

**Peter H.M. Budzelaar**  
**List of Publications**

**2011**

- 134.** Budzelaar P.H.M.  
Mechanisms of branch formation in metal-catalyzed ethene polymerization  
*Comp. Mol. Sci.* **2011**, asap
- 133.** Fowler, K.G.; Littlefield, S.L.; Baird, M.C.; Budzelaar P.H.M.  
Synthesis, Structures, and Properties of the Phosphonium-1-indenylide (PHIN) Ligands 1-C<sub>9</sub>H<sub>6</sub>PPh<sub>3</sub>, 1-C<sub>9</sub>H<sub>6</sub>PMePh<sub>2</sub>, and 1-C<sub>9</sub>H<sub>6</sub>PMe<sub>2</sub>Ph and of the Corresponding Ruthenium(II) Complexes [Ru( $\eta^5$ -C<sub>5</sub>H<sub>5</sub>)( $\eta^5$ -PHIN)]PF<sub>6</sub>  
*Organometallics* **2011**, *30*, 6098-6107
- 132.** Ciancaleoni, G.; Fraldi, N.; Budzelaar, P.H.M.; Busico, V.; Macchioni, A.  
Structure and Dynamics in Solution of Bis(phenoxy-amine)Zirconium Catalysts for Olefin Polymerization  
*Organometallics* **2011**, *30*, 3096-3105
- 131.** Zhu, D.; Thapa, I.; Korobkov, I.; Gambarotta, S.; Budzelaar P.H.M.  
Redox-Active Ligands and Organic Radical Chemistry  
*Inorg. Chem.* **2011**, *50*, 9879-9887
- 130.** Bouwkamp, M.W.; Budzelaar, P.H.M.; Meetsma, A.; Hessen, B.  
Reactivity of cationic decamethylmetallocene complexes towards ketones  
*J. Organomet. Chem.* **2011**, *696*, 1920-1924
- 129.** Budzelaar, P.H.M.  
Radical Chemistry of Iminepyridine Ligands  
*Eur. J. Inorg. Chem.* **2011**, asap
- 128.** Jabri, A.; Budzelaar, P.H.M.  
DFT Study of Pd(PMe<sub>3</sub>)/NMe<sub>3</sub>-Catalyzed Butadiene Telomerization of Methanol  
*Organometallics* **2011**, *30*, 1374-1381
- 127a.** Shamov, G.A.; Schreckenbach, G.; Budzelaar, P.H.M.  
Stability of Hydrocarbons of the Polyhedrane Family Containing Bridged CH Groups: A Case of Failure of the Colle-Salvetti Correlation Density Functionals (erratum)  
*J. Chem. Theory Comput.* **2011**, *7*, 804-806

**2010**

- 127.** Shamov, G.A.; Schreckenbach, G.; Budzelaar, P.H.M.  
Stability of Hydrocarbons of the Polyhedrane Family Containing Bridged CH Groups: A Case of Failure of the Colle-Salvetti Correlation Density Functionals  
*J. Chem. Theory Comput.* **2010**, *6*, 3442-3455
- 126.** Zhu, D.; Budzelaar, P.H.M.  
Binuclear Oxidative Addition of Aryl Halides  
*Organometallics* **2010**, *29*, 5759-5761
- 125.** Ciancaleoni, G.; Fraldi, N.; Budzelaar, P.H.M.; Busico, V.; Cipullo, R.; Macchioni, A.  
Structure-Activity Relationship in Olefin Polymerization Catalysis: Is Entropy the Key?  
*J. Am. Chem. Soc.* **2010**, *132*, 13651-13653

**124.** Sauriol, F.; Sonnenberg, J.F.; Chadder, S.J.; Dunlop-Brière, A.F.; Baird, M.C.; Budzelaar, P.H.M.

Remarkable Reactions and Intermediates in Titanocene(IV) Chemistry: Migratory Insertion Reactions of 2,2-Disubstituted-1-alkenes, Intramolecular 1,5- $\sigma$  Bond Metathesis via  $\epsilon$ -Agostic Interactions, and a Rare Example of a  $\beta$ -Agostic Alkyltitanocene Complex

*J. Am. Chem. Soc.* **2010**, *132*, 13357-13370

**123.** Zhu, D.; Janssen, F.F.B.J.; Budzelaar, P.H.M.

(Py)<sub>2</sub>Co(CH<sub>2</sub>SiMe<sub>3</sub>)<sub>2</sub> As an Easily Accessible Source of "CoR<sub>2</sub>"

*Organometallics* **2010**, *29*, 1897-908

**122.** Shamov, G.A.; Budzelaar, P.H.M.; Schreckenbach, G.

Performance of the Empirical Dispersion Corrections to Density Functional Theory: Thermodynamics of Hydrocarbon Isomerizations and Olefin Monomer Insertion Reactions

*J. Chem. Theory Comput.* **2010**, *6*, 477-90

## 2009

**121.** Ciancaleoni, G.; Fraldi, N.; Budzelaar, P.H.M.; Busico, V.; Macchioni, A.

Activation of a bis(phenoxy-amine) precatalyst for olefin polymerisation: first evidence for an outer sphere ion pair with the methylborate counterion

*Dalton Trans.* **2009**, 8824-7

**120.** Credendino, R.; Busico, V.; Causà, M.; Barone, V.; Budzelaar, P.H.M.; Zicovich-Wilson, C.

Periodic DFT modeling of bulk and surface properties of MgCl<sub>2</sub>

*Phys. Chem. Chem. Phys.* **2009**, *11*, 6525-32

**119.** Budzelaar, P.H.M.

Ethene trimerization at Cr<sup>I</sup>/Cr<sup>III</sup> - A density functional theory (DFT) study

*Can. J. Chem.* **2009**, *87*, 832-7

## 2008

**118.** Talarico, G.; Budzelaar, P.H.M.

Variability of Chain Transfer to Monomer Step in Olefin Polymerization

*Organometallics* **2008**, *27*, 4098-107

**117.** Zhu, D.; Budzelaar, P. H. M.

A Measure for  $\sigma$ -Donor and  $\pi$ -Acceptor Properties of Diiminepyridine-Type Ligands

*Organometallics* **2008**, *27*, 2699-705

**116.** Coussens, B. B.; van Besien, E.; Budzelaar, P. H. M.; Friederichs, N.

Toward a Better Understanding of the Reactivity of Titanium and Zirconium Complexes with an Aryl-Substituted Tripodal Triamido Ligand Derived from cis,cis-1,3,5-Triaminocyclohexane: A Density Functional Study

*Organometallics* **2008**; *27*, 1804-8

**115.** Scott, J.; Vidyaratne, I.; Korobkov, I.; Gambarotta, S.; Budzelaar, P. H. M.

Multiple Pathways for Dinitrogen Activation during the Reduction of an Fe Bis(iminepyridine) Complex

*Inorg. Chem.* **2008**, *47*, 896-911

## 2007

114. Shapiro, P.J.; Sinnema, P.J.; Perrotin, P.; Budzelaar, P.H.M.; Weihe, H.; Twamley, B.; Zehnder, R.A.; Nairn, J.J.  
Ring-Borylated 15-Electron and 17-Electron *ansa*-Chromocene Complexes, their Physical Properties and Molecular Structures  
*Chem. Eur. J.* **2007**, *13*, 6212–22
113. Vidyaratne, I.; Scott, J.; Gambarotta, S.; Budzelaar, P.H.M.  
Dinitrogen Activation, Partial Reduction, and Formation of Coordinated Imide Promoted by a Chromium Diiminepyridine Complex  
*Inorg. Chem.* **2007**, *46*, 7040–49
112. Jellema, E.; Budzelaar, P.H.M.; Reek, J.N.H.; De Bruin, B.  
Rh-Mediated Polymerization of Carbenes: Mechanism and Stereoregulation  
*J. Am. Chem. Soc.* **2007**, *129*, 11631–41
111. Budzelaar, P.H.M.; Coussens, B.B.; Friederichs, N.  
Hydrogen sensitivity – A systematic computational study of electronic effects  
*J. Organomet. Chem.* **2007**, *692*, 4473–80
110. Budzelaar, P.H.M.  
Geometry Optimization Using Generalized, Chemically Meaningful Constraints  
*J. Comput. Chem.* **2007**, *28*, 2226–36
109. Nikiforov, G.B.; Crewdson, P.; Gambarotta, S.; Korobkov, I.; Budzelaar, P.H.M.  
Reduction of Titanium Supported by a  $\sigma$ -/ $\pi$ -Bonded Tripyrrole Ligand: Ligand C-N Bond Cleavage and Coordination of Olefin and Arene with an Inverse Sandwich Structure  
*Organometallics* **2007**, *26*, 48–55

## 2006

108. Knijnenburg, Q.; Gambarotta, S.; Budzelaar, P.H.M.  
Ligand-centred reactivity in diiminepyridine complexes  
*Dalton Trans.* **2006**, 5442–8
107. Phull, H.; Alberti, D.; Korobkov, I.; Gambarotta, S.; Budzelaar, P.H.M.  
Fixation of CO<sub>2</sub> by Magnesium Cations: A Reinterpretation  
*Angew. Chem. I.E.* **2006**, *45*, 5331–4
106. Talarico, G.; Budzelaar, P.H.M.  
A Second Transition State for Chain Transfer to Monomer in Olefin Polymerization Promoted by Group 4 Metal Catalysts  
*J. Am. Chem. Soc.* **2006**, *128*, 4524–5
105. Knijnenburg, Q.; Smits, J. M. M.; Budzelaar, P. H. M.  
Reaction of the Diimine Pyridine Ligand with Aluminum Alkyls: An Unexpectedly Complex Reaction  
*Organometallics* **2006**, *25*, 1036–46
104. Shapiro, P.J.; Zehnder, R.; Foo, D.M.; Perrotin, P.; Budzelaar, P.H.M.; Leitch, S.; Twamley, B.  
*ansa*-Chromocene Complexes. 2. Isocyanide Derivatives of Cr(II) and Cr(III), Their Syntheses, X-ray Crystal Structures, and Physical Properties  
*Organometallics* **2006**, *25*, 719–32

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- 103.** Scott, J.; Gambarotta, S.; Korobkov, I.; Knijnenburg, Q.; De Bruin, B.; Budzelaar, P.H.M.  
Formation of a Paramagnetic Al Complex and Extrusion of Fe during the Reaction of (Diiminepyridine)Fe with  $AlR_3$  (R = Me, Et)  
*J. Am. Chem. Soc.* **2005**, *127*, 17204-6
- 102.** Friederichs, N.; Wang, B.; Budzelaar, P.H.M.; Coussens, B.B.  
A combined experimental-molecular modeling approach for ethene-propene copolymerization with  $C_2$ -symmetric metallocenes  
*J. Mol. Catal. A* **2005**, *242*, 91-104
- 101.** Scott, J.; Gambarotta, S.; Korobkov, I.; Budzelaar, P.H.M.  
Reduction of (Diiminopyridine)iron: Evidence for a Noncationic Polymerization Pathway?  
*Organometallics* **2005**, *24*, 6298-300
- B3.** Drent, E.; Van Broekhoven, J.A.M.; Budzelaar, P.H.M.  
"Alternating copolymers from alkenes and carbon monoxide", p 244-56 in  
"Multiphase Homogeneous Catalysis"  
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- 100.** Scott, J.; Gambarotta, S.; Korobkov, I.; Budzelaar, P.H.M.  
Metal versus Ligand Alkylation in the Reactivity of the (Bis-iminopyridinato)Fe Catalyst  
*J. Am. Chem. Soc.* **2005**, *127*, 13019-29
- 99.** Bouwkamp, M.W.; Budzelaar, P.H.M.; Gercama, J.; Del Hierro Morales, I.; de Wolf, J.; Meetsma, A.; Troyanov, S.I.; Teuben, J.H.; Hessen, B.;  
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*J. Am. Chem. Soc.* **2005**, *127*, 14310-9
- 98.** Nijhuis, C.A.; Jellema, E.; Sciarone, T.J.J.; Meetsma, A.; Budzelaar, P.H.M.; Hessen, B.  
First-Row Transition Metal Bis(amidinate) Complexes; Planar Four-Coordination of  $Fe^{II}$  Enforced by Sterically Demanding Aryl Substituents  
*Eur. J. Inorg. Chem.* **2005**, 2089-99
- 97.** Knijnenburg, Q.; Horton, A.D.; Van der Heijden, H.; Kooistra, T.M.; Hettterscheid, D.G.H.; Smits, J.M.M.; De Bruin, B.; Budzelaar, P.H.M.; Gal, A.W.  
Olefin hydrogenation using diimine pyridine complexes of Co and Rh  
*J. Mol. Catal. A* **2005**, *232*, 151-9
- 96.** Vidyaratne, I.; Gambarotta, S.; Korobkov, I.; Budzelaar, P. H. M.  
Dinitrogen Partial Reduction by Formally Zero- and Divalent Vanadium Complexes Supported by the Bis-iminopyridine System  
*Inorg. Chem.* **2005**, *44*, 1187-9
- 95.** De Pater, B.C.; Frühauf, H.-W.; Goubitz, K.; Fraanje, J.; Budzelaar, P.H.M.; Gal, A.W.; Vrieze, K.  
Crystal structure of the novel neutral octahedral complex  
[ $(4'-(4\text{-}t\text{butylphenyl})-2,2':6',2''\text{-terpyridine})Rh^{III}(\text{Br})(\text{acetylonyl})_2$ ]  
*Inorg. Chim. Acta* **2005**, *358*, 431-6

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*Inorg. Chem.* **2004**, *43*, 5771-9
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*Angew. Chem. I.E.* **2004**, *43*, 4142-57
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Mechanism of oxidation of  $Rh^I$  and  $Ir^I$  olefin complexes by  $H_2O_2$   
*Eur. J. Inorg. Chem.* **2004**, 2385-91
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*Eur. J. Inorg. Chem.* **2004**, 1204-11
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Chemical ligand non-innocence in pyridine diimine Rh complexes  
*Inorg. Chim. Acta* **2004**, *357*, 2945-52
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- P5.** Knijnenburg, Q.; Horton, A.D.; Van der Heijden, H.; Gal, A.W.; Budzelaar, P.H.M.  
Preparation of Co(I), Fe(I) and Fe(II) pyridine diimine complexes as hydrogenation catalysts and process for catalytic hydrogenation of unsaturated organic compounds  
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- 80.** Budzelaar, P.H.M.; Talarico, G.  
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- 79.** Sugiyama, H.; Aharonian, G.; Gambarotta, S.; Yap, G.P.A.; Budzelaar, P.H.M.  
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- 78.** Enright, D.; Gambarotta, S.; Yap, G.P.A.; Budzelaar, P.H.M.  
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- 74.** Borrelli, M.; Busico, V.; Cipullo, R.; Ronca, S.; Budzelaar, P.H.M.  
Selectivity of Metallocene-Catalyzed Olefin Polymerization: A Combined Experimental and Quantum Mechanical Study. 1. Nonchiral Bis(cyclopentadienyl) Systems  
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- 73.** Willems, S.T.H.; Russcher, J.C.; Budzelaar, P.H. M.; De Bruin, B.; De Gelder, R.; Smits, J.M.M.; Gal, A.W.  
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