

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

**2017**

- 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.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

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A Density Functional Theory Investigation of the Cobalt-Mediated η<sup>5</sup>-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 MgCl<sub>2</sub>-supported Ziegler-Natta catalysts - 1: TiCl<sub>4</sub> adsorption on MgCl<sub>2</sub> 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, 1-  
C<sub>9</sub>H<sub>6</sub>Ph<sub>2</sub>PCH<sub>2</sub>PPh<sub>2</sub>  
*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

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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 - 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.  
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*Inorg. Chem.* **2011**, *50*, 9879–9887 - DOI 10.1021/ic2002145

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Reactivity of cationic decamethylmetallocene complexes towards ketones  
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- 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)  
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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.  
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*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- $\sigma$  Bond  
Metathesis via  $\epsilon$ -Agostic Interactions, and a Rare Example of a  $\beta$ -Agostic  
Alkyltitanocene Complex  
*J. Am. Chem. Soc.* **2010**, *132*, 13357-13370 - 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>"  
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- 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  
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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>  
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Variability of Chain Transfer to Monomer Step in Olefin Polymerization  
*Organometallics* **2008**, *27*, 4098-4107 - DOI 10.1021/om800313n
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A Measure for  $\sigma$ -Donor and  $\pi$ -Acceptor Properties of Diiminepyridine-Type Ligands  
*Organometallics* **2008**, *27*, 2699-2705 - DOI 10.1021/om701160b
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Multiple Pathways for Dinitrogen Activation during the Reduction of an Fe Bis(iminepyridine) Complex  
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- 111a. Coussens, B.B.; Budzelaar, P.H.M.; Friederichs, N.  
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Dinitrogen Activation, Partial Reduction, and Formation of Coordinated Imide Promoted by a Chromium Diiminepyridine Complex  
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## 2006

- 108.** Knijnenburg, Q.; Gambarotta, S.; Budzelaar, P.H.M.  
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*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  
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- 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.  
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*Organometallics* **2006**, *25*, 719-732 - DOI 10.1021/om050710j

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