

Curriculum vitae Kenneth Ruud

Name: Kenneth Ruud

Born: September 16 1969, Fredrikstad, Norway

Nationality: Norwegian

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Cand.mag.: June 1990

Cand.scient.: June 1993

Dr.Philos.: October 1998

Military Service:

January—November 1993 at the Norwegian Defense Research Establishment

Positions:

- Director of the Center of Theoretical and Computational Chemistry, a Norwegian Center of Excellence, 2007–
- Head of the Department of Chemistry, University of Tromsø 2005-2007
- Professor, Department of Chemistry, University of Tromsø, 2002-present
- Associate professor (førsteamanuensis), Department of Chemistry, University of Tromsø, 2001-2002
- Postdoctoral researcher at University of Tromsø (awarded by the Norwegian Research Council) 2000-2001
- Postdoctoral researcher at San Diego Supercomputer Center/University of California at San Diego (awarded by the Norwegian Research Council) 1998–2000
- Assistant lecturer, Department of Chemistry, University of Oslo, 1993–1998

Publications:

222 papers published or accepted for publication in international journals with a referee system, and have as of June 21 2012 been cited a total of 6180 times, and have a Hirsch index of 43. The most highly cited paper has received 794 citations.

Awards and Honors:

- Elected member of the Norwegian Academy of Science and Letters 2012
- ERC Starting Grant, 2011 for the project SURFSPEC: “Theoretical multiphoton spectroscopy for understanding surfaces and interfaces”, 1.5 MEuros
- Dirac Medal 2008 “for the outstanding computational chemist in the world under the age of 40” awarded by the World Association of Theoretical and Computation Chemists (WATOC)

- Research Prize for Young Researchers at the University of Tromsø, awarded by the University of Tromsø, 2005.
- Outstanding Young Investigator Award 2004, awarded by the Norwegian Research Council. Research grant of approx. 7 MNok.
- A/S Norsk Varekrigsforsikrings Fonds prize award 1996
- Hafslund/Nycomeds Pris til Unge Forskere 1993 (Hafslund/Nycomeds award to young scientists)
- Norsk Hydros Pris for Fremragende Studieresultater 1991 (Norsk Hydros award for excellent achievements in lower grade studies)
- Bronze medal in the International Chemistry Olympiad, Helsinki (Finland) 1988

Major grants awarded:

- Relativistic two- and four-component density functional theory with periodic boundary conditions, Research Council of Norway 2012-2016, 0.73 Mill. Euros
- Analytic calculations of higher-order molecular properties, Research Council of Norway 2009–2013, 0.85 Mill. Euros
- Project manager of a Norwegian Center of Excellence (Center of Theoretical and Computational Chemistry) established by the Research Council of Norway 2007–2017, annual grant of 1.25 Mill. Euros.
- Vibronic contributions to higher-order molecular properties, Research Council of Norway 2008–2011, 0.67 Mill. Euros
- Coordinator of a strategic University Program in Quantum Chemistry 2003–2007. 1.2 Mill Euros, 4 partners. Awarded by the Norwegian Research Council.
- Partner in a Norwegian theoretical chemistry initiative in Nanomaterial modelling, 1.2 Mill Euros, 2003–2006. 5 partners. Awarded by the Norwegian Research Council.
- Member of the EU Research-Training Network “Nanoquant”, 1.9 Mill.Euros 2004–2007. Awarded by the European Commission
- Partner in a Nordic Research Network “QMMM”, 100 kEuros. 2004–2006. 6 partners. Awarded by the Nordic Research Academy.

Served on the editorial advisory board of:

- International Journal of Quantum Chemistry 2008–
- Research Letters in Physical Chemistry 2009–

Conferences, invited speaker: Invited speaker on 57 occasions from 1997–2011 at international conferences in the domain of computational and theoretical chemistry, of which one as a plenary lecturer.

International schools, organizer:

- “Quantum Chemical Winter School Response Properties of Molecular Materials.” Chamonix January 25–29 2010. Co-organized with Patrick Norman and Trond Saue. 43 participants (9 lectures).

International schools, lecturer:

- Winter school in Theoretical Chemistry (“Calculation of NMR parameters”), Helsinki (Finland), December 11-14, 1995 (2 lectures)

- Workshop on Theoretical Chemistry (Molecular Properties) in Mariapfarr 2006 (Austria), February 14–17 2006.

International schools attended:

- European Summer School in Quantum Chemistry, Tjörnarp (Sweden) 1991, 2 weeks, poster
- Second Sostrup Summer School, Sostrup Slot (Denmark) 1992, 2 weeks, poster
- Ph.D.-course in Parallel Computations — Theory and Practice, Bergen (Norway) 1995, 2 weeks
- Ph.D.-course in Molecular Dynamics, Laser and Photochemistry, Fuglesøcentret (Denmark) 1995, 2 weeks, talk
- Winter school in Theoretical Chemistry (“Solvation”), Helsinki (Finland), December 11–14, 1997
- Winter school in Theoretical Chemistry (“Chemical Reactions”), Helsinki (Finland), December 14–17, 1998

Long-term visits:

- University of Linköping (Sweden), January–December 1997

Referee:

I have acted as a referee of research proposals in Chemistry submitted to the Finnish Academy of Sciences 2004, and as a member in the Scientific Committee for proposal submitted to the Norwegian Research Council in Natural Sciences in 2005.

I have in addition acted as referee of scientific papers for a large number of scientific journals:

- Chemical Physics
- Chemical Physics Letters
- Chemical Communications
- ChemPhysChem
- Chirality
- Collection of Czechoslovak Chemical Communications
- Computer Physics Communications
- Dalton Transactions
- Inorganic Chemistry
- International Journal of Quantum Chemistry
- Journal of the American Chemical Society
- Journal of Chemical Physics
- Journal of Chemical Theory and Computation
- Journal of Computational Chemistry
- Journal of Molecular Structure (THEOCHEM)
- Journal of Organic Chemistry
- Journal of Physical Chemistry (**A** and **B**)
- Macromolecules
- Magnetic Resonance in Chemistry

- Molecular Physics
- New Journal of Chemistry
- Physical Chemistry Chemical Physics
- Physical Chemistry Communications
- Surface Science
- Theoretical Chemistry Accounts
- Tetrahedron Asymmetry

Master students supervised:

- Hanne Heiberg (Cand.Scient.–Dec.96 University of Oslo, cosupervisor with prof.Trygve Helgaker)
- Chris Mohn (Cand.Scient.–June-01 University of Oslo, cosupervisor with prof.Trygve Helgaker)
- Andreas J. Thorvaldsen (Master–November 2003, University of Tromsø)
- Harald Solheim (Cand.Scient.–December 2003 , University of Tromsø, with Prof. Odd Gropen as cosupervisor)
- Marco Anelli (MSc–November 2010, University of Tromsø (physics), with Prof. Trond Saue and Dr. Dan J.Jonsson as cosupervisors)

Ph.D. students supervised:

- Lara Ferrighi (University of Tromsø,PhD dissertation Nov.7 2007)
- Andreas J. Thorvaldsen (University of Tromsø, expected date of dissertation: September 1 2008)
- Dmitry Shcherbin (University of Tromsø, expect date of dissertation: April 1 2010)
- Harald Solheim (University of Tromsø, expect date of dissertation: May 1 2010)
- Arnfinn Hykkerud Steindal (University of Tromsø, expected date of dissertation: February 28 1012, cosupervised with Luca Frediani)
- Magnus Ringholm (University of Tromsø, expected date of dissertation: August 1 2013, cosupervised with Magdalena Pecul)
- Marco Anelli (University of Tromsø, expected date of dissertation: December 31 2014)
- T. B. Demissie (Polish Academy of Sciences, expected date of dissertation: August 31 2013, main supervisor: Helena Dodziuk)
- Maarten T. P. Beerepoot (University of Tromsø, expected date of dissertation: September 30 2016)

Post.docs.:

- Dr. Magdalena Pecul (May 1 2003–June 30 2004, moved to a permanent positions at the University of Warsaw, Poland) – Dr. Jonas Juselius (March 1 2005–June 30 2007)
- Dr. Luca Frediani (April 15 2005–April 15 2007, became associate professor at the University of Tromsø)
- Dr. Eirik Fossgård (University of Tromsø, May 1 2005–August 31 2006, moved to a permanent position at the International Research Center In Stavanger)
- Dr. Maxime Guillaume (October 1 2007–September 30 2009, moved to a postdoc position at the University of Mons (Belgium))
- Dr. Emmanuel Fromager (January 6 2008–October 6 2008, moved to a permanent position at the University of Strasbourg (France))
- Dr. Clemens Woywod (February 1 2008–August 2010, moved to a postdoc position at the University of Tromsø)
- Dr. Radovan Bast (April 1 2008–, moved to a permanent position at the CNRS in Toulouse (France))

- Dr. Adam Chamberlin (September 9 2008–, moved to a postdoc position at the University of Calgary (Canada))
- Dr. Andreas J. Thorvaldsen (March 1 2009–March 1 2011)
- Dr. Dan J. Jonsson (December 1 2011–September 30 2012, moved to a position at the HPC group at the University of Tromsø)
- Dr. Bin Gao (September 24 2008–)
- Dr. Na Lin (January 1 2010–)
- Dr. Michal Repisky (April 1 2010–)
- Dr. Stanislav Komorovsky (May 1 2012–)

Opponent:

- Ole Andreas Andersen, Ph.D.thesis, University of Tromsø (Norway), March 2003 (local member)
- Zilvinas Rinkevicius, Licenciante thesis, KTH, Stockholm (Sweden), May 2003
- Javier Lopez Cacheiro, Ph.D. thesis, University of Santiago de Compostela (Spain), December 2003
- Jonas Jusélius, Ph.D. thesis, University of Helsinki (Finland), December 2004
- Jacob Kongsted, Ph.D. thesis, University of Copenhagen (Denmark), February 2005.
- Lea Thøgersen, Ph.D. thesis, University of Aarhus (Denmark), November 2005.
- Anas Al Natsheh, Ph.D. thesis, University of Kuopio (Finland), June 2006.
- Marianne Sloth, Ph.D. thesis, University of Copenhagen Denmark), October 2006
- Auayporn Jiemchooraj, Ph.D. thesis, Linköping University (Sweden), October 2007.
- Radovan Bast, Ph.D. thesis, Université Louis Pasteur, Strasbourg (France), January 2008
- Maxim Fedorovsky, Ph.D. thesis, Universität Freiburg (Switzerland), April 2008
- Vincent Liegégois, Ph.D. thesis, FUNDP Namur (Belgium), June 2008
- Hans Sverre Smalø, Ph.D. thesis, NTNU (Trondheim, Norway), December 2010

Conferences/meetings organized:

- International Chemistry Olympiad, Oslo (Norway) 1994. 160 students and 80 teachers from 40 different countries. Responsible for the students, their activity program and the 40 different guides.
- Minisymposium on “Computational methods in quantum chemistry”, June 20 2002, 30 participants from 4 countries.
- Sattelite meeting celebrating the 50th birthday of Professor Trygve Helgaker, September 17 2003. 35 partipants from 7 countries.
- “A Coastal Voyage in Quantum Chemistry”. September 18–21 2003. 71 participants from 16 countries.
- COST D26 work group meeting, April 2-3 2004. 18 participants from 6 countries.
- Italian-Norwegian-Swedish Workshop on Quantum Molecular Sciences, September 17-20 2004. 27 participants from 5 countries.
- CDFT 2007 (A Coastal Voyage of Current Density Functional Theory). September 19–22 2007, 43 participants from 15 countries

Positions of trust:

- Chairman of the PCCP Ownership Board, 2012-2013
- Chairman of the The Joint Committee of the Nordic Research Councils for Natural Sciences (NOS-N, 2012–)
- Norwegian representative on the Joint Committee of the Nordic Research Councils for Natural Sciences (2007–).
- Member of the board for e-Infrastructure investments in Sweden, Vetenskapsrådet (2011–)

- Chairman of the Access Committee of the PRACE project (Partnership for Advanced Computing in Europe) (2011–)
- Norwegian representative in the Management Committee of the COST D37 Network “CODECS”, and chairman of working group 1, 2010–
- Member of the Scientific Steering Committee of the PRACE project (Partnership for Advanced Computing in Europe) (2010–)
- President of the Norwegian Chemical Society (2010–)
- Norwegian representative on the Ownership board of the journal Physical Chemistry Chemical Physics (PCCP) (2008–). Core group member (2011–)
- Norwegian representative in the Physical and Engineering Sciences Standing Committee of the European Science Foundation (2007–2012). Core group member (2010–2012)
- Member of the Board of the Division of Science, Research Council of Norway (2007–)
- Member of a national committee proposing a new organization model for the operation of Norwegian eInfrastructure (2011)
- Board member of the Norwegian organizing committee of the International Year of Chemistry 2011 (2009–2011)
- Member of an allocation committee of the Research Council of Norway for granting large infrastructure resources, with a total budget of about 500 MNok (2009–2011)
- Chairman of an international review panel for evaluating basic chemistry research in Finland (2010)
- Member of an committee to evaluate governmental means of increasing energy efficiency appointed by the Ministry of Oil and Energy, Norway (Spring 2009)
- Board member of the Norwegian Chemical Society (2006–2010)
- Board member of TTONord (2005–2011), a company created to facilitate innovation based on University research and collaboration with industry
- Norwegian representative in the Management Committee of the COST D37 Work group “GridChem”, 2006–2010
- *Ex officio* member of the board of the Faculty of Science, University of Tromsø, 2005–2007
- Member of the board for the national research program on nanoscience (NANOMAT), 2006–2007
- Member of the board for supercomputing infrastructure in the Norwegian eScience program (eVITA), 2006–2007
- Member of a project specification committee appointed by the Norwegian Research Council for the implementation of a Norwegian eScience program (2005).
- Board member of Uninett–Sigma (2005–2007), the company running the Norwegian supercomputing program
- Member of a project specification committee appointed by the Norwegian Research Council for the future Norwegian Supercomputing Program (2004)
- Member of the Research and Education Board of the Faculty of Science at the University of Tromsø, (2003–2005)
- Member of the Board of the Department of Chemistry, University of Tromsø (2002–2007)
- Chairman of Oslo Symphony Orchestra 1995–1996
- Treasurer of Oslo Symphony Orchestra 1994

- Member of the organizing committee for the International Chemistry Olympiad, Oslo (Norway) 1994
- Elected member of the student organization at the Faculty of Science and Mathematics at the University of Oslo 1992 as secretary, and member of various boards at Faculty and University levels
- Elected member of the student organization at the Department of Chemistry, 1990-1991, chairman of this organization 1991. Elected to various boards at the Department of Chemistry, University of Oslo

Publication list, Kenneth Ruud

1. *The magnetic hyperpolarizability anisotropy of the neon atom.* M.Jaszunski, H.J.Aa.Jensen, P.Jørgensen, A.Rizzo, T.Helgaker, and K.Ruud. *Chem.Phys.Lett.* **191**, 599 (1992).
2. *Nuclear magnetic shielding tensor for the ethylenic carbon atom in tetrachlorocyclopropene.* M.Jaszunski, K.L.Bak, P.Jørgensen, T.Helgaker, K.Ruud, and H.J.Aa.Jensen. *Chem.Phys.Lett.* **204**, 608 (1993).
3. *Gauge-origin independent multiconfigurational self-consistent-field theory for vibrational circular dichroism.* K.L.Bak, P.Jørgensen, T.Helgaker, K.Ruud, and H.J.Aa.Jensen. *J.Chem.Phys.* **98**, 8873 (1993).
4. *Hartree-Fock limit magnetizabilities from London orbitals.* K.Ruud, T.Helgaker, K.L.Bak, P.Jørgensen, and H.J.Aa.Jensen. *J.Chem.Phys.* **99**, 3847 (1993).
5. *MCSCF calculations of nitrogen NMR shielding constants using London atomic orbitals.* M.Jaszunski, T.Helgaker, K.Ruud, K.L.Bak, and P.Jørgensen. *Chem.Phys.Lett.* **220**, 154 (1994).
6. *MCSCF calculations of Verdet constants.* M.Jaszunski, P.Jørgensen, A.Rizzo, K.Ruud, and T.Helgaker. *Chem.Phys.Lett.* **222**, 263 (1994).
7. *Basis set convergence of atomic axial tensors obtained from self-consistent field calculations using London atomic orbitals.* K.L.Bak, P.Jørgensen, T.Helgaker, K.Ruud, and H.J.Aa.Jensen. *J.Chem.Phys.* **100**, 6620 (1994).
8. *Multiconfigurational self-consistent field calculations of nuclear shieldings using London atomic orbitals.* K.Ruud, T.Helgaker, R.Kobayashi, P.Jørgensen, K.L.Bak, and H.J.Aa.Jensen. *J.Chem.Phys.* **100**, 8178 (1994).
9. *Theoretical calculations of the magnetizability of some small fluorine-containing molecules using London atomic orbitals.* K.Ruud, T.Helgaker, P.Jørgensen, and K.L.Bak. *Chem.Phys.Lett.* **223**, 12 (1994).
10. *An ab initio nuclear magnetic resonance spectrum of vinylolithium.* K.Ruud, T.Helgaker, P.Jørgensen, and K.L.Bak. *Chem.Phys.Lett.* **226**, 1 (1994).
11. *Multiconfigurational self-consistent field calculations of nuclear magnetic resonance indirect spin-spin coupling constants.* A.Barszczewicz, T.Helgaker, M.Jaszunski, P.Jørgensen, and K.Ruud. *J.Chem.Phys.* **101**, 6822 (1994).
12. *Magnetizability of Hydrocarbons.* K.Ruud, H.Skaane, T.Helgaker, K.L.Bak, and P.Jørgensen. *J.Am.Chem.Soc.* **116**, 10135 (1994).
13. *Basis Set Convergence and Correlation Effects in Vibrational Circular Dichroism Calculations using London Atomic Orbitals.* K.L.Bak, P.Jørgensen, T.Helgaker, and K.Ruud. *Faraday Discuss.* **99**, 121 (1994).
14. *Vibrational Raman Optical Activity Calculations Using London Atomic Orbitals.* T.Helgaker, K.Ruud, K.L.Bak, P.Jørgensen, and J.Olsen. *Faraday Discuss.* **99**, 165 (1994).
15. *A numerically stable orbital connection for the calculation of analytical Hessians using perturbation-dependent basis sets.* K.Ruud, T.Helgaker, J.Olsen, P.Jørgensen, and K.L.Bak. *Chem.Phys.Lett.* **235**, 47 (1995).

16. *Orbital connections for perturbation-dependent basis sets.* J.Olsen, K.L.Bak, K.Ruud, T.Helgaker, and P.Jørgensen. *Theor.Chim.Acta* **90**, 421 (1995).
17. *Ab initio calculation of electronic circular dichroism for trans-cyclooctene using London atomic orbitals.* K.L.Bak, Aa.E.Hansen, K.Ruud, T.Helgaker, J.Olsen, and P.Jørgensen. *Theor.Chim.Acta* **90**, 441 (1995).
18. *Loss of H₂ from CH₃NH₃⁺, CH₃OH₂⁺ and CH₃FH⁺. Reaction mechanisms and dynamics from observation of metastable ion fragmentations and ab initio calculations.* E.L.Øiestad, Å.M.L.Øiestad, H.Skaane, K.Ruud, T.Helgaker, E.Uggerud, and T.Vulpus. *Europ.Mass.Spectrom.* **1**, 121 (1995).
19. *NMR Shielding Tensors and Indirect Spin-Spin Coupling Tensors in HCN, HNC, CH₃CN, and CH₃NC Molecules.* A.Barszczewicz, T.Helgaker, M.Jaszunski, P.Jørgensen, and K.Ruud. *J.Magn.Reson. A* **114**, 212 (1995).
20. *Accurate magnetizabilities of the isoelectronic series BeH⁻, BH, and CH⁺. The MCSCF-GIAO approach.* K.Ruud, T.Helgaker, K.L.Bak, P.Jørgensen, and J.Olsen. *Chem.Phys.* **195**, 157 (1995).
21. *Electric field dependence of magnetic properties: Multiconfigurational self-consistent field calculations of hypermagnetizabilities and nuclear shielding polarizabilities of N₂, C₂H₂, HCN, and H₂O.* A.Rizzo, T.Helgaker, K.Ruud, A.Barszczewicz, M.Jaszunski, and P.Jørgensen. *J.Chem.Phys.* **102**, 8953 (1995).
22. *SCF calculations of the NMR shielding tensor for the ethylenic carbon atom in C₃Cl₄.* M.Jaszunski, T.Helgaker, K.Ruud, P.Jørgensen, K.L.Bak, and H.Koch. *Mol.Phys.* **85**, 671 (1995).
23. *NMR properties of N₃⁻. A comparison of theory and experiment.* M.Jaszunski, S.Szymanski, O.Christiansen, P.Jørgensen, T.Helgaker, and K.Ruud. *Chem.Phys.Lett.* **243**, 144 (1995).
24. *Second-Order Methods for the Optimization of Molecular Potential Energy Surfaces.* T.Helgaker, K.Ruud, and P.R.Taylor. In "The Reaction Path in Chemistry: Current Approaches and Perspectives", edited by D.Heidrich, (Kluwer, Netherlands) (1995).
25. *On the Convergence of MBPT and CC Nuclear Magnetic Shielding Constants of BH Toward the Full CI Limit.* J.Gauss, and K.Ruud. *Int.J.Quantum Chem.* **29**, 437 (1995).
26. *Long-range effects of interatomic interactions on NMR shielding constants.* A.Barszczewicz, M.Jaszunski, T.Helgaker, and K.Ruud. *Chem.Phys.Lett.* **250**, 1 (1996).
27. *Efficient parallel implementation of response theory: calculations of the second hyperpolarizability of polyacenes.* P.Norman, D.Jonsson, H.Ågren, P.Dahle, K.Ruud, T.Helgaker, and H.Koch. *Chem.Phys.Lett.* **253**, 1 (1996).
28. *Magnetizability and nuclear shielding constants of solvated water.* K.V.Mikkelsen, K.Ruud, and T.Helgaker. *Chem.Phys.Lett.* **253**, 443 (1996).
29. *MCSCF calculations of hypermagnetizabilities and nuclear shielding polarizabilities of CO and CH₄.* S.Coriani, A.Rizzo, K.Ruud, and T.Helgaker. *Mol.Phys.* **88**, 931 (1996).
30. *Vibrational magnetism of HCN and its isotopomers using rotational London atomic orbitals.* P.A.Braun, T.K.Rebane, and K.Ruud. *Chem.Phys.* **208**, 341 (1996).
31. *Ab Initio Studies of the [AX]₂ Spin Systems of cis- and trans-N₂F₂.* M.Jaszunski, T.Helgaker, and K.Ruud. *Magn.Reson.Chem.* **34**, 646 (1996).

32. *Perturbation-dependent atomic orbitals for the calculation of spin-rotation constants and rotational g tensors.* J.Gauss, K.Ruud, and T.Helgaker. *J.Chem.Phys.* **105**, 2804 (1996).
33. *Energetics and Dynamics of Intermolecular Proton-Transfer Processes. 2. Ab Initio Direct Dynamics Calculations of the Reaction $H_3O^+ + NH_3 \rightarrow NH_4^+ + H_2O$.* H.-H.Bueker, T.Helgaker, K.Ruud, and E.Uggerud. *J.Phys.Chem.* **100**, 15388 (1996).
34. *Full CI calculations of the magnetizability and rotational g factor of the hydrogen molecule.* K.Ruud, P.-O.Åstrand, T.Helgaker, and K.V.Mikkelsen. *J.Mol.Struct. (THEOCHEM)* **388**, 231 (1996).
35. *Magnetizabilities and Nuclear Shielding Constants of the Fluoromethanes in the Gas Phase and Solution.* P.-O.Åstrand, K.V.Mikkelsen, K.Ruud, and T.Helgaker. *J.Phys.Chem.* **100**, 19771 (1996).
36. *The magnetizability, rotational g tensor, and quadrupole moment of PF_3 revisited.* K.Ruud, and T.Helgaker. *Chem.Phys.Lett.* **264**, 17 (1997).
37. *A multipole reaction-field model for gauge-origin independent magnetic properties of solvated molecules.* K.V.Mikkelsen, P.Jørgensen, K.Ruud, and T.Helgaker. *J.Chem.Phys.* **106**, 1170 (1997).
38. *Hyperfine and nuclear quadrupole coupling in chlorine and fluorine dioxides.* B.Fernandez, O.Christiansen, P.Jørgensen, J.Byberg, J.Gauss, and K.Ruud. *J.Chem.Phys.* **106**, 1847 (1997).
39. *Cotton-Mouton effect and shielding polarizabilities in ethylene: an MCSCF study.* S.Coriani, A.Rizzo, K.Ruud, and T.Helgaker. *Chem.Phys.* **216**, 53 (1997).
40. *Mechanisms, energetics and dynamics of a key reaction sequence during the decomposition of nitromethane: $HNO + HNO \rightarrow N_2O + H_2O$.* K.Ruud, T.Helgaker, and E.Uggerud. *J.Mol.Struct. (THEOCHEM)* **393**, 59 (1997).
41. *The magnetizability anisotropy and rotational g factor of deuterium hydride and the deuterium molecule.* P.-O.Åstrand, K.Ruud, K.V.Mikkelsen, and T.Helgaker. *Chem.Phys.Lett.* **271**, 163 (1997).
42. *The Cotton-Mouton effect of liquid water. Part I: The dielectric continuum model.* K.Ruud, T.Helgaker, A.Rizzo, S.Coriani, and K.V.Mikkelsen. *J.Chem.Phys.* **107**, 894 (1997).
43. *Ab initio calculation of the NMR shielding and indirect spin-spin coupling constants of fluoroethylene.* T.Helgaker, M.Jaszunski, and K.Ruud. *Mol.Phys.* **91**, 881 (1997).
44. *Isotope and temperature effects on the ^{13}C and ^{77}Se nuclear shielding in carbon diselenide.* J.Lounila, J.Vaara, Y.Hiltunen, A.Pulkkinen, J.Jokisaari, M.Ala-Korpela, and K.Ruud. *J.Chem.Phys.* **107**, 1350 (1997).
45. *Electric and magnetic properties of the nitroethene molecule.* P.-O.Åstrand, K.Ruud, K.V.Mikkelsen, and T.Helgaker. *Mol.Phys.* **92**, 89 (1997).
46. *The effect of correlation on molecular magnetizabilities and rotational g tensors.* K.Ruud, T.Helgaker, and P.Jørgensen. *J.Chem.Phys.* **107**, 10599 (1997).
47. *The Cotton-Mouton effect of liquid water. Part II: The semi-continuum model.* K.Ruud, H.Ågren, P.Dahle, T.Helgaker, A.Rizzo, S.Coriani, H.Koch, K.O.Sylvester-Hvid, and K.V.Mikkelsen. *J.Chem.Phys.* **108**, 599 (1998).

48. *Solvent effects on nuclear shieldings and spin-spin couplings of hydrogen selenide.* P.-O.Åstrand, K.V.Mikkelsen, P.Jørgensen, K.Ruud, and T.Helgaker. *J.Chem.Phys.* **108**, 2528 (1998).
49. *Saturation of the Optical Band Gap and Properties of Five-Membered Heteroaromatic Oligomers.* Y.Luo, K.Ruud, P.Norman, D.Jonsson, and H.Ågren. *J.Phys.Chem.* **B 102**, 1710 (1998).
50. *The Molecular Zeeman Effect of Norbornadiene, its g-Values, Magnetizability Anisotropies, and Molecular Quadrupole Moment; A High-Resolution Microwave Fourier-Transform Study Combined With Quantum Chemical Calculations.* K.Voges, D.H.Sutter, K.Ruud, and T.Helgaker. *Z.Naturforsch.* **A 53**, 67 (1998).
51. *Molecular length dependence of optical properties of hydrocarbon oligomers.* Y.Luo, P.Norman, K.Ruud, and H.Ågren. *Chem.Phys.Lett.* **285**, 160 (1998).
52. *The Hartree-Fock magnetizability of C₆₀.* K.Ruud, H.Ågren, T.Helgaker, P.Dahle, H.Koch, and P.R.Taylor. *Chem.Phys.Lett.* **285**, 205 (1998).
53. *MCSCF nuclear magnetic shieldings and spin-rotation constants of ¹⁷O in ¹⁶O ¹⁷O ¹⁶O and ¹⁷O ¹⁶O ¹⁶O.* S.Coriani, M.Jaszunski, A.Rizzo, and K.Ruud. *Chem.Phys.Lett.* **287**, 677 (1998).
54. *Generalized integral screening for efficient calculations of nonlinear optical properties of large molecules.* K.Ruud, D.Jonsson, P.Norman, H.Ågren, T.Saue, H.J.Aa.Jensen, P.Dahle, and T.Helgaker. *J.Chem.Phys.* **108**, 7973 (1998).
55. *Basis-set dependence of nuclear spin-spin coupling constants.* T.Helgaker, M.Jaszunski, K.Ruud, and A.Gorska. *Theor.Chem.Acc.* **99**, 175 (1998).
56. *On The Nature and Incidence of -Agostic Interactions in Ethyl Derivatives of Early Transition Metals: Ethyltitanium Trichloride and Related Compounds.* A.Haaland, W.Scherer, K.Ruud, G.S.McGrady, A.J.Downes, and O.Swang. *J.Am.Chem.Soc.* **120**, 3762 (1998).
57. *Calculations of circular intensity differences in electric-field-induced second harmonic generation.* D.Jonsson, Y.Luo, K.Ruud, P.Norman, and H.Ågren. *Chem.Phys.Lett.* **288**, 371 (1998).
58. *Electric and magnetic properties of fullerenes.* D.Jonsson, P.Norman, K.Ruud, H.Ågren, and T.Helgaker. *J.Chem.Phys.* **109**, 572 (1998).
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