

## 1-year Report on the HPRN-Network:

### Molecular Properties and Molecular Materials: MOLPROP

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#### Network Coordinator Data:

Prof. Hans Ågren  
Theoretical Chemistry  
Royal Institute of Technology  
Teknikringen 30  
SE-10044 Stockholm, Sweden  
Tel: +46 87908593  
Fax: +46 87908207  
Mobile: +46 709 885282  
E-mail: [agren@theochem.kth.se](mailto:agren@theochem.kth.se)  
URL-Ågren: <http://www.theochem.kth.se/html/agren>  
URL-MOLPROP: <http://www.theochem.kth.se/molprop>

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## Part A

# Research Results

## A.1 Scientific Highlights

We describe below the scientific highlights from each of the nodes, emphasizing the contracted work plan, the midterm milestones and the collaborative aspects.

**P1 KTH-Stockholm** The Stockholm partner has focused on development and application of response methodology for non-linear optical properties. Much of the research efforts have been devoted to various *optical limiting* processes, with the ultimate goal to derive useful materials for laser protection. This research, which adheres mostly to the second milestone of the mid-term review, has produced predictions of promising materials with multi-dimensional and multi-branched structures, for instance a series of cummulene derived compounds has been proposed for synthesis. We have realized that metallo-organic compounds have outstanding properties for optical limiting and multi-photon absorption, and we have taken interest in the use of approximative relativistic methods for optical properties of such compounds, and obtained some preliminary results in this respect. The main collaborators in this works are Oslo, Odense and Pisa nodes.

**P2 U-Valencia** The goal of enlarging the applicability of coupled cluster methods is being accomplished through the use of techniques based on the Cholesky decomposition of positive definite matrices. First they were applied to the decomposition of the energy denominators appearing in the CCSD(T) formulae. Secondly, a similar technique has been used to Cholesky decompose two-electron integrals taking then profit of their sparsity when considered as a regular matrix with compound indices. This part of the project has been developed in collaboration with the Odense node and will be finished by Thomas Pedersen during his postdoc stay in Valencia from July 1st. We are now starting the study of NMR spectra of HCP and derivatives in collaboration with the Mainz node.

**P3 U-Santiago de Compostela** Development of gauge invariant coupled cluster theory: Using the time-dependent Lagrangian response approach, a gauge invariant coupled cluster model has been formulated based on non-orthogonal orbital rotations. This work has been done in collaboration with the node in Odense. Applications of the coupled cluster theory has also been made for studying van der Waals complexes. We started considering the reduction in the scaling for the SCF and correlated models like the CCSD, using the Cholesky decomposition of the two-electron integrals. Collaboration with the nodes of Odense and Valencia.

**P4 U-Mainz** The node at Mainz investigated the performance of a CC hierarchy consisting of CCSD, C-C3, and CCSDT for the calculation of indirect spin-spin coupling constants. It is concluded that the CC3 model with orbital relaxation effects excluded is well suited for the inclusion of triple excitation effects in coupled-cluster calculation of spin-spin coupling constants. Application of the developed CC schemes in the calculation of spin-spin coupling constants are planned (in collaboration with other nodes) for the next period. The nodes at Mainz and Pisa developed schemes for CC calculations of mixed electric and magnetic properties employing CC response theory techniques. The developed schemes have been ap-

plied to the calculation of shielding polarizabilities. The theory for second energy derivatives for CCSD linear response theory has been worked out and is currently implemented.

**P5-Modena** The analytic procedure of continuous transformation of the origin of the current density-diamagnetic term to zero (CTOCD-DZ) for the calculation of magnetic susceptibility and nuclear magnetic shielding has been implemented within the DALTON code. An extended numerical test has been carried out on a series of molecules. This work is done in collaboration with the University of Copenhagen (Odense node). Implementation of CTOCD-DZ method for hypermagnetizabilities is also being developed. New graphical codes have been implemented for representation of streamlines and modulus of the current density induced by a magnetic field in the electrons of a molecule.

**P6 CNR-Pisa** We have studied electric, magnetic and optical properties in molecules, in collaboration with other nodes. Study of the non-additive two and three body contribution to dispersion energies and electric properties in rare gases, N<sub>2</sub> and H<sub>2</sub>, with CC response techniques (collaboration with the Odense node). Determination of the first virial coefficients for magnetizability, chemical shielding, electric dipole polarizability and Cotton-Mouton birefringence (collaboration with the Oslo node and first results obtained in the training of the YR in Pisa). Study of the effect of static electric fields on the chemical shift of some two- and three-atomic systems (collaboration with Mainz node). Study of the magnetizability and electric dipole polarizability anisotropies of CO<sub>2</sub>, CS<sub>2</sub>, OCS and N<sub>2</sub>O, and of their hypermagnetizability anisotropies. (collaboration with the Stockholm and Oslo nodes).

**P7 U.Helsinki** A new *ab initio* program package for calculation of the optical properties of strain-induced quantum dots is being developed. This is the first *ab initio* program package for large-scale correlated calculations on strain-induced quantum dots. The new program package allows full configuration interaction studies of the energy levels and photoluminescence spectra of quantum dots containing 1-4 excitons. The methods have been used for studying the energy levels, photon relaxation rates, and photon recombination rates of excitons, biexcitons and triexcitons confined a InGaAs/GaAs strain-induced quantum dot. The calculations show that the electron-hole correlation effects increase the radiative recombination rate and significantly affect the recombination trends as a function of the dot size. The calculated stabilization energies suggest the formation of multi-exciton complexes.

**P8 U.Odense** The development of reduced scaling coupled cluster algorithms are proceeding as planned. The Cholesky decomposition of the two-electron integrals is now operational, this part of the project has been delayed due to complications related to numerical stability of the algorithm. Next phase will be the implementation of coupled cluster singles and doubles model using the decomposed integrals. Relativistic 4-component RPA has been implemented, both for frequency dependent properties and for excitation energies and transition moments as well as for quadratic response frequency dependent properties. Relativistic 4-component MCSCF has been implemented and works, work is still needed to optimize some parts of the code. Electron spin resonance Relativistic 4-component calculation of ESR g-tensors has been implemented on the Hartree-Fock level.

**P9 U-Oslo** The Oslo node has worked on the implementation of the fast multipole method (FMM) in Dalton. A model implementation is now in place, in which the non-classical Coulomb contributions are calculated by a naive multipole expansion (which scales quadratically with system size). The FMM method will be implemented in the coming academic year. b) In collaboration with the Aarhus node, the Oslo node has worked on methods for the optimization of Hartree-Fock/DFT without diagonalization.

Our method, which is based on an exponential parametrization of the AO density matrix, now works in a model implementation. True linear scaling will be reached as soon as sparse matrix routines (for addition and multiplications) are implemented in Dalton. c) The Oslo node has implemented in Dalton the integrals that are needed in order to carry out gauge-origin independent magneto-optical activity within the coupled-cluster framework. Calculations are presently being carried out. d) Much work has been devoted to the development of the DFT code, some in collaboration with the Stockholm node.

## A.2 Joint Publications

The partner collaboration is listed. Young Researchers are presented in boldface.

1. P1, P6. **P. Salek**, V. Carravetta, H. Ågren, et al., Dynamical suppression of atomic peaks in resonant dissociative photoemission, *Chem. Phys. Lett.* 00, 000 (2001).
2. P1, P6, P9. **O. Plashkevych**, T. Privalov, H. Ågren, V. Carravetta, and **K. Ruud**, On the validity of the equivalent cores approximation for computing X-ray photoemission and photoabsorption spectral bands, *Chemical Physics*, 260, 11 (2000).
3. P1, P4, P6, P9. **D. Jonsson**, **P. Norman**, H. Ågren, A. Rizzo, **S. Coriani**, and **K. Ruud**, The Cotton-Mouton effect of gaseous CO<sub>2</sub>, N<sub>2</sub>O, OCS and CS<sub>2</sub>. A Cubic Response MCSCF study, *J. Chem. Phys.* 114, 8372 (2001).
4. P1, P8, P9. **P. Norman**, B. Schimmelpfennig, **K. Ruud**, H.J.Aa. Jensen, and H. Ågren, Relativistic effects on linear and non-linear polarizabilities studied by Douglas-Kroll and Dirac-Fock response theory calculations, Submitted.
5. P2, P8. H. Koch and A. Sanchez de Meras, Size-intensive decomposition of orbital energy denominators, *J. Chem. Phys.*, 113(2) 508 (2000).
6. P2, P8. A. Sanchez de Meras, I. Garcia Cuesta and H. Koch, A coupled cluster calculation of the spectrum of urea, *Chem. Phys. Lett.* 00, 000 (2001).
7. P3, P8 **T. B. Pedersen**, B. Fernandez and H. Koch, Comment on 'The importance of higher-order correlation effects for the CO-CO interaction potential', *Chem. Phys. Lett.*, 334, 419-423 (2001).
8. P3, P8 **J.K. Pedersen**, H. Koch and B. Fernandez, Basis set convergence of three-body interactions in He<sub>3</sub>, Ne<sub>3</sub> and Ar<sub>3</sub>, *Theor. Chem. Acta*, in press.
9. P4, P6 A. Rizzo and J. Gauss, CCSD(T) Shielding Polarizabilities, *J. Chem. Phys.*, to be submitted.
10. P4, P8, P9 **K. L. Bak**, P. Jørgensen, J. Olsen, T. Helgaker and J. Gauss, Coupled-cluster singles, doubles and triples (CCSDT) calculations of atomization energies, *Chem. Phys. Lett.* 317, 116-122 (2000).
11. P6, P8 A. Rizzo, **K. Ruud**, D. M. Bishop, Intermolecular interactions and the Cotton-Mouton effect (CME) for helium, *Mol. Phys.*, submitted.

12. P6, P8 M. Jaszunski, A. Rizzo, P. Jørgensen, Coupled Cluster calculation of dispersion contributions to interaction energies and polarizabilities, *Theor. Chem. Acc.*, in print.
13. P7, P8 **M. Braskén, M. Lindberg**, D. Sundholm, J. Olsen, Full Configuration Interaction Calculations of Electron-hole Correlation Effects in Strain-induced Quantum Dots, *Phys. Rev. B* 61 (2000) 7652.
14. P7, P8 **M. Braskén, M. Lindberg**, D. Sundholm, J. Olsen, Carrier-Carrier Correlations in Strain-Induced Quantum Dots, *Phys. Stat. Sol. (b)* 221 (2000) 37.
15. P7, P8 **M. Braskén, M. Lindberg**, D. Sundholm, J. Olsen, Full Configuration Interaction Calculations of Electron-hole Correlation Effects in Strain-induced Quantum Dots, *Phys. Stat. Sol. (b)* 224 (2001) 775.
16. P4, P8 **A. Halkier**, T. Helgaker, W. Klopper, and J. Olsen, Basis-set convergence of the two-electron Darwin term, *Chem. Phys. Lett.* 319, 287-295 (2000).
17. P4, P8 **K. L. Bak**, P. Jørgensen, J. Olsen, T. Helgaker, and W. Klopper, Accuracy of atomization energies and reaction enthalpies in standard and extrapolated electronic wave function/basis set calculations, *J. Chem. Phys.* 112, 9229-9242 (2000).
18. P4, P8 T. Helgaker, **H. Larsen**, J. Olsen, and P. Jørgensen, Direct optimization of the AO density matrix in Hartree-Fock and Kohn-Sham theories, *Chem. Phys. Lett.* 327, 397-403 (2000).
19. P4, P8 **S. Coriani, C. Hättig**, P. Jørgensen, and T. Helgaker, Gauge-origin independent magneto-optical activity within coupled cluster response theory, *J. Chem. Phys.* 113, 3561-3572 (2000).
20. P4, P8 **H. Larsen**, P. Jørgensen, J. Olsen, and T. Helgaker, Hartree-Fock and Kohn-Sham atomic-orbital based time-dependent response theory, *J. Chem. Phys.* 113, 8908-8917 (2000).
21. P4, P8 **K. L. Bak, A. Halkier**, P. Jørgensen, J. Olsen, T. Helgaker, and W. Klopper, Chemical accuracy from "Coulomb-hole" extrapolated molecular quantum-mechanical calculations, *J. Mol. Structure*, in press.

## Part B

# Comparison with the joint program of work

## B.1 Research Objectives

The research objectives - both the low- and the high-end objectives as defined by Annex I of the contract - have been maintained without any significant changes. Thus theoretical work referring to basic science as well as applications of the theory have progressed. This holds for all the milestone items, like coupled cluster theory (milestone 4) and relativistic theory (milestone 2). Many of the remaining "holes" in the 4th order property toolbox (milestone nr 1) have also been filled in. This refers especially to magnetic

and magnetic resonance properties. Several new interaction phenomena have thus been derived and implemented in the response theory framework; magnetic  $g$ -tensors, and new spin-spin coupling modules, to mention two examples. We can here also stress the implementation of relativistic 4-component calculations of ESR parameters as a particularly rewarding example. The computation and the viewing of current densities have progressed along the planned lines of research.

The correlated techniques have been broadened especially concerning the coupled cluster methodologies. The reduced scaling demand has also been met to some extent by means of new algorithms (c.f. milestone 3). The reduced scaling will here also benefit from the so-called density matrix algorithms that now have been derived, and which will have particularly rewarding consequences for density functional applications within the network. Much work is evidently still needed to fulfill this milestone goal, and most of it is still ahead. During the year which has elapsed since the commencement date we have also witnessed an interesting development of *time-dependent* density functional theory and implementations within the network, as was actually envisaged but yet not proven at the time of the contract negotiation. We expect several novel applications to follow from this development, and which are important for the high-end goals of the network.

We emphasize also the development with the relativistic methodologies (milestone 2). The advanced four-component Dirac method now also encompasses multi-configurational self-consistent field wave functions, something truly unique in its kind. Several simplifying relativistic schemes, e.g. the Douglas-Kroll technique, have been tried out in conjunction with property calculations, with the purpose to gain efficiency without losing too much accuracy. With the DIRAC program available these techniques can be thoroughly benchmarked. Although this research focuses on basic matters, the goal of efficiency and applicability evidently holds also for the relativistic methodologies.

Concerning milestone 2, focusing on actual materials applications, we have also advanced our front line. This goes especially for optical limiting applications with the toolbox, as well as with the newly developed methodology for quantum dot systems. In the case of optical limiting, the research has already arrived at some new compounds that have been suggested for synthesis. Much collaborative work is still needed emphasizing also new basic issues in this research. With respect to the milestone point on second harmonic generation we have reached some preliminary results, but most work in this area still lies ahead.

Concerning properties of extended systems and materials the efforts for modeling environmental (solvent) effects should also be stressed, since these give clear possibilities for future large scale applications using the property toolbox. The so-called polarized continuum model has thus been incorporated as well as a new "QM-MM" (Quantum mechanics - molecular mechanics) methodology. We anticipate many useful applications of both these lines of methodological developments.

## B.2 Research Method

The aim with the MOLPROP research is to develop its own research tools. In this sense there will continuously be changes of the research method, or methods, employed. These methods fall under the broad context of first principle "ab initio" methods for molecular modeling. They have during the

passed year been further advanced along the proposed lines, with some obvious corrections and improvements of the original planning. The main project objective for the research methods thus remains as stated, namely to develop them as such, using the tools of quantum theory, algebra and numerical analysis. The method development has followed the proposed hierarchical way with the goal to converge computational results in a controlled manner and so to make possible meaningful interpretations of experimental data and to use rigorous computational criteria for these interpretations. This holds especially for the coupled cluster methodology, on which much efforts are devoted in the network (5 nodes). Our aim to develop the technology necessary for open-ended, ab-initio black-box calculations of molecular properties from first principles thus remains.

The proposed research method of density functional theory (DFT), which at the time of the contract was quite "new" to us, has been pursued along the planned line with an implementation that matches our "ab initio" toolbox to quite a considerable extent. This promising development, which indeed has broadened the scope of the network, thus fits well with our experience with ab initio time-dependent response theory, and will, together with the proposed linear scaling techniques, form a basis for "high end" applications on the outlined technically relevant problems. In this respect our research methodology has developed as proposed, or, in fact, even advanced further than that. Apart for the coupled cluster-, DFT-, relativistic- and solvent methodologies, we also mention briefly the dynamical methods ("direct dynamics") that have been addressed basically along the lines indicated in Annex I of the contract.

A strong focus is still put on the response methods for calculations of *linear and non-linear properties and spectra*. with a wide variety of applications involving linear and non-linear electromagnetic properties, being time-dependent or time-independent, originating from hyperfine interactions or external fields. Some of the properties have a very strong potential for technical applications and for material science. Several new types of such properties have during the passed year been collected in the gauge-invariant fourth order property toolbox, referring to both variational (SCF, MCSCF, DFT) and perturbational (MP, coupled cluster) wave functions. Among them we can also mention the magnetic resonance parameters (NMR and EPR) for which we produced new algorithms and codes.

## **B.3 Work Plan**

### **B.3.1 Breakdown of tasks**

In the following we comment briefly the work plan, in particular any changes from the Technical Annex.

#### **B.3.1.1 Gauge-invariant fourth order property toolbox**

Several new properties have been coded, both for variational and perturbational wave functions. We emphasize several new results with magnetic, hyperfine and excited state properties.

### B.3.1.2 Relativistic formulations

The planned line of research is followed, and has even advanced beyond the plan. For example, the Dirac-Fock implementation of non-linear electric properties is now working. Also several simplifying relativistic models have been implemented and applied.

### B.3.1.3 Linear scaling and density functional theory

New *linear scaling* scaling algorithms have been derived basing on density matrix optimization and tested in model calculations. The goal to derive a new *time-dependent density functional code* has already been fulfilled to a significant extent. Solvent models have been implemented, "PCM", "QCMM" and "semiclassical" models.

### B.3.1.4 Response theory in the time domain

A full-fledged response theory program in the time domain is a considerable undertaking. We have some results with tight-binding models, but not more than that so far.

### B.3.1.5 Direct dynamics

We have derived time-dependent techniques for nuclear dynamics and implemented these for computations in connection with femto-second spectroscopy. We have taken particular interest in wave packet techniques for X-ray Raman scattering used to interpret pulsed synchrotron radiation experiments. The excited state EOM-CC method has benefitted from new algorithms for excited state gradients and Hessians.

### B.3.1.6 Nuclear magnetic spin resonance

We have during the year published several papers for magnetic resonance parameters both within coupled cluster and density functional technologies, the latter represent a development that is very new within the network.

### B.3.1.7 Electron spin resonance

Also ESR theory and codes have been developed to a quite large extent during the year. This goes for g-tensors, spin-spin coupling strengths and zero-field parameters. The diagnostic capability of ESR has been exploited also for bio-radicals as simulated using these new routines. A fully relativistic implementation for g-tensors has also been accomplished.

Table 1: Schedule and fulfillment of tasks during moths 1-12

<i>Months</i>	<i>Projctcs</i>	<i>Comment</i>
<b>1- Fourth order Toolbox</b>		
1-12	MCSCF and CC third and fourth order properties	Going well - 4
1-12	CC applications of excited state properties	New algorithms derived - 4
<b>Relativistic Formulations</b>		
1-12	Relativistic RPA - including applications	Done to the point - 5
6-12	Relativistic four-component, 2nd order MCSCF	Formulation + some results - 3
<b>Reduced Scaling correlated methods</b>		
1-12	TD-DFT spectra and properties	Formulated - 3
1-18	Reduced Scaling in CC	Some reduction obtained - 2
<b>NLO properties and materials</b>		
1-12	Multi-photon and optical limiting	Rich results - 5
1-12	SHG and Kerr materials	No focus yet - 1
<b>Direct Dynamics</b>		
1-12	Interface to EOM-CC	The EOM-CC part developed - 3
<b>Nuclear Magnetic Resonance</b>		
1-12	CC hierarchy for spin-spin couplings	Well met - 4
<b>Electron Spin Resonance</b>		
1-12	Benchmarking	Much development - 5
<b>Non-uniform fields modeling</b>		
1-12	Topological features of current densities	New program - 4
<b>Chirality and Dichroism</b>		
1-12	MCD and Magnetic Optical Dichroism	Several Papers - 3

### B.3.1.8 Non-uniform fields

Development within this area has taken place during the year, especially for the visualization of magnetic field induced current densities. This has been made possible by a production of new graphical codes within the network, giving qualitative interpretations of paths whereby the spin and density information passes through the molecules.

### B.3.1.9 Chirality and dichroism

Dichroic properties -either natural or field induced- can be well studied by the proposed response theory techniques, a fact that has been utilized in some of the network projects. The challenge of using natural dichroism in the X-ray region has also to some extent been met, with applications performed for the common amino acids.

## B.3.2 Schedule

In Table 1 we specify the degree of fulfillment of the Schedule outlined concerning months 1-12 in section 3.2 of the technical Annex. In the rightmost column a comment is given and a digit 0-5, where 5 denotes what we regard as a perfect fulfillment of the plan.

### **B.3.3 Milestones**

The degree of milestone fulfillment was commented already in Part A (Scientific Highlights). We recapitulate the main points here.

#### **B.3.3.1 Fourth order property toolbox**

Several new properties have been included in the toolbox, which basically now is completed for electric field properties. Although outside the midterm milestones, also relativistic and density functional properties - analogous to the non-relativistic ab initio ones - have been put in.

#### **B.3.3.2 Non-linear optical properties and materials**

The midterm milestone for optical limiting has almost been completed already, while only few results have been obtained for second harmonic generation. The codes work excellently for the latter, and we have good faith in fulfilling also this part of the milestone at mid-term.

#### **B.3.3.3 Relativistic formulations**

i) 1-component theory - fulfilled; ii) Electric properties 2-component theory - ground work carried out; iii) Full one-electron implementation for 4-component theory - fulfilled.

#### **B.3.3.4 Reduced scaling in correlated methods**

Most work has focused on the formal part, with the development of new algorithms. For density functional and Hartree-Fock based properties we look optimistic upon fulfilling the midterm milestone. For coupled cluster some reduction has been achieved, but the final amount of reduction obtainable is still difficult to foresee.

### **B.3.4 Research effort of the participants**

Table 2: Professional research effort on the network project (man-months)

<i>Participant</i>	<i>YR Months delivered</i>	<i>From other sources</i>	<i>Total individuals</i>
1	4.5	38	7
2	0	24	5
3	12	16	3
4	2	15	3
5	0	15	3
6	1.5	17	3
7	1.5	15	2
8	3.5	68	12
9	0	36	6
Totals	25	244	42

## B.4 Organization and Management

### B.4.1 Network organization

The possibilities of the international telecommunications have been exploited as much as possible. Firstly, a link has been created from the main CORDIS homepage to a local home page (<http://www.theochem.kth.se/molprop/>) for special and detailed network information. This home page has frequently been used by the participants as a working array to report on employments, organized meetings, meeting attendance, visits, and other network activities. A special part (sealed with a password) of the home page contains financial network information for the node leaders. The home page also provides links to the individual URL addresses of the partners. MOLPROP announcements and information are canalized through this home page (as a complement to the CORDIS page). The home page is thus constantly updated by the partners, but with the coordinator obviously having the overall responsibility.

Secondly, we have used the page/ mailing list that already exists for the DALTON program system, which is the main common main software system of the network. Much of the actual scientific activity, correspondence, results presentations, benchmarking, program discussions, dissemination and updates takes place in connection with the "DALTON" program and through the use of its home page (<http://www.kjemi.uio.no/software/dalton/dalton.html>).

#### B.4.1.1 List of partner home pages

1. P1- Hans Ågren, Royal Institute of Technology, Stockholm  
URL: <http://www.theochem.kth.se/html/agren/>
2. P2-Alfredo M.J. Sanchez de Meras, Universitat de Valencia  
URL: <http://www.uv.es/~uvalen/eng/>
3. P3-Berta Fernandez Rodriguez, Universitat de Santiago de Compostela  
URL: <http://www.usc.es/qfweb/grupesp.html.qch>
4. P4-Jurgen Gauss, Universität Mainz  
URL: <http://www.uni-mainz.de/FB/Chemie/AG-Theoretische/>

5. P5-Paolo Lazzaretti, University of Modena  
URL: <http://www.chimica.unimo.it/lazzaretti.html>
6. P6-Antonio Rizzo, Istituto di Chimica Quantistica ed Energetica Molecolare del C.N.R., Pisa  
URL: <http://www.icqem.pi.cnr.it/rizzo/ar.html>
7. P7-Dr. Dage Sundholm, University of Helsinki  
URL: <http://www.chem.helsinki.fi/~sundholm/>
8. P8-Hans Jørgen Aa. Jensen, University of Southern Denmark  
URL: <http://www.sdu.dk/Nat/Chem/staff/sci/Hja.html>
9. P9-Trygve Helgaker, University of Oslo  
URL: <http://www.uio.no/~trygve/>

## B.4.2 Network meetings

### B.4.2.1 2000-05-28/29: First MOLPROP network meeting

Time : 28-29 May, 2000.

Lectures: 15 lectures plus 2 Discussion sessions

The meeting comprised 43 participants representing all 9 nodes of the Network.

This first MOLPROP network meeting took place in Stockholm, more precisely on the island of Lindingö, which is a suburb located half an hour from Stockholm city. The meeting was run in series with the EU COST/D9 meeting in "Molecules in mixed condensed media", at the Royal Institute of Technology, Stockholm, 26-27 May.

During the meeting talks with recent results were presented on subjects that overlapped with the contracted scientific goals of the network. The final afternoon of the meeting was devoted to discussion and planning of the network, especially on the training content and hiring of Young Researchers.

A full program can be found at: <http://www.theochem.kth.se/events/molprop/program.html>

The full (signed) participant list can be found at: <http://www.theochem.kth.se/molprop/arch/list1.pdf>.

### B.4.2.2 2000-12-11/15 Winter School in Theoretical Chemistry 2000

Time : 11-15 December, 2000.

Title: MAGNETIC PROPERTIES OF MOLECULES

Lectures: 24 lectures plus poster presentations

65 PARTICIPANTS: 35 of them belonging to MOLPROP

11 LECTURERS: 10 of them belonging to MOLPROP

The full program can be found at: <http://www.chem.helsinki.fi/Info/WinterSchool/ws2000.html>

The full (signed) participant list can be found at: <http://www.theochem.kth.se/molprop/arch/list2.pdf>.

This was the first of the yearly Winter Schools organized by partner 7, and with lecturers and participations from the MOLPROP network. It focuses each year on a subject that is central to the network goals and with strong participation of the MOLPROP YRs. The YRs even contribute as lecturers (4 of them this time, see program above).

#### B.4.2.3 2001-01-25/27 First MOLPROP Workshop Meeting in Santiago de Compostela

Time : 25-27 January, 2001.

Lectures: 21 lectures plus 3 Discussion/ Group work sessions

42 Participants.

In this workshop the first new results from the network were presented and discussed. YR presentations were also made. Much of the time was devoted to group work and group presentations focusing on different aspects of the network research goals. Future directions of the work was debated and some revisions and augmentations of the work plan were suggested. Exchange of information was provided, especially concerning the possibilities to fill the remaining holes for the YR employments, for which there was consensus to help each other out.

Full program can be found at: [http://www.theochem.kth.se/molprop/extras/program\\_Santiago2.html](http://www.theochem.kth.se/molprop/extras/program_Santiago2.html)

The full (signed) participant list can be found at: <http://www.theochem.kth.se/molprop/arch/list3.pdf>.

### B.4.3 Networking

The visits among senior and junior researchers have been very frequent. We have 18 longer research visits, node to node, reported, see list below.

1. 2000-11-20: Vincenzo Carravetta (Pisa) visited Stockholm node during 22/9 to 6/10 2000 to work on theory and code for multi-atom resonant photoemission.
2. 2000-07-10: Dr. Henrik Koch (Odense) visited Valencia during three weeks for developing C-holesky decomposition of two-electron
3. 2000-12-02: 2-7/12 Jeppe Olsen visited the Helsinki node for work on quantum dots.
4. 2001-06-07: Visit of Dan Jonsson (YR, Mainz) to Oslo from 2001-03-29 to to work on the implementation of integral direct response theory for high-spin restricted open-shell HF within the Dalton program package travel.
5. 2001-05-29: Visit of J. Gauss (Mainz) to Pisa (5/5/2001-9/5/2001) to collaborate with A. Rizzo on coupled-cluster calculations of mixed electric-magnetic properties.

6. 2001-01-08: Dage Sundholm (Helsinki) visited Mainz 16-23.10.2000
7. 2001-01-28: 28/1 - 11/2. Visit by Antonio Rizzo to Santiago de Compostela, Spain for a total of thirteen days.
8. 2001-05-22: 22-28/5 Hans Ågren (Stockholm) visit to Pisa, in collaboration with the V. Carravetta and A. Rizzo.
9. 2001-05-27: 27/5-3/6 Helena Larsen (YR, Odense) visited the Oslo node to work with Trygve Helgaker.
10. 2001-01-02: Visit of Christof Hättig (YR) to Oslo 12.11.00-24.11.00
11. 2001-01-02: Visit of Mark Watson (YR) to Oslo 10.10.00 - 24.10.00
12. 2001-01-02: Visit of Sonia Coriani(YR, Odense) to Oslo 12.11.00-24.11.00
13. 2001-01-02: Mark Watson (YR): Visit to Oslo 08.12.00-21.12.00
14. 2001-02-28: Visit of Torgeir Ruden (YR, Oslo) to Aarhus, Denmark 05.02.01 - 17.02.01
15. 2001-04-30: Jeppe Olsen (Odense) visited Helsinki 3.12.2000-7.12.2000.
16. 2001-01-16: 16-21/1 Kenneth Ruud (YR, Oslo), visited Stockholm to work on electron spin spin coupling integrals.
17. 2001-02-19: 19/2 -3/3 Oscar Rubio (YR, Valencia) visited Stockholm to do response calculations on some naphthalene species.
18. 2001-04-26: 26/4-5/5 Kenneth Ruud (YR, Oslo), visited Stockholm to work on Douglas-Kroll implementation in Dalton.

## B.5 Training

### B.5.1 Vacancies

Vacancies in the YR program have been advertised on the MOLPROP home page, with links from the personal home pages of the individual scientists in the network and from the pages of the institutions to which they belong. Proper advertisement has also been made through the channels provided by CORDIS. The frequent meeting attendance by MOLPROP members has given give special possibilities to announce the positions.

### B.5.2 Recruitment of YRs

Despite some initial recruitment problems and the early commencement date, it seems that to date all recruitment have been made, and the empty boxes in the Table above have been filled (some discussion about the candidature to the Post-Doc position at node 8 is still being made). Thus Oslo

Table 3: Hiring of Young Researchers (Months)

Participant	Contract deliverable of Young Researchers to be financed by the contract (person-months)			Young Researchers financed by the contract so far (person-months)		
	Pre-doc (a)	Post-doc (b)	Total (a+b)	Pre-doc (c)	Post-doc (d)	Total (c+d)
P1-Stockholm	4.5		4.5	24		24
P2-Valencia					24	24
P3-Santiago		12	12		24	24
P4-Mainz		2	2		24	24
P5-Modena					24	24
P6-Pisa		1.5	1.5	24		24
P7-Helsinki	1.5		1.5		24	24
P8-Odense	3.5		3.5	36	12	48
P9-Oslo				36		36
Total	9.5	15.5	25	120	132	252

node (P9) has hired a Post-Doc from 1/7 2001 (Mark Watson, England); the Valencia node has hired a Post-Doc Tomas Pedersen (Odense, Denmark) from 1/7 and the Modena node has contact with an Hungarian female PhD student who most likely will start there in August 2001.

### B.5.3 Integration of YRs

As shown in B.4.3 there has been a strong participation of YRs in the visit program (11 Young Researcher visits). The participation of the YRs in the 3 network meetings has amounted to about 30 each (more if YRs not affiliated with the network nodes are counted). Several publications have been outlined involving the YRs, 17 such publications have already been obtained.

### B.5.4 Special measures

Apart from the integration of the YRs in the specified network research projects, we have actively stimulated the YRs to participate in the meetings (especially the 3 network meetings), and to give talks or posters at these meetings. About 15 YR oral presentations have been made so far. All this have been accounted for in the foregoing. We have also tried to activate them as much as possible in the editing and preparation of the research papers which they coauthor.

We have faced problems to fulfill the rather ambitious twinning program, mostly due to that the recruitment dates have come out so different. The early commencement date was also an obstacle in this respect.

### B.5.5 Equal opportunities

We do have made special efforts to recruit female students, however, since the recruitment situation initially was problematic we were forced to take a somewhat pragmatic view in this context. Node 5 will now recruit a female pre-doctor.

### B.5.6 Multidisciplinarity

The fields covered by the network projects are quite versatile; mathematics, numerical analysis, quantum mechanics, and scientific computing. We have objectives covering basic science as well as materials applications. We have tried to emphasize this in the network meetings and visits involving the YRs, so they are trained (at least) in computing and programming as well as in theory.

### B.5.7 Industrial connections

No connections utilized so far.

## B.6 Difficulties

We, ourselves, consider the network already to be a success in most aspects; science, training, meetings, visits, and collaboration in general. There has been a lot of enthusiasm and good spirits among the partners. This, we feel, is not surprising since it owes to the close connections between most of the nodes that already were established, in some cases since a long time. This fact has also greatly alleviated the coordination of the network. We have great confidence in the further success in the scientific part and in the training.

The major difficulty is, or was, the recruitment. After the contract negotiation it took a long time to sign the contract (almost a year, which is along time compared to the duration time of three years), and to settle the commencement date. This date was finally moved to an early, "immediate", date in order to allow for the first network meeting to take place at a suitable time. In retrospect this was a mistake. The initial problems to hire the YRs to the network refer to great extent to these planning issues which initially created confusion when to start. This also rendered difficulties in implementing our quite ambitious twinning program and to send network YRs to the first summer school (SOSTRUP), staffed and organized by the partners, and which took place only 1.5 months after the pre-dated commencement. A further, somewhat smaller, problem was the delay in two months of forwarding of advanced payments to the nodes, which owes to a failure at the local administration office at the university of the coordinator.

Now with all positions filled, we are fully confident that, if not something unexpected happens, the full quota of 252 YR months *will* be delivered by the network.

### B.6.1 Explanation of Cost Statement Summary - Part E-3

The fact that the first network meeting took place before the advanced payment was delivered changed the advanced payment as follows: Of the full cost of this meeting (25,975 Euro), 8,035 Euro was covered directly by the arranging node (node 1). The remaining part was allocated to each node according to their meeting costs, and then subtracted from their coming advanced payments. This is the reason that the nodes are allocated a somewhat smaller advanced payment than the 40 % of their contracted total contribution, see Part E-3 in the cost statement summary. The corresponding cost 17,939 Euro is reported in E-3 as an extra network cost for node 1.