricting the

research activities for graduate students and employees and hindering recruitment. In general, the age of the building and the construction materials used-combined with insufficient maintenance-has led to a deterioration of the working conditions that has led to health problems for several of the employees at the department. These problems arise from moisture damage and mold in walls and flooring, asbestos in the outer walls and an insufficient ventilation system.

The general layout of the building neither reflects the nature nor the level of the activity performed in the Department. This has been so obvious as to have generated comments in the popular press regarding the contrast between the high quality of research and the appearance of the offices and laboratories.

Relocation of the department or a major renovation of the building is of utmost importance and is therefore of high priority for the department. However, the department is concerned with the potential problems of temporary relocation of an advanced experimental department with high demands on laboratory quality. The department is also concerned that urgent but minor alterations in the building will not get priority by the University, leaving the department in an unacceptable status quo where maintenance is ignored and the future is, at best, uncertain.

With the engagement of the Department in a Center for Research-based innovation and in a Center of Excellence, the Department is furthermore in dire need of more office space, and a rough estimate indicates a shortage of office space by about 15 offices, or about 30 work places. There is no possibility to accommodate these needs within the current chemistry building, and an expansion outside the current chemistry building is required. A challenge will then be to keep the researchers at the Department in touch with each other if the activity of the Department is divided into several different physical locations.

7.2 Scientific equipment

The field of chemistry is highly dependent on advanced scientific equipment. Chemistry is an experimental research field and it is impossible to carry out this research without the availability of analytical instruments. All three experimental research groups (inorganic, organic and structural chemistry) depend on a series of central instrument systems with high investments costs (1-15 MNOK). These equipments are also characterized by relatively high running and maintenance costs. In addition, a pool of equipment with investment costs in the range 0.1 - 1.0 MNOK is necessary on a daily basis for experimental research in chemistry, along with well-equipped laboratories. A stock of less expensive laboratory articles (glassware, etc.) must be available, but an opportunity of combining the stockroom needs of the Department of chemistry with the facilities of the Faculty of medicine should be explored.

7.2.1 Instruments with investment costs >1.0 Mill NOK

Nuclear Magnetic Resonance (NMR) spectrometers: The department has recently purchased a new NMR system and upgraded its old system at a total cost of 10 MNOK. These systems are now of state of the art quality and in addition to internal use also serves as the NMR laboratory for the department of Pharmacy. However, the magnet on the routine NMR spectrometer will have to be replaced at some point.

Raman spectrophotometer: The inorganic chemistry group has a small-frame Coherent Innova 70 mixed Ar-Kr laser, a single monochromator, and a Dilor triple spectrograph for resonance Raman studies. Although the spectrometer is excellent, the laser (purchased in 1997) offers only a modest selection of excitation wavelengths. A mainframe Kr laser and a dye laser are necessary for a broader range of resonance Raman measurements.

X-ray instruments for macromolecular and chemical crystallography: The structural biology group has replaced the X-ray generators for macromolecular crystallography in 2006, and the group is now equipped with state-of the art facilities for in-house X-ray data collection. However, the group will have to modernize the facilities/robots for crystallization in the near future.

Mass spectrometers: A new MS instrumental laboratory will be purchased and installed at the Department

in 2007 as replacement for a failed MS apparatus. After this installation is completed, the department should be well equipped with necessary MS equipment.

As pointed out above, several of these units are outdated and due for replacement and the development in modern chemistry requires new equipment, presently not available at the department. Based on this, the future investment plan for new equipment with a budget above 1 Mill NOK has been decided in a prioritized order to be:

Priority	Equipment	Estimated costs
1	Kr-ion laser and dye laser for resonance Raman	3.0
2	New magnet for routine NMR	1.2

7.2.2 Instruments with investment costs 0.1 - 1.0 Mill NOK

The equipment with investment costs below 1.0 Mill NOK cannot be financed through the national program for scientific instruments in the RCN. Therefore, instruments in this cost range can only be financed by the University or as parts of grant applications to the RCN. The department strongly encourages their staff members to include extraordinary equipment needed for the completion of a project in the project applications, though the Department may offer partial in-cash contributions to such equipment requests in application to the RCN.

The **infrared spectrophotometer** and **polarimeter** are also both victims of frequent breakdowns, and only the skills of the technical staff have made it possible for these instruments to stay operational. A new IR spectrometer will be installed during 2007.

Equipment for combinatorial synthesis: New equipment for combinatorial synthesis has been bought and installed in 2006, and the Department is now well equipped on this field.

A large number of instruments are in need of rather urgent upgrade/replacement, and a prioritized list for medium-cost scientific equipment is in prioritized order:

Priority	Equipment	Estimated costs (kNOK)
1	Crystallization robot	1.0-1.5
2	Polarimeter	0.2
3	Automated preparative column chromatographer	0.25
4	High-speed solvent removal system	0.2
5	Hydrogenation equipment	0,25
6	Stopped-flow UV	0.5
7	Spectrophotometer	0.5
8	Guoy balance	0.2
9	Shaking incubator	0.19-0.29
10	Diamond anvil for HPIR	0.2
11	Photochemical reactor	0.5

7.2.3 Upgrading of standard laboratory equipments \$<\$ 0.1 Mill NOK

The annual budget for a researcher in experimental sciences at the Department is set to 70 kNOK, and common experimental equipment may remain too expensive to be purchased by the individual users of these instruments. The Department will there try to establish routines for replacing such instruments on departmental funds. The current prioritized list of such "low-cost items" are:

<i>Priority</i>	<i>Equipment</i>	<i>Estimated costs (kNOK)</i>
	Thermometers without mercury	10
	Oil pumps (3)	60
	Freezer -80C for crystallization	80
	Rotavapor	27
	Ultrasound horn	42
	Samle holder for crystal aquisition	50
	Heating mantle/lab jacks	14
	Equipment for pump tables	28
	Syringe pump	18
	Vacuum lines (2)	35
	Stirrer/heating plate	15
	Automatic flash column	28
	Fiber-optic mobile spectrometer	35
	Cold UV-Vis cells	20
	Microscope	80
	Weights	20
	Multichannel pipettes	20
	Pipettes (2 sets)	24

7.3 Computing facilities

The theoretical and inorganic chemistry group is a major consumer of computing facilities. The main source of CPU time is the National and regional supercomputing facilities, the former operated by Uninett-Sigma in the NOTUR-II project. The department will continuously contribute to securing national and regional supercomputer facilities.

7.4 Participation in large scale international facilities

The structural chemistry group is dependent on the availability of synchrotron radiation sources for X-ray data collection in addition to the home source. Beam time is obtained by peer reviewed proposals to European synchrotron radiation facilities such as ESRF (Grenoble), BESSY (Berlin) and SLS (Zürich). The Swiss-Norwegian BeamLine (SNBL) at ESRF has been the main source of synchrotron radiation for routine data collection for the structural chemistry group to date. A membership fee of 180,000 NOK is currently

paid to SNBL by the University of Tromsø. SNBL is a multi-purpose beam line and not specifically designed for crystallography. The need for dedicated and specialized macromolecular crystallography beam lines is however increasing, and the gap in technology between SNBL and the dedicated beam lines is now evident. Therefore, the structural chemistry group is in the process of looking for alternatives-both for its own research but also through the national responsibility of NorStruct.

7.5 Other important infrastructures

The Department is currently very happy with the services provided by the University library. The wide selection of journal titles available electronically in chemistry and related fields of science, as well as the access to important databases such as Chemical Abstracts and ISI is very important to ensure that the research conducted at the Department is of the highest international quality. In case economically feasible, the Department would encourage the University library to consider the inclusion also of indexing services such as Crossfire (Beilstein).

Although the Department to an increasing extent orders equipment and chemicals when need arises, the Department is in need of a small stockroom for the most basic supply of office equipment, glassware and simple laboratory supplies. In addition, the Department has a fairly extensive collection of chemicals that need to be maintained in a proper manner. This services need to be maintained, although the department should continuously evaluate the possible benefits of obtaining these services from the Medical Faculty, freeing man power for other services at the Department.

8 Internal and external collaborations

8.1 Internal collaborations

The general shift, both at the national and international levels, toward favoring larger research applications makes it imperative that the researchers join forces in writing common, larger, research proposals. However, such initiatives should be taken by the researchers themselves and not be created in an *ad hoc* manner by the department. However, the department will actively seek to support such larger research proposal initiatives through the possibilities of offering in-kind and in-cash contributions to such research proposals should they be successful. The strategic funds available at the department will be actively used for these purposes.

8.2 External collaborations

The individual research groups have an extensive network of collaborative partners within the University, nationally and internationally.

The groups in organic chemistry and structural chemistry have well established connections with the Faculty of medicine. In the case of the organic chemistry group this has resulted in the establishment of a limited company, Lytix A/S. In the case of the structural chemistry group, a joint proposal with the Faculty of Medicine was submitted for the establishment of a Center of Excellence.

The structural chemistry group has extensive national collaborations through its responsibilities as a technology platform for the structure determination of macromolecules, and proteins in particular. This gives the group the possibility of acquiring competence in a wide field of molecular biology/biological chemistry, as well as knowledge about where expertise for selected tasks necessary for local projects may be found in Norway.

Through the participation in the European Synchrotron Radiation Facilities (ESRF) and the Swiss-Norwegian beam line, the structural chemistry group also has easy access to extensive collaborative

networks at the European level, which has resulted in joint EU proposals and other collaborations. The group's expertise in protein-ligand structures is expected to attract national and international collaboration in fields such as structure based drug design. The group should seek to take a stronger lead in such international collaborative efforts.

Theoretical chemistry has an extensive European collaborative network through its central role in the development of in particular the quantum chemistry program Dalton, but as of late also through Dirac and ACESII. The group has been very loosely associated with a European research and training network, and is actively seeking to gain a stronger position in such networks. New initiatives to start collaborations with Poland and Canada will be/has been initiated.

The inorganic chemistry and materials science group has an extensive international network of collaborators, though largely located outside of Norway and Europe making the cost of maintaining active collaborations high.

Considering the geographical location of the Department, external collaborations are considered important, and the department will support initiatives to establish new collaborations, within the University, at a national level, and at the international level through the use of strategic funds. The Department may also support particularly well-functioning collaborations, though it is in general assumed that alternative sources of funding should be sought to enable and secure long-term collaborative projects.

9 External funding

The large scientific activity at the Department is extensive due to successful proposals to external funding agencies, in particular the RCN, at a success rate which is much higher than the average for proposals granted by the RCN. It is a priority for the Department to secure the extent of external funding.

The success in attracting external funds is ultimately in the hands of the individual researchers in their ability to do excellent research and propose excellent new research projects. The general atmosphere of the Department must therefore be one in which externally funded projects are given support. The researchers must be given as much possible support as needed from the Department and from the Faculty to write proposals, and particularly large and promising proposals may be supported by the Department through in-kind contributions. In particular, the Department must provide the necessary support for proposals that were found to be of high scientific quality but were not get funded due to limited resources at the external funding agencies, so that these proposals can be further strengthened in a renewed application.

The Department is very dependent on funding from the RCN. Initiatives to attract funding from industry should be given particularly high priority. The Department should actively support initiatives to attract funding from the EU, in particular for initiatives where researchers at the Department have a leading position in the proposal. However, it does not appear possible for such a small department, by the standards of chemistry departments in Europe, to support the large administrative overheads following EU initiatives. Support for such initiatives must in these cases come from the Faculty of Sciences and from the University of Tromsø.