

Curriculum Vitae for Per-Ola Norrby

Name	Title	Date of birth	Marital Status
Per-Ola Norrby	Professor	May 8, 1962	Married, two children

Affiliation	Home address
University of Gothenburg Department of Chemistry & Molecular Biology Kemigården 4, SE-412 96 Göteborg, Sweden Phone: +46 31 7869034. Fax +46 31 7723840 Email: pon@chem.gu.se WWW: http://www.cmb.gu.se/english/staff/norrby-per-ola/	Synemansv. 23 SE-43341 Partille, Sweden

Examina

Royal Institute of Technology, Stockholm, Sweden; M.Sc.; 1984; Chemistry and Chemical Engineering.
Royal Institute of Technology, Stockholm, Sweden; Ph.D.; 1992; Organic Chemistry.
Royal Institute of Technology, Stockholm, Sweden; Docent; 1995; Organic Chemistry.

Honors

Ernst Jonsson Graduate Fellowship 1985-1989.
Bengt Lundqvist Memory Award 1992.
Syntheses, Inc. Lecturer at Notre Dame University, In, USA, 2000
Eli Lilly Lecturer at Notre Dame University, In, USA, 2004

Professional Memberships

Swedish Chemical Society
American Chemical Society

Professional Experience

1984-89 Synthetic Heterocyclic Chemistry. Advisor: Jan Bergman.
1989-92 Res. Assist., Organometallic Molecular Mechanics. Advisor: Björn Åkermark.
1992-93 Postdoc, Scripps Research Institute. Advisor: K. Barry Sharpless.
1994-96 Research Associate, Royal Danish School of Pharmacy (DFH), Copenhagen, Denmark.
1997-2000 Associate Professor, Royal Danish School of Pharmacy, Copenhagen, Denmark.
2000-2006 Associate Professor, Technical University of Denmark
2006- Professor, University of Gothenburg

Commissions of trust

Editorial Board, "Journal of Molecular Catalysis A: Chemical" (Elsevier)
Editorial Board, "ChemCatChem" (Wiley)
Editorial Board, "Theoretical Chemistry Accounts" (Springer)

Conference organization

1998 Co-organizer, "12th European Symposium on Quantitative Structure-Activity Relationships; Molecular Modelling and Prediction of Bioactivity" in Copenhagen
2001 Organizer, "Drug Design Copenhagen 2001" in Copenhagen.
2002 Symposium co-organizer, "New developments in force fields for molecular modeling", fall ACS meeting in Boston, USA
2002 Co-organizer, "Trends in Organic Chemistry: Computational Organic Chemistry" in Uppsala, Sweden.
2004 COST symposium organizer, "Sustainable Chemistry and Catalysis" in Copenhagen
2004 COST D24 WG 0013-02 meeting organizer, "Sustainable Chemical Processes: Stereoselective Transition Metal-Catalysed Reactions" in Copenhagen
2005 Organizer, "Stereoselective Synthesis" in Copenhagen
2007 Co-organizer, "Trends in Organic Chemistry: Metal-Mediated Reactions" in Gothenburg
2009 Co-organizer, "Organkemiska vintermötet 2009" in Åre

- 2009 Organizer, "The 1st Åbo-Gothenburg organic chemistry meeting" in Gothenburg
2009 Organizer, EuCOMC XVIII in Gothenburg, Sweden:
<http://www.chemsoc.se/sidor/KK/comc18/index.htm>
2012 Co-organizer, the 23rd "Organikerdagarna" in Gothenburg: <http://www.organikerdagarna.se/>

Teaching Experience

- Laboratory assistant, organic chemistry, KTH 1985-1987.
Teaching assistant, physical chemistry, KTH 1985.
Laboratory assistant, advanced organic chemistry, KTH 1987.
Production of an instruction video (2 h. 10 min.) for use in laboratory teaching, KTH, 1989.
Teaching assistant, organic chemistry, KTH 1989-1991, DFH 1997-2000.
Lecturer, advanced organic chemistry, DTU, 2001-2006
Undergraduate project supervision, DTU, 2001-2006
Lecturer, spectroscopy, DTU, 2002-2006
Lecturer, basic and advanced organic chemistry, GU, 2007-2011
Lecturer at graduate summer schools: Heidelberg: 2003, 2006, 2009, 2010; Lugano: 2004; Villars-sur-Ollon: 2008; Doorn (AMOC): 2010; Bressanone (WISPOC): 2012.

Participation in and coordination of several Ph.D. level courses in molecular modelling at DFH (now KU), Lund University, Notre Dame University, and DTU.

The Ph.D. course "Molecular Modelling for experimental chemists", a two-week intensive course which was given 2001, 2003, and 2005 at DTU, 2007 and 2010 at GU, and 2011 at University of West Indies, Jamaica. Shorter versions, ranging from 2 days to a week, have been given at Heidelberg (Germany, 2000), Madison (WI, USA, 2001), KTH (2002), Stockholm University (2004), Uppsala University (2005), and Aalto University (Helsinki, 2011).

Supervisor in M.Sc. thesis projects:

- "N-etylering av indol", Eva Näsman, KTH 1991.
"Bestämning av molekylmekaniska parametervärden för palladium- π -allylkomplex", Fredrik Häffner, KTH 1991.
"Conformational Calculations on some Palladium π -allyl Complexes with Internal Ligands", Bruno Paul, KTH 1992.
"Bestämning av molekylmekaniska parametervärden för palladium-olefinkomplex", Mattias Ekman, KTH 1992
Co-supervisor, with Mikael Begtrup, Tommy Liljefors, Ebbe Kelstrup (DTU), and Helge Johansen (DTU): "Beregnet og eksperimentel reaktivitet i pyrazoler", Thomas Balle, DFH 1996.
Co-supervisor, with Tommy Liljefors: "Conformational Energy Penalties of Protein-Bound Ligands", Jonas Boström, DFH 1996.
Co-supervisor, with Tommy Liljefors and Stephan Sauer (KU), "Investigations of Coenzyme B₁₂ Structure and Function", Kasper Planeta Jensen, DFH 1999-2000.
Main supervisor, with David Tanner, "Studies on the Asymmetric Osmium-catalyzed Dihydroxylation", Peter Fristrup, DTU, 2002.
Main supervisor, with Janne E. Tønder, "Brug af chirale auxiliaries i Peterson olefineringsreaktionen", Elena Redondo, DTU, 2002.
Co-supervisor, with Knud J. Jensen, KVL, "Total Chemical Synthesis of Model Proteins", Pernille Tofteng, DTU, 2003-4.
Co-supervisor, with John Nielsen, KVL, "Synthesis of phenazine natural product analogues", Jakob Ewald Rasmussen, DTU, 2003-2004.
Co-supervisor, with Knud J. Jensen, KVL, "Thioesters in peptides", Lotte Harlou, DTU, 2003-2004.
Co-supervisor, with Rasmus P. Clausen and Jesper L. Kristensen, DFU, "Development of New Glutamic Acid Receptor Ligands", Signe Holmegaard, DTU, 2004.
Main supervisor, with Klaus Gundertofte, Lundbeck A/S, "Force field parameterization of heteroaromatic systems for use in docking studies", Sune A. Pedersen, DTU, 2004.

“Virtual screening of ligands in palladium-catalyzed allylic alkylation”, Lars Rasmussen, DTU, 2004-2005.

Main supervisor, with David Tanner, DTU, "Enantiospecificity in Palladium-Catalyzed Allylic Alkylations", Nina Svensen, DTU, 2006.

Co-supervisor, with Peder Svensson, NeuroSearch Sweden AB, "New quantum chemically derived QSAR descriptors of substituent effects on the interaction between aromatic systems and their surroundings", Ylva Sunesson, Umeå University, 2007.

"Reactivity in Fe-catalyzed coupling reactions", Parisa Emamy, GU, 2009

"Ligands for Fe-catalyzed coupling reactions", Kenan Asenov, GU, 2010

"Condition dependence of the allylic alkylation reaction", Franziska Grafe, GU, 2011

"Reducing Iron; creating pandemonium", Erik Lindstedt, GU, 2012

Supervisor, Ph.D. projects:

Co-supervisor, with Björn Åkermark, KTH: “Palladium-Catalyzed Aromatic Coupling and Allylic Substitution – An Experimental and Theoretical Study”, Helena Hagelin, Ph.D.Thesis, KTH, Stockholm, May 1999.

Co-supervisor, with Tommy Liljefors and Povl Krogsgaard-Larsen, “A pharmacophore model for GABA_A receptor agonists”, Lena Tagmose, DFH, May 2000.

Co-supervisor, with Tommy Liljefors and Jerzy Jaroszewski, “Konformationelle egenskaber af polære molekyler i vandig opløsning undersøgt ved NMR-spektroskopi og computational chemistry”, Peter Aadal Nielsen, DFH, Oct. 2000.

Main supervisor, with Mikael Begtrup, “Molekylmodellering i asymmetrisk katalyse”, Torben Rasmussen, DFH, May 2001.

Co-supervisor, with Fredrik Björkling and David Tanner, “Synthesis of Anti-inflammatory aminothiazoles”, Thomas Hansen, DTU, March 2002.

Main supervisor, with David Tanner, “Selective homogeneous catalysis in asymmetric synthesis”, Peter Fristrup, DTU, 2003-2006

Co-supervisor, with Lars Hemmingsen, “Structural characterization of chiral molecules using vibrational circular dichroism (VCD) spectroscopy”, Peter R. Lassen, DTU, 2003-2006

Co-supervisor, with Paul Helquist and Olaf Wiest, Notre Dame University (ND), “Computer-aided design of chiral phenanthroline ligands for use in asymmetric catalysis”, Elsa Kieken, ND, 2003-

Supervisor, “Mechanistic investigation of metal-catalyzed formation of three-membered rings”, Henriette Holm, DTU, 2003-

Main supervisor, with David Tanner, “Mechanistic Investigation of Organometallic Addition Reactions”, Mårten Ahlquist, DTU, 2004-2007

Co-supervisor, with Tommy Liljefors, Morten Langgård, and Lena Tagmose, “Flexible Pseudo Receptor Docking”, Sune Askjær Pedersen, DUPS and Lundbeck A/S, 2005-2008

Main supervisor, with David Tanner, “Investigation of Pd(0) Complexes in Homogeneous Catalysis”, Signe Teuber Henriksen, DTU, 2006-2009

Supervisor, "Mechanistic investigations of metal-catalyzed reactions", Anna Hedström, GU, 2007-2013

Supervisor, "Mechanistic investigations of transition metal catalyzed reactions", Jonatan Kleimark, GU, 2007-2012

Supervisor, "Mechanistic investigations of metal-catalyzed reactions", Per-Fredrik Larsson, GU, 2007-2012

Supervisor, "Ligand Dependent Regioselectivity in Palladium Mediated Allylic Alkylation", Charlotte Johansson, GU, 2007-2010

Co-supervisor, with Jürgen Gräfenstein, and Sten O. Nilsson Lill, "Chiral Lithium N,P-amide Complexes, Synthesis, applications and structural studies by NMR and DFT", Petra Rönnholm, GU, 2010-2011.

Invited lectures (not including departmental invitations and contributed talks)

- 1996**
 April CERC3 Workshop on Catalytic Asymmetric Synthesis in Dublin: “Computational Tools in Asymmetric Catalysis”
- 2000**
 March ASC spring meeting in San Francisco: “QM-guided molecular mechanics as a tool for selectivity predictions in asymmetric catalysis”
- 2001**
 June European Schrödinger User Group Meeting in Frankfurt: “A computational investigation of the addition of dialkyl zinc to aldehydes”
- 2002**
 July The 6th European Conference on Bioinorganic Chemistry in Lund, tutorial lecture: “Molecular modeling of coordination complexes”
 Aug. ACS fall meeting in Boston: “Selectivity in the addition of dialkyl zinc to aldehydes from Q2MM force field modelling”
 Sept. COST D24 MC meeting in Dublin: “Selectivity in asymmetric catalysis from molecular modeling”
- 2003**
 Aug. XVth FEICHEM Conference on Organometallic Chemistry in Zürich, plenary lecture: “Opportunities and Limitations in Computational Transition Metal Chemistry”
- 2004**
 Jan. COST D24 meeting in Barcelona: “Accurate Predictions of Selectivity in Catalytic Reactions from Molecular Modeling”
 Sept. 5th RSC International Symposium on Transition Metals in Organic Synthesis (TMOS-5) in Glasgow: “Selectivity Predictions in Asymmetric Catalysis”
 Sept. COST D24 meeting in Copenhagen: “Reactivities and Selectivities from Molecular Modeling”
- 2005**
 Sept. COST D24 meeting in Barcelona: “Mechanistic Investigations of Palladium-Catalyzed Reactions”
 Dec. Pacificchem inorganic symposium “The future of force field Modeling of Metal Complexes in the DFT Age” in Honolulu: “Reaction selectivities from force fields”
- 2006**
 May Swedish Theoretical Chemistry meeting in Stockholm: “A Paradigm Change in Transition Metal Chemistry, No More 18-electron rule”
 July XXII International Conference on Organometallic Chemistry, Zaragoza: “A new view on palladium-catalyzed coupling reactions, memory effects, and halide acceleration; no more 18-electron rule”
 Oct. COST D24 meeting in Rome: “Selectivity and reactivity in transition metal catalysis”
- 2007**
 May COST D40 kickoff meeting in Dublin: “Modeling of Metal-catalyzed Coupling Reactions”
 Aug. EuCOMC XVII in Sofia: “Mechanistic Investigations of Metal-catalyzed Couplings”
 Sept. First annual symposium , division of theoretical chemistry, the Swedish chemical society, Örebro: “Unusual selectivity-determining factors in the Heck arylation of allylic ethers”
 Nov. Christina Moberg birthday symposium: “Mechanistic investigation of transition metal catalyzed couplings”
- 2008**
 May COST D40 meeting in Tarragona: “Recent Adventures with the Heck Reaction”
- 2009**
 Jan. Organic Chemistry winter meeting in Åre, “Övergång” (in Swedish)
 April COST D40 meeting in Bratislava: “A Smörgåsbord of Homogeneous Catalysis”
 May COST D40 meeting in Turku: “Mechanism of Iron-Catalyzed Couplings”
 Aug. IUPAC meeting in Glasgow: "Accurate reaction selectivities from force fields"
 Nov. The 5th Global Process R&D External Science Symposium at AstraZeneca, Charnwood: “Selectivities in Homogeneous Catalysis”
- 2010**

March Organic Chemistry winter meeting in Laisaliden, "Sustainable Catalytic Chemistry"
March ACS Spring meeting in San Francisco: "18e R.I.P"
May COST D40 meeting in Ankara: "18e R.I.P"
Aug. EuCheMS meeting in Nürnberg: "Mechanistic Investigations in Homogeneous Catalysis"
2011
March Organic Chemistry winter meeting in Åre: "Worth Waiting For"
June The Tage Erlander Professor Installation 2011, Gothenburg: "Mechanistic Investigations in Homogeneous Catalysis"
June COST D40 meeting in Valetta: "Reaction Selectivity from Q2MM Modeling"
Aug. Challenges in Computational Homogeneous Catalysis in Stockholm: "Selectivities in Homogeneous Catalysis"
Oct. Modeling of Molecular Properties, MOLMOD2011 in Heidelberg: "Accurate Energies in Homogeneous Catalysis"
2012
June FeUR symposium in Regensburg: "The Catalyst in Fe-catalyzed C-C-coupling"
Sept. ICCOS meeting in Moscow: "Mechanistic Investigations in Homogeneous Catalysis"

Publications in international, refereed journals

A total of 4297 citations in Jan 2013; *h-value* 41. ResearcherID: <http://www.researcherid.com/rid/A-3399-2009>

- 1) "Structure Elucidation of Some Products Obtained by Acid-Catalyzed Condensation of Indole with Acetone." Jan Bergman, Per-Ola Norrby, Ulf Tilstam, and Lennart Venemalm, *Tetrahedron* **1989**, *45*, 5549-5564.
- 2) "Alkylation with Oxalic Esters. Scope and Mechanism." Jan Bergman, Per-Ola Norrby, and Peter Sand, *Tetrahedron* **1990**, *46*, 6113-6124.
- 3) "Selective Stabilization of the Anti Isomer of (η^3 -Allyl) palladium and -platinum Complexes." Magnus Sjögren, Sverker Hansson, Per-Ola Norrby, Björn Åkermark, Maria Elena Cucciolito, and Aldo Vitagliano, *Organometallics* **1992**, *11*, 3954-3964.
- 4) "Calculation of NMR Observables from Computed Conformers as a Tool of Structure Verification. Conformation of the Stereochemistry of trans-Methyl 2,3-dimethyl-5-methoxy-2-cyclohexene-1-carboxylate." Jeffrey T. Martin, Per-Ola Norrby, and Björn Åkermark, *J. Org. Chem.* **1993**, *58*, 1400-1406.
- 5) "Molecular Mechanics (MM2) Parameters for the η^3 -Allyl Palladium Moiety." Per-Ola Norrby, Björn Åkermark, Fredrik Hæffner, Sverker Hansson, and Margareta Blomberg, *J. Am. Chem. Soc.* **1993**, *115*, 4859-4867.
- 6) "Effects of Phenanthroline Type Ligands on the Dynamic Processes of (η^3 -Allyl) palladium Complexes. Molecular Structure of (2,9-Dimethyl-1,10-phenanthroline)[(1,2,3- η)-3-methyl-2-butenyl]chloropalladium." Sverker Hansson, Per-Ola Norrby, Magnus P.T. Sjögren, Björn Åkermark, Maria Elena Cucciolito, Federico Giordani, and Aldo Vitagliano, *Organometallics* **1993**, *12*, 4940-4948.
- 7) "Calculations on the Reaction of Ruthenium Tetroxide with Olefins Using Density Functional Theory (DFT). Implications for the Possibility of Intermediates in the Osmium-Catalyzed Asymmetric Dihydroxylation (AD)." Per-Ola Norrby, Hartmuth C. Kolb, and K. Barry Sharpless, *Organometallics* **1994**, *13*, 344-347.
- 8) "Towards an Understanding of the High Enantioselectivity in the Osmium Catalyzed Asymmetric Dihydroxylation (AD). 2. A Qualitative Molecular Mechanics Approach." Per-Ola Norrby, Hartmuth C. Kolb, and K. Barry Sharpless, *J. Am. Chem. Soc.* **1994**, *116*, 8470-8478.
- 9) "Comparing Two Models for the Selectivity in the Asymmetric Dihydroxylation Reaction (AD)." Heinrich Becker, Pui-Tong Ho, Hartmuth Kolb, Stefan Loren, Per-Ola Norrby, and K. Barry Sharpless, *Tetrahedron Letters* **1994**, *35(40)*, 7315-7318.
- 10) "Unusual Conformational Determining Interactions in Oxymethylpyridines. An Ab Initio Study and an Improved Method for Refining Molecular Mechanics Parameters." Per-Ola Norrby, Kenneth Wärnmark, Björn Åkermark, and Christina Moberg, *J. Comput. Chem.* **1995**, *16*, 620-627.
- 11) "Studies of Allylic Substitution Catalyzed by a Palladium Complex of a C2-Symmetric Bis(aziridine). Preparation and NMR Spectroscopic Investigation of a Chiral π -Allyl Species." Pher G. Andersson, Adrian Harden, David Tanner, and Per-Ola Norrby, *Chem. Eur. J.* **1995**, *1*, 12-16
- 12) "Conformations of (η^3 -Cyclohexenyl)Palladium Systems. A Molecular Mechanics (MM2) Study" Björn Åkermark, Johan D. Oslob, and Per-Ola Norrby, *Organometallics* **1995**, *14*, 1688-1693
- 13) "On the Chirality Transfer in the Epoxidation of Alkenes Catalyzed by Manganese(salen) Complexes." Per-Ola Norrby, Christian Linde, and Björn Åkermark, *J. Am. Chem. Soc.* **1995**, *117*, 11035-11036
- 14) "A Detailed Study of the (η^3 -Cyclohexenyl)Palladium Systems." Jeffrey T. Martin, Johan D. Oslob, Björn Åkermark, and Per-Ola Norrby, *Acta Chem. Scand.* **1995**, *49*, 888-893
- 15) "Kinetic Constraints on Possible Reaction Pathways for the Osmium Catalyzed Asymmetric Dihydroxylation (AD)" Per-Ola Norrby and Kevin P. Gable, *J. Chem. Soc., Perkin Trans. 2* **1996**, 171-178
- 16) "Towards an Understanding of the High Enantioselectivity in the Osmium Catalyzed Asymmetric Dihydroxylation (AD). Part 3. New Insights into Isomeric Forms of the Putative Osmaoxetane Intermediate" Per-Ola Norrby, Heinrich Becker, and K. Barry Sharpless, *J. Am. Chem. Soc.* **1996**, *118*, 35-42
- 17) "A Comparison of Conformational Energies Calculated by Several Molecular Mechanics Methods" Klaus Gundertofte, Tommy Liljefors, Per-Ola Norrby, and Ingrid Pettersson, *J. Comput. Chem.* **1996**, *17*, 429-449
- 18) "Conformational Preference of 2-(Halomethyl)- and 2-(Oxomethyl)pyridines. Microwave Spectrum, Ab Initio and MM3 Studies of 2-(Fluoromethyl)pyridine" Christina Moberg, Hans Adolfsson, Kenneth Wärnmark, Per-Ola Norrby, Karl-Magnus Marstokk, and Harald Møllendal, *Chem. Eur. J.* **1996**, *2*, 516-522
- 19) "Molecular Mechanics Predictions and Experimental Testing of Asymmetric Palladium-Catalyzed Allylation Reactions Using New Chiral Phenanthroline Ligands" Eduardo Peña-Cabrera, Per-Ola Norrby, Magnus Sjögren, Aldo Vitagliano, Vincenzo deFelice, Johan Oslob, Shingo Ishii, Björn Åkermark, and Paul Helquist, *J. Am. Chem. Soc.* **1996**, *118*, 4299-4313

- 20) "An *ab initio* study of the trimethylamine - formic acid and the trimethylammonium ion - formate anion complexes, their monohydrates and their interactions with a dielectric continuum "
Tommy Liljefors and Per-Ola Norrby, *J. Am. Chem. Soc.* **1997**, *119*, 1052-1058
- 21) "Toward an Understanding of the High Enantioselectivity in the Osmium-Catalyzed Asymmetric Dihydroxylation. 4. Electronic Effects in Amine-Accelerated Osmylations"
Derek W. Nelson, K. Barry Sharpless, Andreas Gypser, Pui Tong Ho, Hartmuth C. Kolb, Teruyuki Kondo, Hoi-Lun Kwong, Dominic V. McGrath, A. Erik Rubin, Per-Ola Norrby, and Kevin P. Gable, *J. Am. Chem. Soc.* **1997**, *119*, 1840-1858.
- 22) "Molybdenum-Catalyzed Allylic Substitution. Influence of 1,10-Phenanthroline Ligands on Reactivity and Selectivity"
Magnus P.T. Sjögren, Håkan Frisell, Björn Åkermark, Per-Ola Norrby, Lars Eriksson, and Aldo Vitagliano, *Organometallics* **1997**, *16*, 942-950
- 23) "The Theoretical Basis of the Isoinversion Principle"
Andreas Gypser and Per-Ola Norrby, *J. Chem. Soc., Perkin Trans. 2* **1997**, 939-943
- 24) "Steric Influences on the Selectivity in Palladium-Catalyzed Allylation"
Johan D. Oslob, Björn Åkermark, Paul Helquist, and Per-Ola Norrby, *Organometallics* **1997**, *16*, 3015-3021
- 25) "High yield preparation of 4'-(4-bromophenyl)-2,2':6',2"-terpyridine by a condensation reaction. Determination of the stereochemistry of two complex byproducts by a combination of molecular mechanics and NMR"
Peter Korall, Anna Börje, Per-Ola Norrby, and Björn Åkermark, *Acta Chem. Scand.* **1997**, *51*, 760-766
- 26) "Is There a Radical Intermediate in the Jacobsen-Katsuki Epoxidation of Alkenes?"
Christian Linde, Moritz Arnold, Per-Ola Norrby, and Björn Åkermark, *Angew. Chem.* **1997**, *109*, 1802-1803; *Angew. Chem., Int. Ed. Engl.* **1997**, *36*, 1723-1725
- 27) "Structural Features of Muscimol, a Potent GABA_A Receptor Agonist, Crystal Structure and Quantum Chemical *Ab Initio* Calculations"
Lotte Brehm, Karla Frydenvang, Lene Merete Hansen, Per-Ola Norrby, Povl Krogsgaard-Larsen, and Tommy Liljefors, *Structural Chemistry* **1997**, *8*, 443-451
- 28) "Structural characteristics of isoxazol-3-ol and isothiazol-3-ol, carboxy group bioisosteres examined by X-ray crystallography and *ab initio* calculations"
Karla Frydenvang, Lisa Matzen, Jerzy Jaroszewski, Per-Ola Norrby, Tommy Liljefors, and Povl Krogsgaard-Larsen, *J. Chem. Soc., Perkin Trans. 2* **1997**, 1783-1791
- 29) "A Quantum Chemical Exploration of the Horner-Wadsworth-Emmons Reaction"
Peter Brandt, Per-Ola Norrby, Ivar Martin, and Tobias Rein, *J. Org. Chem.* **1998**, *63*, 1280-1289
- 30) "Automated Molecular Mechanics Parameterization with Simultaneous Utilization of Experimental and Quantum Chemical Data"
Per-Ola Norrby and Tommy Liljefors, *J. Comput. Chem.* **1998**, *19*, 1146-1166
- 31) "A Bis(Crown-Ether) Analogue of Tröger's Base: Recognition of Achiral and Chiral Primary Bisammonium Salts"
Anna P. Hansson, Per-Ola Norrby, and Kenneth Wärnmark, *Tetrahedron Letters* **1998**, *39*, 4565-4568
- 32) "Molecular Mechanics (MM3*) Parameters for Ruthenium(II) Pyridyl complexes"
Peter Brandt, Thomas Norrby, Björn Åkermark, and Per-Ola Norrby, *Inorg. Chem.* **1998**, *37*, 4120-4127
- 33) "Conformational Energy Penalties of Protein-Bound Ligands"
Jonas Boström, Per-Ola Norrby, and Tommy Liljefors, *J. Comp.-Aid. Mol. Des.* **1998**, *12*, 383-396
- 34) "Reagent Control of Geometric Selectivity and Enantiotopic Group Preference in Asymmetric Horner-Wadsworth-Emmons Reactions with meso-Dialdehydes"
Joshua S. Tullis, Lauri Vares, Nina Kann, Per-Ola Norrby, and Tobias Rein, *J. Org. Chem.* **1998**, *63*, 8284-8294
- 35) "A Solvated Transition State for the Nucleophilic Attack on Cationic η^3 -Allylpalladium Complexes"
Helena Hagelin, Björn Åkermark, and Per-Ola Norrby, *Chem. Eur. J.* **1999**, *5*, 902-909
- 36) "Strong Decrease of the Benzene-Ammonium Ion Interaction upon Complexation with a Carboxylate Anion"
Per-Ola Norrby and Tommy Liljefors, *J. Am. Chem. Soc.*, **1999**, *121*, 2303-2306
- 37) "Timing Is Critical: Effect of Spin Changes on the Diastereoselectivity in Mn(salen)-Catalyzed Epoxidation"
Christian Linde, Björn Åkermark, Per-Ola Norrby, and Mats Svensson, *J. Am. Chem. Soc.*, **1999**, *121*, 5083-5084
- 38) "New Molecular Mechanics (MM3*) Force Field Parameters for Calculations on (η^3 -Allyl)palladium Complexes with Nitrogen and Phosphorus Ligands"
Helena Hagelin, Björn Åkermark, and Per-Ola Norrby, *Organometallics*, **1999**, *18*, 2884-2895
- 39) "Asymmetric Horner-Wadsworth-Emmons reactions with meso-dialdehydes: Scope, mechanism, and synthetic applications"
Tobias Rein, Lauri Vares, Ikuo Kawasaki, Torben M. Pedersen, Per-Ola Norrby, Peter Brandt, and David Tanner, *Phosphorus Sulfur and Silicon and the related elements* **1999**, *146*, 169-172

- 40) "Rationalization of Product Selectivities in Asymmetric Horner-Wadsworth-Emmons Reactions by Use of a New Method for Transition-State Modeling"
Per-Ola Norrby, Peter Brandt, and Tobias Rein, *J. Org. Chem.*, **1999**, *64*, 5845-5852
- 41) "Molecular Mechanics (MM3*) Force Field Parameters for Calculations on Palladium Olefin Complexes with Phosphorus Ligands"
Helena Hagelin, Mats Svensson, Björn Åkermark, and Per-Ola Norrby, *Organometallics*, **1999**, *18*, 4574-4583
- 42) "Rationalizing the Stereoselectivity of Osmium Tetroxide Asymmetric Dihydroxylations with Transition State Modeling Using Quantum Mechanics-Guided Molecular Mechanics"
Per-Ola Norrby, Torben Rasmussen, Jan Haller, Thomas Strassner, and K. N. Houk, *J. Am. Chem. Soc.*, **1999**, *121*, 10186-10192.
- 43) "Selectivity and Reactivity in Asymmetric Allylic Alkylation"
Christina Moberg, Ulf Bremberg, Kristina Hallman, Mats Svensson, Per-Ola Norrby, Anders Hallberg, Mats Larhed, and Ingeborg Csöreg, *Pure Appl. Chem.*, **1999**, *71*, 1477-1483
- 44) "Quantum Mechanical Conformational Analysis of β -Alanine Zwitterion in Aqueous Solution"
Peter Aadal Nielsen, Per-Ola Norrby, Tommy Liljefors, Nadia Rega, and Vincenzo Barone, *J. Am. Chem. Soc.*, **2000**, *122*, 3151-3155
- 45) "Selectivity in asymmetric synthesis from QM-guided molecular mechanics"
Per-Ola Norrby, *J. Mol. Struct. (Theochem)*, **2000**, *506*, 9-16
- 46) "Mechanistic Studies of Copper-Catalyzed Alkene Aziridination"
Peter Brandt, Mikael J. Södergren, Pher G. Andersson, and Per-Ola Norrby, *J. Am. Chem. Soc.*, **2000**, *122*, 8013-8020
- 47) "Chiral Recognition Among Trisdiimine-Metal Complexes, 7. Racemic Compound Formation versus Conglomerate Formation with $[M(\text{bpy})_3](\text{PF}_6)_2$ ($M = \text{Ni, Zn, Ru}$); Lattice Energy Minimisations and Implications for Structure Prediction"
Josef Brey, Holger Domel, and Per-Ola Norrby, *Eur. J. Inorg. Chem.* **2000**, 2409-2419
- 48) "Theoretical Investigation of Steric and Electronic Effects in Coenzyme B₁₂ Models"
Kasper P. Jensen, Stephan P. A. Sauer, Tommy Liljefors, and Per-Ola Norrby, *Organometallics* **2001**, *20*, 550-556
- 49) "Unprecedented Migration of *N*-Alkoxy carbonyl Groups in Protected Pyroglutaminol"
Lennart Bunch, Per-Ola Norrby, Karla Frydenvang, Povl Krogsgaard-Larsen, and Ulf Madsen, *Org. Lett.* **2001**, *3*, 433-435
- 50) "Deriving Force Field Parameters for Coordination Complexes"
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