

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

**2017**

- 174.** Zhang, N.; Sherbo, R.S.; Bindra, G.S.; Zhu, D.; Budzelaar, P.H.M.  
Rh and Ir beta-Diiminato Complexes of Boranes, Silanes, Germanes, and Stannanes  
*Organometallics* **2017**, *36*, 4123–4135 - DOI 10.1021/acs.organomet.7b00469
- 173.** Rocchigiani, L.; Fernandez-Cestau, J.; Agonigi, G.; Chambrier, I.; Budzelaar, P. H. M.;  
Bochmann, M.  
Gold(III) Alkyne Complexes: Bonding and Reaction Pathways  
*Angew. Chem. Int. Ed.* **2017**, *56*, 13861–13865 - DOI 10.1002/anie.201708640
- 172.** Zaccaria, F.; Cipullo, R.; Budzelaar, P.H.M.; Busico, V.; Ehm, C.  
Backbone rearrangement during olefin capture as the rate limiting step in molecular  
olefin polymerization catalysis and its effect on comonomer affinity  
*J. Polymer Sci. A* **2017**, *55*, 2807–2814 - DOI 10.1002/pola.28685
- 171.** Ehm, C.; Budzelaar, P.H.M.; Busico, V.  
Tuning the Relative Energies of Propagation and Chain Termination Barriers in  
Polyolefin Catalysis through Electronic and Steric Effects  
*Eur. J. Inorg. Chem.* **2017**, *27*, 3343–3349 - DOI 10.1002/ejic.201700398
- 170.** Manzoor, A.; Wienefeld, P.; Baird, M.C.; Budzelaar, P.H.M.  
Catalysis of Cross-Coupling and Homocoupling Reactions of Aryl Halides Utilizing  
Ni(0), Ni(I), and Ni(II) Precursors; Ni(0) Compounds as the Probable Catalytic  
Species but Ni(I) Compounds as Intermediates and Products  
*Organometallics* **2017**, *36*, 3508–3519 - DOI 10.1021/acs.organomet.7b00446
- 169.** Rahimi, N.; de Bruin, B.; Budzelaar, P.H.M.  
Balance between Metal and Ligand Reduction in Diiminepyridine Complexes of Ti  
*Organometallics* **2017**, *35*, 3189–3198 - DOI 10.1021/acs.organomet.7b00239  
(also issue cover)
- 168.** Rocchigiani, L.; Fernandez-Cestau, J.; Budzelaar, P.H.M.; Bochmann, M.  
Arene C–H activation by gold(III): solvent-enabled proton shuttling, and observation  
of a pre-metallation Au–arene intermediate  
*Chem. Commun.* **2017**, *53*, 4358–4361 - DOI 10.1039/c7cc01628j
- 167.** Ehm, C.; Budzelaar, P.H.M.; Busico, V.  
Metal–carbon bond strengths under polymerization conditions: 2,1-insertion as a  
catalyst stress test  
*J. Catal.* **2017**, *351*, 146–152 - DOI 10.1016/j.jcat.2017.04.013
- 166.** Talarico, G.; Budzelaar, P.H.M.  
Ligand Coordination Driven by Monomer and Polymer Chain: The Intriguing Case of  
Salalen–Ti Catalyst for Propene Polymerization  
*Macromolecules* **2017**, *50*, 5332–5336 - DOI 10.1021/acs.macromol.7b00846
- 165.** Zaccaria, F.; Ehm, C.; Budzelaar, P.H.M.; Busico, V.  
Accurate Prediction of Copolymerization Statistics in Molecular Olefin Polymerization  
Catalysis: The Role of Entropic, Electronic, and Steric Effects in Catalyst  
Comonomer Affinity  
*ACS Catal.*, **2017**, *7*, 1512–1519 - DOI 10.1021/acscatal.6b03458

164. Chambrier, I.; Roşca, D.A.; Fernandez-Cestau, J.; Hughes, D.L.; Budzelaar, P.H.M.; Bochmann, M.  
Formation of Gold(III) Alkyls from Gold Alkoxide Complexes  
*Organometallics*, **2017**, *36*, 1358–1364 - DOI 10.1021/acs.organomet.7b00077

## 2016

163. Boulho, C.; Zijlstra, H.S.; Hofmann, A.; Budzelaar, P.H.M.; Harder, S.  
Insight into Oxide-Bridged Heterobimetallic Al/Zr Olefin Polymerization Catalysts  
*Chem. Eur. J.* **2016**, *22*, 17450–17459 - DOI 10.1002/chem.201602674
162. Ehm, C.; Cipullo, R.; Budzelaar, P. H. M.; Busico, V.  
Role(s) of TMA in polymerization  
*Dalton Trans.* **2016**, *45*, 6847–6855 - DOI 10.1039/c5dt04895h
161. Ehm, C.; Cipullo, R.; Passaro, M.; Zaccaria, F.; Budzelaar, P. H. M.; Busico, V.  
Chain Transfer to Solvent in Propene Polymerization with Ti Cp-phosphinimide Catalysts: Evidence for Chain Termination via Ti–C Bond Homolysis  
*ACS Catalysis* **2016**, *6*, 7989–7993 - DOI 10.1021/acscatal.6b02738
160. Pintus, A.; Rocchigiani, L.; Fernandez-Cestau, J.; Budzelaar, P.H.M.; Bochmann, M.  
Stereo- and Regioselective Alkyne Hydrometallation with Gold(III) Hydrides  
*Angew. Chem. Int. Ed.* **2016**, *55*, 12321–12324 - DOI 10.1002/anie.201607522  
(VIP, highlighted in "Chemistry Views")
159. Yu, Y.; Busico, V.; Budzelaar, P.H.M.; Vittoria, A.; Cipullo, R.  
Of Poisons and Antidotes in Polypropylene Catalysis  
*Angew. Chem. Int. Ed.* **2016**, *55*, 8590–8594 - DOI 10.1002/anie.201602485
158. Sherbo, R.S.; Bindra, G.S.; Budzelaar, P.H.M.  
Square-Planar–Tetrahedral Interconversion without Spin Flip in ( $\beta$ -diimine)Rh(1,3-diene) Complexes  
*Organometallics* **2016**, *35*, 2039–2048 - DOI 10.1021/acs.organomet.6b00328
157. Talarico, G.; Budzelaar, P.H.M.  
 $\alpha$ -Agostic Interactions and Growing Chain Orientation for Olefin Polymerization Catalysts  
*Organometallics* **2016**, *35*, 47–54 - DOI 10.1021/acs.organomet.5b00866

## 2015

156. Dunlop-Briere, A.F.; Baird, M.C.; Budzelaar, P.H.M.  
[Cp<sub>2</sub>TiCH<sub>2</sub>CH<sub>2</sub>(SiEt<sub>2</sub>CHMe<sub>2</sub>)]<sup>+</sup>, an Alkyl-titanocene(IV) Complex Containing an Unconventional Ti  $\leftarrow$  C( $\beta$ )-Si Mode of Bonding  
*Organometallics* **2015**, *34*, 5245–5253 - DOI 10.1021/acs.organomet.5b00675
155. Zhu, D.; Sharma, A.Z.; Wiebe, C.R.; Budzelaar, P.H.M.  
Rhodium(II) dimers without metal-metal bonds  
*Dalton Trans.* **2015**, *44*, 13460–13463 - DOI 10.1039/c5dt02218e
154. Dunlop-Briere, A.F.; Baird, M.C.; Budzelaar, P.H.M.  
Mechanisms of  $\alpha$ -,  $\beta$ -, and  $\gamma$ -H(D) Exchange Processes in the  $\alpha$ -Agostic Alkyltitanocene(IV) Complexes [Cp<sub>2</sub>TiCH<sub>2</sub>CH(CH<sub>3</sub>)(CMe<sub>3</sub>)]<sup>+</sup> and [Cp<sub>2</sub>TiCH<sub>2</sub>CH(CD<sub>3</sub>)(CMe<sub>3</sub>)]<sup>+</sup>: Stark Contrasts with Their  $\gamma$ -SiMe<sub>3</sub> Analogue  
*Organometallics* **2015**, *34*, 2356–2368 - DOI 10.1021/om5011462

**153.** Purdavaie, K.; Baird, M.C.; Budzelaar, P.H.M.  
Synthesis and structure of a new phosphonium-1-indenylide (PHIN) ligand, 4,7-dimethyl-1-C<sub>9</sub>H<sub>4</sub>PMePh<sub>2</sub>, and of new PHIN complexes of rhodium and iridium  
*New J. Chem.* **2015**, *39*, 9429-9441 - DOI 10.1039/c5nj01756d

**152.** Ehm, C.; Budzelaar, P.H.M.; Busico, V.  
Calculating accurate barriers for olefin insertion and related reactions  
*J. Organomet. Chem.* **2015**, *775*, 39-49 - DOI 10.1016/j.jorganchem.2014.10.019

## 2014

**151.** Ehm, C.; Antinucci, G.; Budzelaar, P.H.M.; Busico, V.  
Catalyst activation and the dimerization energy of alkylaluminium compounds  
*J. Organomet. Chem.* **2014**, *772*, 161-171 - DOI 10.1016/j.jorganchem.2014.09.013

**150.** Talarico, G.; Budzelaar, P.H.M.  
Analysis of Stereochemistry Control in Homogeneous Olefin Polymerization Catalysis  
*Organometallics* **2014**, *33*, 5974-5982 - DOI 10.1021/om5003655

**149.** Alzamly, A.; Gambarotta, S.; Korobkov, I.; Murugesu, M.; Le Roy, J.J.H.; Budzelaar, P.H.M.  
Isolation of a Hexanuclear Chromium Cluster with a Tetrahedral Hydridic Core and Its Catalytic Behavior for Ethylene Oligomerization  
*Inorg. Chem.* **2014**, *53*, 6073-6081 - DOI 10.1021/ic500445b

**148.** Langer, N.N.P.; Bindra, G.S.; Budzelaar, P.H.M.  
C-H and C-O bond activation with a rhodium(I) beta-diiminate complex  
*Dalton Trans.* **2014**, 11286-11294 - DOI 10.1039/c4dt00309h

## 2013

**147.** Capone, F.; Rongo, L.; D'Amore, M.; Budzelaar, P.H.M.; Busico, V.  
Periodic Hybrid DFT Approach (Including Dispersion) to MgCl<sub>2</sub>-Supported Ziegler-Natta Catalysts. 2. Model Electron Donor Adsorption on MgCl<sub>2</sub> Crystal Surfaces  
*J. Phys. Chem.* **2013**, *117*, 24345-24353 - DOI 10.1021/jp406977h

**146.** Dunlop-Briere, A.F.; Baird, M.C.; Budzelaar, P.H.M.  
[Cp<sub>2</sub>TiCH<sub>2</sub>CHMe(SiMe<sub>3</sub>)]<sup>+</sup>, an Alkyl-Titanium Complex Which (a) Exists in Equilibrium between a β-Agostic and a Lower Energy γ-Agostic Isomer and (b) Undergoes Hydrogen Atom Exchange between α-, β-, and γ-Sites via a Combination of Conventional β-Hydrogen Elimination-Reinsertion and a Nonconventional CH Bond Activation Process Which Involves Proton Tunnelling  
*J. Am. Chem. Soc.* **2013**, *135*, 17514-17527 - DOI 10.1021/ja4092775

**145.** Zhu, D.; Budzelaar, P.H.M.  
N-Aryl β-diiminate complexes of the platinum metals  
*Dalton Trans.* **2013**, *42*, 11343-11354 - DOI 10.1039/c3dt50715g

**144.** Shuster, V.; Gambarotta, S.; Nikiforov, G.B.; Budzelaar, P.H.M.  
Heterometallic Aluminum-Chromium Phenazine and Thiophenazine Complexes. Formation of a Tetranuclear Chromium(I) Sandwich Complex  
*Organometallics* **2013**, *32*, 2329-2335 - DOI 10.1021/om3012097

## 2012

- 143.** Ylijoki, K.E.O.; Budzelaar, P.H.M.; Stryker, J.M.  
A Density Functional Theory Investigation of the Cobalt-Mediated  $\eta^5$ -Pentadienyl/Alkyne [5+2] Cycloaddition Reaction: Mechanistic Insight and Substituent Effects  
*Chem. Eur. J.* **2012**, *18*, 9894–9900 - DOI 10.1002/chem.201200319
- 142.** D'Amore, M.; Credendino, R.; Budzelaar, P.H.M.; Causa, M.; Busico, V.  
A periodic hybrid DFT approach (including dispersion) to  $\text{MgCl}_2$ -supported Ziegler-Natta catalysts - 1:  $\text{TiCl}_4$  adsorption on  $\text{MgCl}_2$  crystal surfaces  
*J. Catal.* **2012**, *286*, 103–110 - DOI 10.1016/j.jcat.2011.10.018
- 141.** Hussain, R.; Fowler, K.G.; Sauriol, F.; Baird, M.C.; Budzelaar, P.H.M.  
Synthesis and Ruthenium Coordination Complexes of the Chelating Phosphine Phosphonium-1-indenylide 1,1-Bis(diphenylphosphino)methane-1-indenylide,  $\text{C}_9\text{H}_6\text{Ph}_2\text{PCH}_2\text{PPh}_2$   
*Organometallics* **2012**, *31*, 6926–6932 - DOI 10.1021/Om300715a
- 140.** Zhu, D.; Kozera, D.J.; Enns, K.D.; Budzelaar, P.H.M.  
Cascade Activation of SiH, CH, and SiC Bonds at a Rhodium  $\beta$ -Diiminate Complex  
*Angewandte Chemie IE* **2012**, *51*, 12211–12214 - DOI 10.1002/anie.201206751
- 139.** Ciancaleoni, G.; Fraldi, N.; Cipullo, R.; Busico, V.; Macchioni, A.; Budzelaar, P.H.M.  
Structure/Properties Relationship for Bis(phenoxyamine)Zr(IV)-Based Olefin Polymerization Catalysts: A Simple DFT Model To Predict Catalytic Activity  
*Macromolecules* **2012**, *45*, 4046–4053 - DOI 10.1021/Ma300343c
- 138.** Shuster, V.; Gambarotta, S.; Nikiforov, G.B.; Korobkov, I.; Budzelaar, P.H.M.  
Radical Cleavage of Al–C Bonds Promoted by Phenazine: From Noninnocent Ligand to Radical Abstractor  
*Organometallics* **2012**, *31*, 7011–7019 - DOI 10.1021/Om300889m
- 137.** Zhu, D.; Korobkov, I.; Budzelaar, P.H.M.  
Radical Mechanisms in the Reaction of Organic Halides with Diiminepyridine Cobalt Complexes  
*Organometallics* **2012**, *31*, 3958–3971 - DOI 10.1021/Om300182c
- 136.** Dunlop-Brière, A.F.; Budzelaar, P.H.M.; Baird, M.C.  
 $\alpha$ - and  $\beta$ -Agostic Alkyl–Titanocene Complexes  
*Organometallics* **2012**, *31*, 1591–1594 - DOI 10.1021/Om3001197
- 135.** Thapa, I.; Gambarotta, S.; Korobkov, I.; Murugesu, M.; Budzelaar, P.H.M.  
Isolation and Characterization of a Class II Mixed-Valence Chromium(I)/(II) Self-Activating Ethylene Trimerization Catalyst  
*Organometallics* **2012**, *31*, 486–494 - DOI 10.1021/Om201181n
- 134.** Budzelaar, P.H.M.  
Radical Chemistry of Iminepyridine Ligands  
*Eur. J. Inorg. Chem.* **2012**, 530–534 - DOI 10.1002/ejic.201100698
- 133.** Budzelaar P.H.M.  
Mechanisms of branch formation in metal-catalyzed ethene polymerization  
*WIREs Comput. Mol. Sci.* **2012**, 221–241 - DOI 10.1002/Wcms.79

## 2011

- 132.** 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(η<sup>5</sup>-C<sub>5</sub>H<sub>5</sub>)(η<sup>5</sup>-PHIN)]PF<sub>6</sub>  
*Organometallics* **2011**, *30*, 6098-6107 - DOI 10.1021/om200545j
- 131.** 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 - DOI 10.1021/om2001926
- 130.** 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 - DOI 10.1021/ic2002145
- 129.** 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 - DOI 10.1016/j.jorganchem.2011.02.023
- 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 - DOI 10.1021/om1008617
- 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 - DOI - DOI 10.1021/ct200004s

## 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 - DOI 10.1021/ct100389d
- 126.** Zhu, D.; Budzelaar, P.H.M.  
Binuclear Oxidative Addition of Aryl Halides  
*Organometallics* **2010**, *29*, 5759-5761 - DOI 10.1021/om100811f
- 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 - DOI 10.1021/ja105965x
- 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-σ Bond Metathesis via ε-Agostic Interactions, and a Rare Example of a β-Agostic Alkyltitanocene Complex  
*J. Am. Chem. Soc.* **2010**, *132*, 13357-13370 - DOI 10.1021/ja104526v
- 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*, 1897-1908 - DOI 10.1021/om901045s

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*, 477–490 - DOI 10.1021/ct9005135

## 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**, 8824–8827 - DOI 10.1039/b908805a
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*, 6525–6532 - DOI 10.1039/b905676a
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*, 832–837 - DOI 10.1139/V09-022

## 2008

118. Talarico, G.; Budzelaar, P.H.M.  
Variability of Chain Transfer to Monomer Step in Olefin Polymerization  
*Organometallics* **2008**, *27*, 4098–4107 - DOI 10.1021/om800313n
117. Zhu, D.; Budzelaar, P. H. M.  
A Measure for  $\sigma$ -Donor and  $\pi$ -Acceptor Properties of Diiminepyridine-Type Ligands  
*Organometallics* **2008**, *27*, 2699–2705 - DOI 10.1021/om701160b
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*, 1804–1808 - DOI 10.1021/om7010744
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 - DOI 10.1021/ic701643d
- 111a. Coussens, B.B.; Budzelaar, P.H.M.; Friederichs, N.  
A systematic computational study of electronic effects on hydrogen sensitivity of olefin polymerization catalysts  
*J. Phys.-Condens. Matter* **2008**, *20*, 064241 - DOI 10.1088/0953-8984/20/6/064241

## 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*, 6212–6222 - DOI 10.1002/chem.200601901

- 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*, 7040-7049 - DOI 10.1021/ic700810f
- 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*, 11631-11641 - DOI 10.1021/ja073897+
- 111.** Budzelaar, P.H.M.; Coussens, B.B.; Friederichs, N.  
Hydrogen sensitivity – A systematic computational study of electronic effects  
*J. Organomet. Chem.* **2007**, *692*, 4473–4480 - DOI 10.1016/j.jorganchem.2007.04.030
- 110.** Budzelaar, P.H.M.  
Geometry Optimization Using Generalized, Chemically Meaningful Constraints  
*J. Comput. Chem.* **2007**, *28*, 2226–2236 - DOI 10.1002/jcc.20740
- 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 - DOI 10.1021/om060908j

## 2006

- 108.** Knijnenburg, Q.; Gambarotta, S.; Budzelaar, P.H.M.  
Ligand-centred reactivity in diiminepyridine complexes  
*Dalton Trans.* **2006**, 5442–5448 - DOI 10.1039/b612251e
- 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*, 5331–5334 - DOI 10.1002/anie.200601834
- 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*, 4524-4525 - DOI 10.1021/ja0586034
- 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*, 1036-1046 - DOI 10.1021/om050936m
- 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*, 719-732 - DOI 10.1021/om050710j

## 2005

- 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<sub>3</sub> (R = Me, Et)  
*J. Am. Chem. Soc.* **2005**, *127*, 17204-17206 - DOI 10.1021/ja056135s

- 102.** Friederichs, N.; Wang, B.; Budzelaar, P.H.M.; Coussens, B.B.  
A combined experimental-molecular modeling approach for ethene-propene copolymerization with C<sub>2</sub>-symmetric metallocenes  
*J. Mol. Catal. A* **2005**, *242*, 91-104 - DOI 10.1016/j.molcata.2005.06.066
- 101.** Scott, J.; Gambarotta, S.; Korobkov, I.; Budzelaar, P.H.M.  
Reduction of (Diiminopyridine)iron: Evidence for a Noncationic Polymerization Pathway?  
*Organometallics* **2005**, *24*, 6298-6300 - DOI 10.1021/om0507833
- B3.** Drent, E.; Van Broekhoven, J.A.M.; Budzelaar, P.H.M.  
"Alternating copolymers from alkenes and carbon monoxide", p 244-256 in "Multiphase Homogeneous Catalysis"  
eds Cornils, B.; Hermann, W.A.; Horváth, I.T.; Mecking, S.; Olivier-Bourbigou, H.; Vogt, D., VCH, Weinheim, **2005** - DOI
- 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*, 13019-13029 - DOI 10.1021/ja054152b
- 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.  
Naked (C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>M Cations (M = Sc, Ti, and V) and Their Fluoroarene Complexes  
*J. Am. Chem. Soc.* **2005**, *127*, 14310-14319 - DOI 10.1021/ja054544i
- 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<sup>II</sup> Enforced by Sterically Demanding Aryl Substituents  
*Eur. J. Inorg. Chem.* **2005**, 2089-2099 - DOI 10.1002/ejic.200500094
- 97.** Knijnenburg, Q.; Horton, A.D.; Van der Heijden, H.; Kooistra, T.M.; Hetterscheid, 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*, 151-159 - DOI 10.1016/j.molcata.2004.12.039
- 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*, 1187-1189 - DOI 10.1021/ic048358+
- 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-*t*butylphenyl)-2,2':6',2''-terpyridine)Rh<sup>III</sup>(Br)(acetylonyl)<sub>2</sub>]  
*Inorg. Chim. Acta* **2005**, *358*, 431-436 - DOI 10.1016/j.ica.2004.08.019

## 2004

- 94.** Sugiyama, H.; Korobkov, I.; Gambarotta, S.; Möller, A.; Budzelaar, P.H.M.  
Preparation, Characterization, and Magnetic Behavior of the Ln Derivatives (Ln = Nd, La) of a 2,6-Diiminepyridine Ligand and Corresponding Dianion  
*Inorg. Chem.* **2004**, *43*, 5771-5779 - DOI 10.1021/ic049820t
- 93.** Knijnenburg, Q.; Smits, J.M.M.; Budzelaar, P.H.M.  
Reaction of AlEt<sub>2</sub>Cl with the diiminepyridine ligand: an unexpected product  
*C. R. Chimie* **2004**, *7*, 865-869 - DOI 10.1016/j.crci.2004.03.012



92. De Bruin, B.; Budzelaar, P.H.M.; Gal, A.W.  
Functional models for rhodium-mediated olefin oxygenation catalysis  
*Angew. Chem. I.E.* **2004**, *43*, 4142-4157 - DOI 10.1002/anie.200300629
91. Budzelaar, P.H.M.; Blok, A.N.J.  
Mechanism of oxidation of Rh<sup>I</sup> and Ir<sup>I</sup> olefin complexes by H<sub>2</sub>O<sub>2</sub>  
*Eur. J. Inorg. Chem.* **2004**, 2385-2391 - DOI 10.1002/ejic.200300546
90. Knijnenburg, Q.; Hetterscheid, D.G.H.; Kooistra, T.M.; Budzelaar, P.H.M.  
The Electronic Structure of (Diiminopyridine)cobalt(I) Complexes  
*Eur. J. Inorg. Chem.* **2004**, 1204-1211 - DOI 10.1002/ejic.200300569
89. Kooistra, T.M.; Hetterscheid, D.G.H.; Schwartz, E; Knijnenburg, Q.; Budzelaar, P.H.M.; Gal, A.W.  
Chemical ligand non-innocence in pyridine diimine Rh complexes  
*Inorg. Chim. Acta* **2004**, *357*, 2945-2952 - DOI 10.1016/j.ica.2004.02.012
88. Budzelaar, P.H.M.  
CO/Ethene Copolymerization at Zirconocene Centers?  
*Organometallics* **2004**, *23*, 855-860 - DOI 10.1021/om0342863
87. De Pater, B.C.; Zijp, E.J.; Frühauf, H.-W.; Ernsting, J.M.; Elsevier, C.J.; Vrieze, K.; Budzelaar, P.H.M.; Gal, A.W.  
Oxidative Addition Reactions of [Rh<sup>I</sup>(Br)(Tpy\*)] (Tpy\* = 4'-(4-*tert*-Butylphenyl)-2,2':6',2''-terpyridine) with Alkyl Bromides  
*Organometallics* **2004**, *23*, 269-279 - DOI 10.1021/om0305418

## 2003

86. 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. The *ansa*-Me<sub>2</sub>Si(Ind)<sub>2</sub>Zr and Me<sub>2</sub>C(Cp)(Flu)Zr Systems  
*Macromolecules* **2003**, *36*, 8171-8177 - DOI 10.1021/ma034990v
85. Budzelaar, P.H.M.; Talarico, G.  
Insertion and β-hydrogen transfer at aluminium  
Group 13 Chemistry III: Industrial Applications:  
*Structure and Bonding* **2003**, *105*, 141-165 - DOI
84. Blok, A.N.J.; Budzelaar, P.H.M.; Gal, A.W.  
Mechanism of Ethene Trimerization at an *ansa*-(Arene)(cyclopentadienyl) Titanium Fragment  
*Organometallics* **2003**, *22*, 2564-2570 - DOI 10.1021/om030049o
83. Budzelaar, P.H.M.; Engelberts, J.J.; Van Lenthe, J.H.  
Trends in Cyclopentadienyl-Main-Group-Metal Bonding  
*Organometallics* **2003**, *22*, 1562-1576 - DOI 10.1021/om020928v
82. Kooistra, T.M.; Hekking, K.F.W.; Knijnenburg, Q.; De Bruin, B.; Budzelaar, P.H.M.; De Gelder, R.; Smits, J.M.M.; Gal, A.W.  
Cobalt Chloride Complexes of N3 and N4 Donor Ligands  
*Eur. J. Inorg. Chem.* **2003**, 648-655 - DOI
- 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  
*Int. Pat. Appl. WO2003042131 A1 20030522 (2003)*

81. Zhang, Y.; Budzelaar, P.H.M.; Smits, J.M.M.; De Gelder, R.; Hageman, P.R.; Gal, A.W. Reactions of cis-2,3-Dimethylaziridine, 3-Pyrroline and Pyrrolidine with Me<sub>3</sub>Al and Me<sub>3</sub>Ga: Adducts and Dimeric Amides  
*Eur. J. Inorg. Chem.* **2003**, 656-665 - DOI

## 2002

80. Budzelaar, P.H.M.; Talarico, G.  
Mono- and dinuclear olefin polymerization at aluminum  
*ACS Symposium Series* **2002**, 822, 142-152 - DOI
79. Sugiyama, H.; Aharonian, G.; Gambarotta, S.; Yap, G.P.A.; Budzelaar, P.H.M.  
Participation of the  $\alpha,\alpha'$ -diiminopyridine ligand system in reduction of the metal center during alkylation  
*J. Am. Chem. Soc.* **2002**, 124, 12268-12274 - DOI 10.1021/ja020485m
78. Enright, D.; Gambarotta, S.; Yap, G.P.A.; Budzelaar, P.H.M.  
The ability of the  $\alpha,\alpha'$ -diiminopyridine ligand system to accept negative charge: Isolation of paramagnetic and diamagnetic trianions  
*Angew. Chem. I.E.* **2002**, 41, 3873-3876 - DOI 10.1002/1521-3773(20021018)41:20<3873::AID-ANIE3873>3.0.CO;2-8
77. Khorobkov, W.; Gambarotta, S.; Yap, G.P.A.; Budzelaar, P.H.M.  
Reversible Alkylation at the Pyridine Nitrogen in a  $\alpha,\alpha'$ -Diimine Pyridine Ligand System  
*Organometallics* **2002**, 21, 3088-3090 - DOI 10.1021/om020349q
76. Willems, S.T.H.; Budzelaar, P.H. M.; Moonen, N.N.P.; De Gelder, R.; Smits, J.M.M.; Gal, A.W.  
Coordination and Oxidative addition at a Low-coordinate Rhodium(I)  $\beta$ -Diiminate Centre  
*Chem. Eur. J.* **2002**, 8, 1310-1320 - DOI 10.1002/1521-3765(20020315)8:6<1310::AID-CHEM1310>3.0.CO;2-U
75. Drent, E.; Mul, W.P.; Budzelaar, P.H.M.  
Teaching a palladium polymerization catalyst to mono-oxygenate olefins  
*Comm. Inorg. Chem.* **2002**, 23, 127-147 - DOI
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  
*Macromolecules* **2002**, 35, 2835-2844 - DOI 10.1021/ma011557h
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.  
Spontaneous disproportionation of rhodium(I) bisoxazolinates to rhodium(II)  
*Chem. Commun.* **2002**, 148-149 - DOI 10.1039/b110183h
72. Sciarone, T.; Hoogboom, J.; Schlebos, P.P.J.; Budzelaar, P.H.M.; De Gelder, R.; Smits, J.M.M.; Gal, A.W.  
(Diene)rhodium and -iridium Complexes of Pyridinophane Ligands  
*Eur. J. Inorg. Chem.* **2002**, 457-464 - DOI
71. Talarico, G.; Budzelaar, P.H.M.  
Mono- and Dinuclear Olefin Reactions at Aluminium  
*Organometallics* **2002**, 21, 34-38 - DOI 10.1021/om010606b

## 2001

70. Busico, V.; Cipullo, R.; Ronca, S.; Budzelaar, P.H.M.  
Mimicking Ziegler-Natta Catalysts in Homogeneous Phase, 1.  $C_2$ -Symmetric Octahedral Zr(IV) Complexes with Tetradentate [ONNO]-Type Ligands  
*Macromol. Rapid Commun.* **2001**, *22*, 1405-1410 - DOI 10.1002/1521-3927(20011101)22:17<1405::AID-MARC1405>3.0.CO;2-H
69. Kooistra, T.M.; Knijnenburg, Q.; Smits, J.M.M.; Horton, A.D.; Budzelaar, P.H.M.; Gal, A.W.  
Olefin Polymerization with  $[\{\text{bis}(\text{imino})\text{pyridyl}\}\text{Co}^{\text{II}}\text{Cl}_2]$ : Generation of the Active Species Involves  $\text{Co}^{\text{I}}$   
*Angew. Chem. I.E.* **2001**, *40*, 4719-4722 - DOI 10.1002/1521-3773(20011217)40:24<4719::AID-ANIE4719>3.0.CO;2-O
68. Talarico, G.; Busico, V.; Budzelaar, P.H.M.  
Olefin Polymerization at Aluminium? A Theoretical Study  
*Organometallics* **2001**, *20*, 4721-4726 - DOI 10.1021/om010696k
67. Talarico, G.; Barone, V.; Budzelaar, P.H.M.; Adamo, C.  
Modeling Polymerization Reactions at Aluminum-Based Catalysts: Is DFT a Reliable Computational Tool?  
*J. Phys. Chem. A* **2001**, *105*, 9014-9023 - DOI 10.1021/jp011334t
66. Budzelaar, P.H.M.; De Bruin, B.; Gal, A.W.; Wieghardt, K.; Van Lenthe, J.H.  
Metal-to-Ligand Electron Transfer in Diiminopyridine Complexes of Mn-Zn. A Theoretical Study  
*Inorg. Chem.* **2001**, *40*, 4649-4655 - DOI 10.1021/ic001457c

## 2000

65. Talarico, G.; Budzelaar, P.H.M.  
Ethene Polymerization at Cationic Aluminum Amidinate and Neutral Aluminum Alkyl. A Theoretical Study  
*Organometallics* **2000**, *19*, 5691-5695 - DOI 10.1021/om000622t
64. Talarico, G.; Budzelaar, P. H. M.; Barone, V.; Adamo, C.  
A theoretical study of the competition between ethylene insertion and chain transfer in cationic Aluminum systems.  
*Chem Phys. Lett.* **2000**, *329*, 99-105 - DOI 10.1016/S0009-2614(00)00981-7
63. Burns, C.T.; Shapiro, P.J.; Budzelaar, P.H.M.; Willett, R.; Vij, A.  
Bis(permethylcyclopentadienyl)aluminum compounds: Precursors to  $[\text{Cp}^*_2\text{Al}]^+$  but not to  $\text{Cp}^*_3\text{Al}$   
*Organometallics* **2000**, *19*, 3361-3367 - DOI 10.1021/om000173x
62. Budzelaar, P.H.M.; Moonen, N.N.P.; De Gelder, R.; Smits, J.M.. M.; Gal, A.W.  
Steric Control over Arene Coordination to  $\beta$ -Diiminate Rhodium(I) Fragments  
*Chem. Eur. J.* **2000**, *6*, 2740-2747 - DOI 10.1002/1521-3765(20000804)6:15<2740::AID-CHEM2740>3.0.CO;2-0
61. Budzelaar, P.H.M.; Moonen, N.N.P.; De Gelder, R.; Smits, J.M.. M.; Gal, A.W.  
Rhodium and Iridium  $\beta$ -Diiminate Complexes – Olefin Hydrogenation Step by Step  
*Eur. J. Inorg. Chem.* **2000**, 753-769 - DOI

60. Talarico, G.; Budzelaar, P.H.M.; Gal, A.W.  
Ethylene coordination, insertion, and chain transfer at a cationic aluminum center: A comparative study with ab initio correlated level and density functional methods  
*J. Comp. Chem.* **2000**, *21*, 398-410 - DOI 10.1002/(SICI)1096-987X(20000415)21:5<398::AID-JCC6>3.0.CO;2-I

59. Drent E., Budzelaar P.H.M.  
The oxo-synthesis catalyzed by cationic palladium complexes, selectivity control by neutral ligand and anion  
*J. Organomet. Chem.* **2000**, *594*, 211-225 - DOI 10.1016/S0022-328X(99)00554-9

## 1999

58. Klooster, W.T.; Brammer, L.; Schaverien, C.J.; Budzelaar, P.H.M.  
C-H Bonds are not Elongated by Coordination of Lanthanide Metals: Single-Crystal Neutron Diffraction Structures of  $(C_5Me_5)Y(OC_6H_3^tBu_2)(CH(SiMe_3)_2)$  at 20 K and  $(C_5Me_5)La\{CH(SiMe_3)_2\}_2$  at 15 K  
*J. Am. Chem. Soc.* **1999**, *121*, 1381-1382 - DOI 10.1021/ja983068b

## 1998

57. Budzelaar, P.H.M.; Van Oort, A.B.; Orpen, A.G.  
 $\beta$ -Diiminato Complexes of  $V^{III}$  and  $Ti^{III}$  - Formation and Structure of Stable Paramagnetic Dialkylmetal Compounds  
*Eur. J. Inorg. Chem.* **1998**, 1485-1494 - DOI

56. Budzelaar, P.H.M.; De Gelder, R.; Gal, A.W.  
A Stable Three-Coordinate Rhodium(I) Olefin Complex  
*Organometallics* **1998**, *17*, 4121-4123 - DOI 10.1021/om980580x

55. Groen, J.H.; De Zwart, A.; Vlaar, M.J.M.; Van Leeuwen, P.W.N.M.; Vrieze, K.; Kooijman, H.; Smeets, W.J.J.; Spek, A.L.; Budzelaar, P.H.M.; Xiang, Q.; Thummel, R.P.  
Insertion Reactions into Palladium-Carbon Bonds of Complexes Containing Terdentate Nitrogen Ligands; Experimental and Ab initio MO Studies  
*Eur. J. Inorg. Chem.* **1998**, 1129-1143 - DOI

54. Budzelaar, P.H.M.  
Theoretical Study of the Reaction of Alkylolithium with Pyridylphosphines  
*J. Org. Chem.* **1998**, *63*, 1131-1137 - DOI 10.1021/jo9716136

53. Fisher, J.D.; Shapiro, P.J.; Budzelaar, P.H.M.; Staples, R.J.  
Heteroatom Derivatives of Cyclopentadienylaluminum: X-ray Crystal Structure of  $(\eta^5-C_5H_5)(2,6-t-Bu-4-Me-C_6H_2O)_2Al$   
*Inorg. Chem.* **1998**, *37*, 1295-1298 - DOI 10.1021/ic970376m

52. Schaverien, C.J.; Ernst, R.; Terlouw, W.; Schut, P.; Sudmeijer, O.; Budzelaar, P.H.M.  
Phosphorus-bridged metallocenes: New homogeneous catalysts for the polymerization of propene  
*J. Mol. Catal.* **1998**, *128*, 245-256 - DOI 10.1016/S1381-1169(97)00178-7

## 1997

51. Witte, P.T.; Meetsma, A.; Hessen, B.; Budzelaar, P.H.M.  
Coordination of Ethene and Propene to a Cationic  $d^0$  Vanadium Center  
*J. Am. Chem. Soc.* **1997**, *119*, 10561-10562 - DOI 10.1021/ja972219s

50. Fisher, J.D.; Budzelaar, P.H.M.; Shapiro, P.J.; Staples, R.J.; Yap G.P.A.; Rheingold, A.L.  
Regarding the Structures and Fluxionality of Tricyclopentadienylaluminium  
Compounds  
*Organometallics* **1997**, *16*, 871-879 - DOI 10.1021/om9610049
49. Van der Kerk, S.M.; Budzelaar, P.H.M.  
A Simple Model for Resonant Tunnelling in Multi-Well Systems  
*Proc. Royal Dutch Acad.* **1997**, *100*, 67-78 - DOI

## 1996

48. Janiak, C.; Lange, K.C.H.; Versteeg, U.; Lentz, D.; Budzelaar, P.H.M.  
Ethene Polymerization Activity and Coordination Gap Aperture in non-ansa Alkyl-  
Substituted Cyclopentadienyl- and Phospholyl-Zirconium/MAO Catalysts  
*Chem. Ber.* **1996**, *129*, 1517-1529 - DOI 10.1002/cber.19961291219
- B2. Drent, E.; Van Broekhoven, J.A.M.; Budzelaar, P.H.M.  
"The Alternating Copolymerization of Alkenes and Carbon Monoxide", ch 2.3.4 of  
"Applied Homogeneous Catalysis with Organometallic Compounds"  
eds Cornils, B.; Hermann, W.A., VCH, Weinheim, **1996**
47. Drent, E.; Budzelaar, P.H.M.  
Palladium-Catalyzed Alternating Copolymerization of Alkenes and Carbon Monoxide  
*Chem. Rev.* **1996**, *96*, 663-681 - DOI 10.1021/cr940282j
46. Drent, E.; Van Broekhoven, J.A.M.; Budzelaar, P.H.M.  
Alternating copolymerization of alkenes and carbon monoxide catalyzed by cationic  
palladium complexes  
*Recl. Trav. Chim. Pays-Bas* **1996**, *115*, 263-270 - DOI

## 1995

- B1. Budzelaar, P.H.M.; Van Lenthe, J.H.  
"An introduction to quantumchemical organometallic chemistry", introductory chapter  
of "Theoretical aspects of homogeneous catalysis"  
eds Van Leeuwen, P.W.N.M.; Morokuma, K.; Van Lenthe, J.H., Kluwer, Dordrecht, **1995**

## 1994

45. Drent, E.; Arnoldy, P.; Budzelaar, P.H.M.  
Homogeneous catalysis by cationic palladium complexes. Precision catalysis in the  
carbonylation of alkynes  
*J. Organomet. Chem.* **1994**, *475*, 57-63 - DOI 10.1016/0022-328X(94)84007-5

## 1993

44. Drent, E.; Arnoldy, P.; Budzelaar, P.H.M.  
Efficient palladium catalysts for the carbonylation of alkynes  
*J. Organomet. Chem.* **1993**, *455*, 247-253 - DOI 10.1016/0022-328X(93)80406-2

## 1992

43. Budzelaar, P.H.M.; Van Leeuwen, P.W.N.M.; Roobeek, C.F.; Orpen, A.G.  
[(dppp)Pd]<sub>2</sub>(SO<sub>3</sub>CF<sub>3</sub>)<sub>2</sub>: a palladium(I) dimer with side-on phosphine coordination  
*Organometallics* **1992**, *11*, 23-25 - DOI 10.1021/om00037a012

## 1991

- P4.** Drent, E.; Budzelaar, P.H.M.; Jager, W.W.; Stapersma, J.  
Carbonylation catalysts  
Shell Internationale Research Maatschappij B. V., Neth.  
*Eur. Pat. Appl.* EP 441447 A1 910814 (1991)
- 42.** Budzelaar, P.H.M.; Van Doorn, J.A.; Meijboom, N.  
Reductive cleavage of the carbon-phosphorus bond with alkali metals. I. Cleavage of functionalized triphenylphosphines; formation of secondary and primary phosphines  
*Recl. Trav. Chim. Pays-Bas* **1991**, *110*, 420-432 - DOI

## 1990

- P3.** Drent, E.; Budzelaar, P.H.M.  
Group VIII metal-phosphine catalysts for carbonylation of unsaturated hydrocarbons  
Shell Internationale Research Maatschappij B. V., Neth.  
*Eur. Pat. Appl.* EP 386834 A1 900912 (1990)
- P2.** Drent, E.; Budzelaar, P.H.M.; Jager, W.W.  
Group VIII metal-phosphine catalysts for carbonylation of unsaturated hydrocarbons  
Shell Internationale Research Maatschappij B. V., Neth.  
*Eur. Pat. Appl.* EP 386833 A1 900912 (1990)
- 41.** Fennis, P.J.; Budzelaar, P.H.M.; Frijns, J.H.G.; Orpen, A.G.  
Dichloromethane addition to rhodium- $\beta$ -diketonate complexes of diphosphines and pyridyl-substituted diphosphines  
*J. Organomet. Chem.* **1990**, *393*, 287-298 - DOI 10.1016/0022-328X(90)80205-E
- 40.** Van Oort, A.B.; Budzelaar, P.H.M.; Frijns, J.H.G.; Orpen, A.G.  
Mono- and binuclear molybdenum complexes of 2,6-bis(diphenylphosphino)-N-methylaniline  
*J. Organomet. Chem.* **1990**, *396*, 33-47 - DOI
- 39.** Budzelaar, P.H.M.; Van Doorn, J.A.; Meijboom, N.  
Orbital control in the reductive cleavage of tris(methoxyphenyl)phosphines  
*Recl. Trav. Chim. Pays-Bas* **1990**, *109*, 253-254 - DOI
- 38.** Budzelaar, P.H.M.; Van Doorn, J.A.  
Selective nucleophilic displacement of a methoxy group in 1,2,3-trimethoxybenzenes  
*Recl. Trav. Chim. Pays-Bas* **1990**, *109*, 443-445 - DOI
- 37.** Budzelaar, P.H.M.; Boersma, J.  
Metal-metal interactions in indium(I) and thallium(I) cyclopentadienyls  
*Recl. Trav. Chim. Pays-Bas* **1990**, *109*, 187-189 - DOI
- 36.** Budzelaar, P.H.M.; Frijns, J.H.G.; Orpen, A.G.  
Synthesis and coordination chemistry of a new class of binucleating ligands: pyridyl-substituted diphosphines  
*Organometallics* **1990**, *9*, 1222-1227 - DOI 10.1021/om00118a050

## 1989

- 35.** Fischer, B.; Wijkens, P.; Boersma, J.; Van Koten, G.; Smeets, W.J.J.; Spek, A.L.; Budzelaar, P.H.M.  
The unusual solid state structures of the pentasubstituted bis(cyclopentadienyl)zinc compounds bis(pentamethylcyclopentadienyl)zinc and bis(tetramethylphenylcyclopentadienyl)zinc  
*J. Organomet. Chem.* **1989**, *376*, 223-233 - DOI

- P1.** Van Doorn, J.A.; Budzelaar, P.H.M.; Wife, R.L.  
Catalytic compositions for the polymerization of carbon monoxide with an olefin  
Shell Internationale Research Maatschappij B. V., Neth.  
*Eur. Pat. Appl.* EP 305012 A2 890301 (1989)

## 1987

- 34.** Budzelaar, P.H.M.; Timmermans, P.J.J.A.; Mackor, A.; Baerends, E.J.  
Bonding in the ground state and excited states of copper-alkene complexes  
*J. Organomet. Chem.* **1987**, *331*, 397-407 - DOI
- 33.** Budzelaar, P.H.M.; Timmermans, P.J.J.A.; Mackor, A.; Spek, A.L.; Duisenberg, A.J.  
Bis(cyclooctene)copper(I) trifluoromethanesulfonate  
*Acta Crystallogr. C* **1987**, *43*, 2298-2300 - DOI
- 32.** Dekker, J.; Schouten, A.; Budzelaar, P.H.M.; Boersma, J.; Van der Kerk, G.J.M.; Spek, A.L.; Duisenberg, A.J.  
Zinc enolates. C- or O-metallation?  
*J. Organomet. Chem.* **1987**, *320*, 1-12 - DOI
- 31.** Budzelaar, P.H.M.; Cremer, D.; Wallasch, M.; Würthwein, E.U.; Schleyer, P.v. R.  
Dioxetenes and diazetines: nonaromatic  $6\pi$ -systems in four-membered rings  
*J. Am. Chem. Soc.* **1987**, *109*, 6290-6299 - DOI
- 30.** Verbeek, J.; Van Lenthe, J.H.; Timmermans, P.J.J.A.; Mackor, A.; Budzelaar, P.H.M.  
On the existence of *trans*-cyclohexene  
*J. Org. Chem.* **1987**, *52*, 2955-2957 - DOI

## 1986

- 29.** Blom, R.; Boersma, J.; Budzelaar, P.H.M.; Fischer, B.; Haaland, A.; Volden, H.V.; Weidlein, J.  
The preparation of bis(pentamethylcyclopentadienyl)zinc and bis(trimethylsilylcyclopentadienyl)zinc, and their molecular structures determined by gas electron diffraction  
*Acta Chem. Scand. A* **1986**, *40*, 113-120 - DOI
- 28.** Budzelaar, P.H.M.; Van der Kerk, S.M.; Krogh-Jespersen, K.; Schleyer, P.v. R.  
Dimerization of borirene to 1,4-diboracyclohexadiene. Structures and stabilities of  $(\text{CH})_4(\text{BH})_2$  molecules  
*J. Am. Chem. Soc.* **1986**, *108*, 3960-3967 - DOI
- 27.** Budzelaar, P.H.M.; Schleyer, P.v.R.  
Azadiboridine and diazaboridine: aromatic and antiaromatic three-membered-ring prototypes  
*J. Am. Chem. Soc.* **1986**, *108*, 3967-3970 - DOI
- 26.** Budzelaar, P.H.M.; Kraka, E.; Cremer, D.; Schleyer, P.v.R.  
Long interbridgehead bonds in acceptor-substituted bicyclobutanes  
*J. Am. Chem. Soc.* **1986**, *108*, 561-567 - DOI

## 1985

- 25.** Budzelaar, P.H.M.; Boersma, J.; Van der Kerk, G.J.M.; Spek, A.L.; Duisenberg, A.J.M.  
Preparation and crystal structure of  $[\mu\text{-Ni}(\text{C}_5\text{H}_5)\text{P}(\text{C}_6\text{H}_5)_3][\mu\text{-C}_5\text{H}_5][\text{ZnC}_5\text{H}_5]_2$ , a nickel-bridged cyclopentadienylzinc dimer  
*J. Organomet. Chem.* **1985**, *287*, C13-C17 - DOI

24. Budzelaar, P.H.M.; Dietrich, H.; Macheleid, J.; Weiss, R.; Schleyer, P.v.R.  
The molecular and electronic structure of dipiperidinosquaraine  
*Chem. Ber.* **1985**, *118*, 2118-2126 - DOI
23. Budzelaar, P.H.M.; Krogh-Jespersen, K.; Clark, T.; Schleyer, P.v.R.  
Remarkable structures of C<sub>2</sub>B<sub>2</sub>H<sub>4</sub> isomers  
*J. Am. Chem. Soc.* **1985**, *107*, 2773-2779 - DOI
22. Würthwein, E.U.; Kupfer, R.; Budzelaar, P.H.M.; Strobel, C.; Beck, H.P.  
A new, simple route to 2-azaallenium salts - bis(2-adamantylidene)ammonium hexachloroantimonate  
*Angew. Chem.* **1985**, *97*, 327-8; *I.E.* **1985**, *24*, 340-341 - DOI
21. Budzelaar, P.H.M.; Boersma, J.; Van der Kerk, G.J.M.; Spek, A.L.; Duisenberg, A.J.M.  
Cp<sub>6</sub>Ni<sub>2</sub>Zn<sub>4</sub> - an unusually electron-rich octahedral cluster  
*Organometallics* **1985**, *4*, 680-683 - DOI
20. Budzelaar, P.H.M.; Kos, A.J.; Clark, T.; Schleyer, P.v.R.  
Effects of boron substituents in borirenes, boriranes, and boranes. The energies of B-X bonds  
*Organometallics* **1985**, *4*, 429-437 - DOI
19. Budzelaar, P.H.M.; Boersma, J.; Van der Kerk, G.J.M.; Spek, A.L.; Duisenberg, A.J.M.  
The structure of dicyclopentadienylzinc  
*J. Organomet. Chem.* **1985**, *281*, 123-130 - DOI

## 1984

18. Budzelaar, P.H.M.; Schleyer, P.v.R.; Krogh-Jespersen, K.  
Diboramethylenecyclopropane, theoretical studies on the structure and mechanism of topomerization  
*Angew. Chem.* **1984**, *96*, 809-10; *I.E.* **1984**, *23*, 825-826 - DOI
17. Cremer, D.; Gauss, J.; Schleyer, P.v.R.; Budzelaar, P.H.M.  
1,2-Dihydroborete: structure of a potential homoaromatic system  
*Angew. Chem.* **1984**, *96*, 370-1; *I.E.* **1984**, *23*, 370-371 - DOI
16. Van der Kerk, S.M.; Budzelaar, P.H.M.; Van Eekeren, A.L.M.; Van der Kerk, G.J.M.  
The addition of methylborylene to acetylenes. Synthesis of 1,4-diboracyclohexa-2,5-dienes, and of a borirene and a diboretene derivative  
*Polyhedron* **1984**, *3*, 271-280 - DOI
15. Dekker, J.; Budzelaar, P.H.M.; Boersma, J.; Van der Kerk, G.J.M.; Spek, A.J.  
The nature of the Reformatsky reagent. Crystal structure of (BrZnCH<sub>2</sub>COO-*t*-Bu.THF)<sub>2</sub>  
*Organometallics* **1984**, *3*, 1403-1407 - DOI
14. Budzelaar, P.H.M.; Boersma, J.; Van der Kerk, G.J.M.; Spek, A.L.  
A novel type of cyclopentadienyl bridge - structure of (μ-C<sub>5</sub>H<sub>5</sub>)[μ-N(SiMe<sub>3</sub>)<sub>2</sub>](ZnC<sub>5</sub>H<sub>5</sub>)<sub>2</sub>  
*Organometallics* **1984**, *3*, 1187-1190 - DOI
13. Schleyer, P.v.R.; Cremer, D.; Kraka, E.; Budzelaar, P.H.M.  
Puckered structures of 1,3-dihydro-1,3-diboretates and bicyclobutane-2,4-dione: nonplanar 2π-Hückel aromatic molecules  
*Angew. Chem.* **1984**, *96*, 374-5; *I.E.* **1984**, *23*, 374-375 - DOI
12. Budzelaar, P.H.M.; Den Haan, K.H.; Boersma, J.; Van der Kerk, G.J.M.; Spek, A.L.  
Reaction of (C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>NbH<sub>3</sub> with (C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>Zn - structure of (C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>NbH<sub>2</sub>ZnC<sub>5</sub>H<sub>5</sub>  
*Organometallics* **1984**, *3*, 156-159 - DOI



11. Budzelaar, P.H.M.; Van der Zeijden, A.A.H.; Boersma, J.; Van der Kerk, G.J.M.; Spek, A.L.; Duisenberg, A.J.M.  
Tantalum-zinc compounds - structure of  $(\text{CH}_3\text{C}_5\text{H}_4)_2\text{TaH}(\text{ZnC}_5\text{H}_5)_2$   
*Organometallics* **1984**, 3, 159-163 - DOI

## 1983

10. Budzelaar, P.H.M.; De Koning, A.J.; Van Aarssen, B.G.K.  
Reduction of pyridinoid heterocyclic compounds. A MINDO/3 study  
*J. Chem. Soc. Perkin 2* **1983**, 989-992 - DOI
9. Budzelaar, P.H.M.; Boersma, J.; Van der Kerk, G.J.M.  
Hexacyclopentadienylnickelzinc  $((\text{C}_5\text{H}_5)_6\text{Ni}_2\text{Zn}_4)$  - the first zinc-containing mixed metal cluster  
*Angew. Chem.* **1983**, 95, 335-6; *I.E.* **1983**, 22, 329 - DOI
8. Budzelaar, P.H.M.; Alberts-Jansen, H.J.; Mollema, K.; Boersma, J.; Van der Kerk, G.J.M.; Spek, A.L.; Duisenberg, A.J. M.  
Internally coordinated organozinc-transition metal compounds. Crystal structure of  $(\text{CH}_3)_2\text{N}(\text{CH}_2)_3\text{ZnW}(\eta\text{-C}_5\text{H}_5)(\text{CO})_3$   
*J. Organomet. Chem.* **1983**, 243, 137-148 - DOI
7. Van der Kerk, Sies M.; Budzelaar, P.H.M.; Van der Kerk-Van Hoof, A.C.T.H.; Van der Kerk, G.J.M.; Schleyer, P.v.R.  
Syntheses of borirenes and diboretenes, a new class of  $2\pi$ -aromatic compounds  
*Angew. Chem.* **1983**, 95, 61; *I.E.* **1983**, 22, 48 - DOI

## 1982

6. Budzelaar, P.H.M.; Alberts-Jansen, H.J.; Boersma, J.; Van der Kerk, G.J.M.  
Reactions of allylic and propargylic amines and ethers with zinc bis(tetracarbonylcobaltate)  $(\text{Zn}[\text{Co}(\text{CO})_4]_2)$   
*Polyhedron* **1982**, 1, 563-566 - DOI
5. Budzelaar, P.H.M.; Boersma, J.; Van der Kerk, G.J.M.; Spek, A.L.; Duisenberg, A.J.M.  
Cyclopentadienylzinc-transition metal compounds. Structure of  $(\text{C}_5\text{H}_5\text{Zn})_2\text{Co}(\text{C}_5\text{H}_5)\text{P}(\text{C}_6\text{H}_5)_3$   
*Inorg. Chem.* **1982**, 21, 3777-3780 - DOI

## 1981

4. De Koning, A.J.; Budzelaar, P.H.M.; Van Aarssen, B.G.K.; Boersma, J.; Van der Kerk, G.J.M.  
Reaction of magnesium hydride with pyridine  
*J. Organomet. Chem.* **1981**, 217, C1-C4 - DOI

## 1980

3. Budzelaar, P.H.M.; Boersma, J.; Van der Kerk, G.J.M.  
Cyclopentadienylzinc derivatives of manganese, molybdenum and tungsten: the first examples of stable organozinc-transition metal compounds  
*J. Organomet. Chem.* **1980**, 202, C71-C72 - DOI
2. De Koning, A.J.; Budzelaar, P.H.M.; Boersma, J.; Van der Kerk, G.J.M.  
Specific and selective reduction of aromatic nitrogen heterocycles with the bis-pyridine complexes of bis(1,4-dihydro-1-pyridyl)zinc and bis(1,4-dihydro-1-pyridyl)magnesium  
*J. Organomet. Chem.* **1980**, 199, 153-169 - DOI

1. De Koning, A.J.; Budzelaar, P.H.M.; Brandsma, L.; De Bie, M.J.A.; Boersma, J.  
Synthesis and NMR spectroscopic properties of some methyl-substituted 1-methyl-  
1,4-dihydropyridines  
*Tetrahedron Lett.* **1980**, *21*, 2105-2108 - DOI