

Peter H.M. Budzelaar
List of Publications

2018

182. Breuza, E.; Antinucci, G.; Budzelaar, P.H.M.; Busico, V.; Correa, A.; Ehm, C.
MgCl₂-Supported Ziegler-Natta Catalysts: a DFT-D "Flexible-Cluster" Approach to Internal Donor Adducts.
Phys. Chem. C **2018**, *122*, 9046-9053 - DOI 10.1021/acs.jpcc.8b01500
181. Chambrier, I.; Rocchigiani, L.; Hughes, D.L.; Budzelaar, P.H.M.; Bochmann, M.
Thermally Stable Gold(III) Alkene and Alkyne Complexes: Synthesis, Structures, and Assessment of the trans-Influence on Gold-Ligand Bond Enthalpies
Chem. Eur. J. **2018**, *24* (44), 11467-11474 - DOI 10.1002/chem.201802160
180. Chehal, N.K.; Budzelaar, P.H.M.; Hultin, P.G.
E-Z isomerization in Suzuki cross-couplings of haloenones: ligand effects and evidence for a separate catalytic cycle
Org. Biomol. Chem. **2018**, *16*, 1134-1143 - DOI
179. Kehoe, R.; Mahadevan, M.; Manzoor, A.; McMurray, G.; Wienefeld, P.; Baird, M.C.; Budzelaar, P.H.M.
Reactions of the Ni(0) Compound Ni(PPh₃)₄ with Unactivated Alkyl Halides: Oxidative Addition Reactions Involving Radical Processes and Nickel(I) Intermediates.
Organometallics **2018**, *37*, 2450-2467 - DOI 10.1021/acs.organomet.8b00244
178. Rocchigiani, L.; Fernandez-Cestau, J.; Budzelaar, P.H.M.; Bochmann, M.
Reductive Elimination Leading to C-C Bond Formation in Gold(III) Complexes: A Mechanistic and Computational Study.
Chem. Eur. J. **2018**, *24*, 8893-8903 - DOI 10.1002/chem.201801277
177. Zaccaria, F.; Ehm, C.; Budzelaar, P.H.M.; Busico, V.; Cipullo, R.
Catalyst Mileage in Olefin Polymerization: The Peculiar Role of Toluene.
Organometallics **2018**, *37*, 2872-2879 - DOI 10.1021/acs.organomet.8b00393
176. Zaccaria, F.; Vittoria, A.; Correa, A.; Ehm, C.; Budzelaar, P.H.M.; Busico, V.; Cipullo, R.
Internal Donors in Ziegler-Natta Systems: is Reduction by AlR₃ a Requirement for Donor Clean-Up?
Chemcatchem **2018**, *10*, 984-988 - DOI 10.1002/cctc.201701422
175. Zhang, N.; Zhu, D.; Herbert, D.E.; van Leest, N.P.; de Bruin, B.; Budzelaar, P.H.M.
Reactivity of Rhodium(II) amido/Rhodium(I) aminyl complexes
Inorg. Chim. Acta **2018**, *482*, 709-716 - DOI 10.1016/j.ica.2018.06.015

2017

174. Zhang, N.; Sherbo, R.S.; Bindra, G.S.; Zhu, D.; Budzelaar, P.H.M.
Rh and Ir β-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

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- 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 (β -diiminate)Rh(1,3-
diene) Complexes
Organometallics **2016**, *35*, 2039–2048 - DOI 10.1021/acs.organomet.6b00328
- 157.** Talarico, G.; Budzelaar, P.H.M.
 α -Agostic Interactions and Growing Chain Orientation for Olefin Polymerization
Catalysts
Organometallics **2016**, *35*, 47–54 - DOI 10.1021/acs.organomet.5b00866

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- 156.** Dunlop-Briere, A.F.; Baird, M.C.; Budzelaar, P.H.M.
[Cp₂TiCH₂CH₂(SiEt₂CHMe₂)]⁺, an Alkyl-titanocene(IV) Complex Containing an
Unconventional Ti \leftarrow C(β)-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 α -, β -, and γ -H(D) Exchange Processes in the α -Agostic
Alkyltitanocene(IV) Complexes [Cp₂TiCH₂CH(CH₃)(CMe₃)]⁺ and
[Cp₂TiCH₂CH(CD₃)(CMe₃)]⁺: Stark Contrasts with Their γ -SiMe₃ 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-C₉H₄PMePh₂, 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
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- 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
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Organometallics **2014**, *33*, 5974–5982 - DOI 10.1021/om5003655

- 149.** Alzamy, 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

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- 147.** Capone, F.; Rongo, L.; D'Amore, M.; Budzelaar, P.H.M.; Busico, V.
Periodic Hybrid DFT Approach (Including Dispersion) to MgCl₂-Supported Ziegler-Natta Catalysts. 2. Model Electron Donor Adsorption on MgCl₂ 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.
[Cp₂TiCH₂CHMe(SiMe₃)]⁺, 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
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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.
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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-C₉H₆Ph₂PCH₂PPh₂
Organometallics **2012**, *31*, 6926-6932 - DOI 10.1021/Om300715a
- 140.** Zhu, D.; Kozera, D.J.; Enns, K.D.; Budzelaar, P.H.M.
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- 136.** Dunlop-Brière, A.F.; Budzelaar, P.H.M.; Baird, M.C. α - and β -Agostic Alkyl–Titanocene Complexes
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- 134.** Budzelaar, P.H.M. Radical Chemistry of Iminepyridine Ligands
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A Case of Failure of the Colle–Salvetti Correlation Density Functionals (erratum)
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- 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.
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Key?
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P.H.M.
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Insertion Reactions of 2,2-Disubstituted-1-alkenes, Intramolecular 1,5- σ Bond
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