TREVOR A. HAMLIN

PERSONAL DETAILS

Full Name: Trevor Alexander Hamlin
Website: www.theochem.nl/tahamlin
ORCID: 0000-0002-5128-1004
E-mail: t.a.hamlin@vu.nl

PROFESSIONAL EXPERIENCE

Assistant Professor (with tenure) **2019-Present**
Vrije Universiteit Amsterdam Amsterdam (NL)
Research focus: Theory-Driven Experimentation, Physical Organic Chemistry, Computational Chemistry

Postdoctoral Research Fellow **2015-2019**
Vrije Universiteit Amsterdam Amsterdam (NL)
Principal Investigator: Professor F. M. Bickelhaupt
Research focus: Theory-Driven Experimentation and Computational Chemistry

EDUCATION

Ph.D. in Physical Organic Chemistry **2010-2015**
University of Connecticut **GPA: 3.88/4.00** Storrs, CT (USA)
Principal Investigator: Professor Nicholas E. Leadbeater
Research focus: Organofluorine, Oxoammonium Salt Chemistry, Continuous-Flow Processing

B.S. in Biochemistry **2006-2010**
Albright College **GPA: 3.73/4.00** (*cum laude*) Reading, PA (USA)
Principal Investigator: Professor Christian S. Hamann
Research focus: Terpene Biosynthesis and Computational Chemistry

AWARDS and DISTINCTIONS

2024	Completed VU Course: “Supervising Ph.D. Students”
2023	Fellow of the Royal Society of Chemistry
2023	Editorial Advisory Board of *Chemistry—A European Journal*
2023	Editorial Advisory Board of *ChemPhysChem*
2023	Member of the American Chemical Society (ACS)
2022	Microsoft Research Grant for Catalyst Design Using AI
2021	Track Coordinator of the MSc Chemistry Program
2020	University Teaching Qualification (Basiskwalificatie Onderwijs)
2020	Member of the MSc Chemistry Program Committee
2020	Early Career Advisory Board of *Chemistry—A European Journal*
2020	Member of the Royal Netherlands Chemical Society (KNCV)
2019	Member of the Holland Research School of Molecular Chemistry (HRSMC)
2016	Pi Kappa Phi: 30 Under Thirty Award
2014	Doctoral Dissertation Fellowship
2013	Zaiput Flow Technologies Challenge Grant
2011	Chemistry Alumni Outstanding Teaching Assistant Award
2010	Benjamin H. Handorf Chemistry Prize
2010	Eileen Walker Memorial Award
2009	Undergraduate Student Travel Award: Division of Organic Chemistry of the ACS
2006-2010	The Presidential Scholarship
2006-2010	The Cecilia Hand and Morgan Hand, II Memorial Scholarship Award
2006-2010	Ocean City Masonic Club “Foster Karney” Foundation Scholarship

2006-2010 National Honor Society Scholar

TEACHING DUTIES

Vrije Universiteit Amsterdam

Analytical NMR Spectroscopy – Developer, Coordinator, and Lecturer	**2020-Present**
Molecular Moleculing (52548MOC6Y) – Developer, Coordinator and Lecturer	**2019-Present**
Physical Organic Chemistry (52548POC6Y) – Developer, Coordinator, Lecturer	**2018-Present**
Molecular Modeling (HRSMC) – Developer, Coordinator and Lecturer	**2019-Present**
Advanced Computational Chemistry (5254ADCC6Y) – Lecturer	**2019-Present**
Molecular Computational Chemistry (51128COC6Y) – Lecturer	**2017-Present**
Computational Pharmcochemistry (X_435350) – Lecturer	**2019-Present**

University of Connecticut

Physical Chemistry – Teaching Assistant	**2013-2015**
Organic Chemistry – Teaching Assistant	**Summer 2014**
General Chemistry – Teaching Assistant	**2010-2013**

ACADEMIC STAFF SUPERVISED

Vrije Universiteit Amsterdam

***Postdoctoral Fellows* (Total = 6)** – M. Dalla Tiezza, T. Hansen, X. Sun, T. Sergeleva, D. Svatunek, O. Larrañaga

***PhD Students* (Total = 19)** – Y. Hordijk *(Co-promoter)*, S. Beutick *(Co-promoter)*, E. Tiekink *(Co-promoter)*, N. Roig Vidal, K. Yamazaki, B. Moloto *(Co-promoter)*, T. Hansen, E. Blokker *(Co-promoter)*, X. Sun *(Co-promoter)*, L. de Azevedo Santos *(Co-promoter)*, A. Castro *(Co-promoter)*, D. Rodrigues Silva *(Co-promoter)*, S. Yu *(Co-promoter)*, P. Vermeeren *(Co-promoter)*, A. K. Narsaria, M. Bortoli, S. Wan, R. P. Orenha, Z. Liu

***MSc Students* (Total = 41)** – Matthijs Kragtwijk, A. van Velzen, K. Salimans, V. Aleksic, D. Bodenstaff, N. Pujmbroeck, L. de Jong, K. Salimans, A. van Velzen, V. Aleksic, R. Verdijk, M. van Dongen, S. Lekanne Deprez, S. Vega Ces, J. Roozee, Y. Hordijk, T. Gijzen, T. Kaptein, L. Tian, S. Beutick, R. van de Ven, K. Zijderveld, R. Ham, M. ten Brink, W. Kossen, B. Waaijer, M. Doppert, M. Grasser, G. Tsitropoulos, E. Tenkink, A. Eisses, R. Yoshisada, B. de Tobel, K. van Dommelen, T. Verdonshot, B. van Beek, P. Laan, T. Bettens, A. S. J. Jaarsma, S. Jiménez Jiménez, K. de Groot

***BSc Students* (Total = 26)** – L. de Jong, M. van Dongen, B. Kras, D. Etnel, L. van Dissel, R. Wagemakers, H. van Overeem, L. van der Zee, A. Landbrug, D. van Raamsdonk, E. Tiekink, D. Jelema, N. Schut, M. Stoop, M. Koning, J. Meijer, M. van Dorp, A. Haim, F. Brinkhuis, D. Jellema, J. Norbury, T. van Heezch, O. Spinnewijn, J. Burg, A. Visscher, E. Blokker

ORGANIZATIONAL DUTIES

Co-Chair: 4th European Symposium on Chemical Bonding (CBOND2024)	**2024**
Organizer: 19th European Symposium on Organic Reactivity (ESOR2023)	**2023**
Chair: 3rd European Symposium on Chemical Bonding (CBOND2022)	**2022**
Organizer: 18$_{th}$ European Symposium on Organic Reactivity (ESOR2021)	**2021**
Track Coordinator (Molecular Sciences) of MSc Chemistry	**2021-Present**
Member: Program Committee of VU and UvA	**2019-2021**
Organizer: 23rd International Conference on “Horizons in Hydrogen Bond Research”	**2019**

INDUSTRY EXPERIENCE

Innospec Fuel Specialties **Summer: 2008 & 2009**
Laboratory Technicians Newark, DE (USA)
Job description: Analyzed customer fuel samples (Sunoco, CononoPhillips, Valero) to determine optimal fuel additive treatment rates for peak combustion performance.

PUBLICATIONS, JOURNAL ARTICLES

[117] Radical Addition Reactions: Hierarchical *Ab initio* Benchmark and DFT Performance Study
Y. Hordijk, M. Dalla Tiezza, D. Rodrigues Silva, **T. A. Hamlin***
ChemPhysChem. **2024**, DOI: 10.1002/cphc.202400728

[116] Concise Synthesis of Cyctetryptomycin A and B Enabled by Zr-catalyzed Dimerization
L. Yu, H. Ogawa, S. Li, T. L. Cheung, W. Liu, D. Yan, Y. Matsuda, Y. Kobayashi, Z. Guo, K. Ikeda, **T. A. Hamlin**, K. Yamazaki, P.-Y. Qian, H. Nakamura
Angew. Chem. Int. Ed. **2024**, DOI: 10.1002/anie.202414295

[115] C1-4 Alkylation of Aryl Bromides with Light Alkanes enabled by Metallaphotocatalysis in Flow
A. Pulcinella, P. C. Tiwari, A. Luridiana, K. Yamazaki, D. Mazzarella, A. K. Sadhoe, A. I. Alfano, E. H. Tiekink, **T. A. Hamlin,*** T. Noël
Angew. Chem. Int. Ed. **2024**, DOI: 10.1002/anie.202413846

[114] Retro-Cope Elimination of Cyclic Alkynes: Reactivity Trends and Rational Design of Next-Generation Bioorthogonal Reagents
S. E. Beutick, S. Yu, L. Orian, F. M. Bickelhaupt, **T. A. Hamlin***
Chem. Sci. **2024**, DOI: 10.1039/D4SC04211E

[113] Rational Design of Metallylenes for Hydrogenation Reactions
E. H. Tiekink, S. Lekanne Deprez, P. Vermeeren, **T. A. Hamlin***
Eur. J. Org. Chem. **2024**, 27, e202400069
Special issue on Physical Organic Chemistry
Spotlight in KNCV Society Volume
Highlighted in C2W
Highlighted in C2W International

[112] Nature and Strength of Group-14 A–A' Bonds
D. Rodrigues Silva, E. Blokker, J. M. van der Schuur, **T. A. Hamlin**, F. M. Bickelhaupt
Chem. Sci. **2024**, *15*, 1648-1656
Highlighted in C2W
Highlighted in C2W International

[111] Cobalt-Catalyzed Enantio- and Regioselective C(sp3)–H Alkenylation of Thioamides
L. Staronova, K. Yamazaki, X. Xu, H. Shia, F. M. Bickelhaupt, **T. A. Hamlin,*** D. J. Dixon
Angew. Chem. Int. Ed. **2024**, *63*, e202316021

[110] Role of Alkaline-Earth Metal in Catalysed Imine Hydrogenations
B. De Tobel, **T. A. Hamlin**, C. Fonseca Guerra, S. Harder, F. De Proft, M. Alonso
Polyhedron **2024**, *248*, 116751

[109] Understanding the Retro-Cope Elimination Reaction of Linear Alkynes
S. E. Beutick, S. Yu, L. Orian, F. M. Bickelhaupt, **T. A. Hamlin***
ChemistryEurope **2024**, *2*, e202300072

[108] Palladium-Catalyzed Activation of HnA–AHn bonds (AHn = CH3, NH2, OH, F)
B. P. Moloto, P. Vermeeren, M. Dalla Tiezza, T. Bouwens, C. Esterhuysen, **T. A. Hamlin,*** F. M. Bickelhaupt
Pure Appl. Chem. **2023**, *95*, 181-191

[107] Solvent Effects on the Sodium Borohydride Reduction of 2-Halocyclohexanones
D. Rodrigues Silva, L. A. Zeoly, P. Vermeeren, R. A. Cormanich, **T. A. Hamlin**, C. Fonseca Guerra, M. P. Freitas
J. Phys. Org. Chem. **2023**, *36*, e4556

[106] S_N2 versus E2 Competition of Cyclic Ethers
T. A. Hansen, P. Vermeeren, K. W. J. Zijderveld, F. M. Bickelhaupt, **T. A. Hamlin***
Chem. Eur. J. **2023**, *29*, e202301308

[105] Catalytic Enantioselective Intramolecular Oxa-Michael Reaction to α,β-Unsaturated Esters and Amides
G. Su, M. Formica, K. Yamazaki, **T. A. Hamlin,*** D. J. Dixon
J. Am. Chem. Soc. **2023**, *145*, 12771–12782
Highlighted in Synfacts
Highlighted in Org. Process Res. Dev.
Highlighted in Organic Chemistry Portal

[104] Origin of the Captodative Effect: The Lone-Pair Shielded Radical
E. Blokker, M. ten Brink, J. M. van der Schuur, **T. A. Hamlin**, F. M. Bickelhaupt
ChemistryEurope **2023**, *1*, e202300006
Highlighted in C2W
Highlighted in C2W International

[103] The Origin of Catalysis and Regioselectivity of Lewis Acid-Catalyzed Diels-Alder Reactions with Tropone
E. H. Tiekink, P. Vermeeren, **T. A. Hamlin***
Chem. Eur. J. **2023**, *29*, e202301223

[102] Not Antiaromaticity Gain, but Increased Asynchronicity Enhances the Diels-Alder Reactivity of Tropone
E. H. Tiekink, P. Vermeeren, **T. A. Hamlin***
Chem. Commun. **2023**, *59*, 3703–3706

[101] Enantioselective Total Synthesis of (–)-Himalensine A via a Palladium and 4-Hydroxyproline Co-catalyzed Desymmetrization of Vinyl-Bromide-tethered Cyclohexanones
R. Kučera, S. R. Ellis, K. Yamazaki, J. H. Cooke, N. Chekshin, K. E. Christensen, **T. A. Hamlin**,* D. J. Dixon
J. Am. Chem. Soc. **2023**, *145*, 5422-5430

[100] The Search for Enhanced σ-Donor Ligands to Stabilize Boron–Boron Multiple Bonds
D. E. Trujillo-González, G. González-García, **T. A. Hamlin**, F. Matthias Bickelhaupt, H. Braunschweig, J. O. C. Jiménez-Halla, M. Solà
Eur. J. Inorg. Chem. **2023**, *26*, e202200767

[99] Origin of Stereoselectivity in SE2' Reactions of Six-membered Ring Oxocarbenium Ions
W. A. Remmerswaal, T. Hansen, **T. A. Hamlin**,* J. D. C. Codée
Chem. Eur. J. **2023**, *29*, e202203490

[98] Intermolecular Covalent Interactions: Nature and Directionality
L. de Azevedo Santos, T. C. Ramalho, **T. A. Hamlin**,* F. M. Bickelhaupt
Chem. Eur. J. **2023**, *29*, e202203791

[97] C(sp^n)–X (n = 1–3) Bond Activation by Iron
M. Bołt, E. H. Tiekink, T. Hansen, F. M. Bickelhaupt, **T. A. Hamlin**,*
Eur. J. Org. Chem **2022***, 46*, e202201144

[96] How Bases Catalyze Diels-Alder Reactions
S. Yu, E. H. Tiekink, P. Vermeeren, F. M. Bickelhaupt, **T. A. Hamlin***
Chem. Eur. J. **2022***, 29*, e202203121

[95] Iron-Catalysed Carbene Transfer to Isocyanides as a Platform for Heterocycle Synthesis
T. R. Roose, H. D. Preschel, H. M. Tejedor, J. C. Roozee, **T. A. Hamlin**,* B. U. W. Maes, E. Ruijter, R. V. A. Orru
Chem. Eur. J. **2022**, *29*, e202203074

[94] Stability of Alkyl Carbocations
T. Hansen, P. Vermeeren, F. M. Bickelhaupt, **T. A. Hamlin***
Chem. Commun. **2022**, *58*, 12050–12053

[93] Rational Tuning of the Reactivity of Three-Membered Heterocycle Ring-Openings via S_N2 Reactions
T. Hansen, A. Nin-Hill, J. D. C. Codée, **T. A. Hamlin**, C. Rovira
Chem. Eur. J. **2022**, *28*, e202201649

[92] Pericyclic reaction benchmarks: hierarchical computations targeting CCSDT(Q)/CBS and analysis of DFT performance
P. Vermeeren, M. Dalla Tiezza, M. E. Wolf, M. E. Lahm, W. D. Allen, H. F. Schaefer, III, **T. A. Hamlin**,* F. M. Bickelhaupt
Phys. Chem. Chem. Phys. **2022**, *24*, 18028-18042

[91] Methyl Substitution Destabilizes Alkyl Radicals
E. Blokker, W.-J. van Zeist, X. Sun, J. Poater, J. M. van der Schuur, **T. A. Hamlin**, F. M. Bickelhaupt
Angew. Chem. Int. Ed. **2022**, *61*, e202207477

[90] The 1,3-Dipolar Cycloaddition: From Conception to Quantum Chemical Design
S. E. Beutick, P. Vermeeren, **T. A. Hamlin***
Chem. Asian J. **2022**, *17*, e202200553

[89] Palladium-Catalyzed Activation of Carbon–Halogen Bonds: Electrostatics-Controlled Reactivity
B. P. Moloto, P. Vermeeren, M. Dalla Tiezza, C. Esterhuysen, F. M. Bickelhaupt, **T. A. Hamlin**,*
Eur. J. Org. Chem. **2022**, *26*, e202200722

[88] SN2 versus SN2' Competition
T. Hansen, P. Vermeeren, L. de Jong, F. M. Bickelhaupt, **T. A. Hamlin***
J. Org. Chem. **2022**, *87*, 8892–8901

[87] How Ionization Catalyzes Diels-Alder Reactions
P. Vermeeren, **T. A. Hamlin**,* F. M. Bickelhaupt
Chem. Eur. J. **2022**, *28*, e202200987

[86] C–X Bond Activation by Palladium: Steric Shielding versus Steric Attraction
T. Hansen, X. Sun, M. Dalla Tiezza, W.-J. van Zeist, J. N. P. van Stralen, D. P. Geerke, L. P. Wolters, J. Poater, **T. A. Hamlin**,* F. M. Bickelhaupt
Chem. Eur. J. 2022, e202201093

[85] B-DNA Structure and Stability: The Role of Nucleotide Composition and Order
C. Nieuwland, **T. A. Hamlin**, C. Fonseca Guerra, G. Barone, F. M. Bickelhaupt
ChemistryOpen **2022**, *11*, e202100231

[84] Rational Design of Iron Catalysts for C–X Bond Activation
X. Sun, T. Hansen, J. Poater, **T. A. Hamlin**,* F. M. Bickelhaupt
J. Comput. Chem. **2022**, *43*, 495-505

[83] $C(sp^n)$–X (n = 1–3) Bond Activation by Palladium
T. Hansen, X. Sun, M. Dalla Tiezza, W.-J. van Zeist, J. Poater, **T. A. Hamlin**,* F. M. Bickelhaupt
Chem. Eur. J. **2022**, *28*, e202103953

[82] Bifunctional Iminophosphorane Catalyzed Enantioselective Sulfa-Michael Addition to Unactivated α,β-Unsaturated Amides
D. Rozsar, M. Formic, K. Yamazaki, **T. A. Hamlin**,* D. J. Dixon
J. Am. Chem. Soc. **2021**, *144*, 1006–1015

[81] How Solvation Influences the S_N2 versus E2 Competition
T. Hansen, J. Roozee, F. M. Bickelhaupt, **T. A. Hamlin***
J. Org. Chem. **2021**, *87*, 1805–1813

[80] A New Organocatalytic Desymmetrization Reaction Enables the Enantioselective Total Synthesis of Madangamine E
S. Shiomi, B. D. A. Shennan, K. Yamazaki, A. L. Fuentes de Arriba, D. Vasu, **T. A. Hamlin**,* D. J. Dixon
J. Am. Chem. Soc. **2021**, *144*, 1407–1415

[79] The Chemical Bond: When Atom Size Instead of Electronegativity Difference Determines Trends in Bond Strength

E. Blokker, X. Sun, J. Poater, J. M. van der Schuur, **T. A. Hamlin**, F. M. Bickelhaupt
Chem. Eur. J. **2021**, *27*, 15616–15622
Highlighted by ChemistryViews
Highlighted by C2W
Highlighted by Chemistry World
Highlighted by VU News
Highlighted by Nature

[78] Radical Scavenging Potential of the Phenothiazine Scaffold: A Computational Analysis
M. Dalla Tiezza, **T. A. Hamlin**,* F. M. Bickelhaupt, L. Orian
ChemMedChem **2021**, *16*, 3763–3771

[77] Switch from Pauli-Lowering to LUMO-Lowering Catalysis in Brønsted Acid-Catalyzed Aza-Diels-Alder Reactions
S. Yu, F. M. Bickelhaupt, **T. A. Hamlin***
ChemistryOpen **2021**, *10*, 784–789

[76] How Lewis Acids Catalyze Ene Reactions
E. H. Tiekink, P. Vermeeren, F. M. Bickelhaupt, **T. A. Hamlin***
Eur. J. Org. Chem. **2021**, 5275–5283

[75] Origin of Asynchronicity in Diels-Alder Reactions
P. Vermeeren, **T. A. Hamlin**,* F. M. Bickelhaupt
Phys. Chem. Chem. Phys. **2021**, *23*, 20095–20106

[74] Dipolar Repulsion in α-Halocarbonyl Compounds Revisited
D. Rodrigues Silva, L. de Azevedo Santos, **T. A. Hamlin**, F. M. Bickelhaupt, M. P. Freitas, C. Fonseca Guerra
Phys. Chem. Chem. Phys. **2021**, *23*, 20883–20891

[73] Switchable, Reagent-Controlled Diastereodivergent Photocatalytic Carbocyclisation of Imine-Derived α-Amino Radicals
J. A. P. Maitland, J. A. Leitch, K. Yamazaki, K. E. Christensen, D. J. Cassar, **T. A. Hamlin**,* D. J. Dixon
Angew. Chem. Int. Ed. **2021**, *60*, 24116–24123

[72] How Divalent Cations Interact with the Internal Channel Site of Guanine Quadruplexes
F. Zaccaria, S. C. C. van der Lubbe, C. Nieuwland, **T. A. Hamlin**,* C. Fonseca Guerra
ChemPhysChem **2021**, *22*, 2265–2266

[71] Boron Tunneling in the "Weak" Bond-Stretch Isomerization of N–B Lewis Adducts
A. Nandi, N. Tarannam, D. Rodrigues Silva, C. Fonseca Guerra, **T. A. Hamlin**,* S. Kozuch
ChemPhysChem **2021**, *22*, 1857–1862

[70] Origin of the α-Effect in S_N2 Reactions
T. Hansen, P. Vermeeren, F. Matthias Bickelhaupt, **T. A. Hamlin***
Angew. Chem. Int. Ed. 2021, *60*, 20840–20848
Highlighted by ChemistryViews

[69] The Pnictogen Bond: A Quantitative Molecular Orbital Picture
L. de Azevedo Santos, **T. A. Hamlin**, T. C. Ramalho, F. M. Bickelhaupt
Phys. Chem. Chem. Phys. **2021**, *23*, 13842–13852

[68] Chemical Reactivity from an Activation Strain Perspective
P. Vermeeren, **T. A. Hamlin**,* F. M. Bickelhaupt
Chem. Commun. **2021**, *57*, 5880–5896

[67] A General Pyrrolidine Synthesis via Iridium-Catalyzed Reductive Azomethine Ylide Generation from Tertiary Amides & Lactams
K. Yamazaki, P. Gabriel, G. Di Carmine, J. Pedroni, M. Farizyan, **T. A. Hamlin**,* D. J. Dixon
ACS Catal. **2021**, *11*, 7489–7497

[66] Pd-Catalyzed Cascade to Benzoxepins by Using Vinyl-Substituted Donor-Acceptor Cyclopropanes
M. Faltracco, K. N. A. van de Vrande, M. Dijkstra, J. M. Saya, **T. A. Hamlin**,* E. Ruijter
Angew. Chem. **2021**, *133*, 14531–14535; *Angew. Chem. Int. Ed.* **2021**, *60*, 14410–14414

[65] The Pauli-Repulsion Lowering Concept in Catalysis
T. A. Hamlin,* I. Fernandez, F. M. Bickelhaupt
Acc. Chem. Res. **2021**, *54*, 1972–1981

[64] A Bifunctional Iminophosphorane Squaramide Catalyzed Enantioselective Synthesis of Hydroquinazolines via Intramolecular Aza-Michael Addition to α,β-Unsaturated Esters
G. Su, C. J. Thomson, K. Yamazaki, D. Rozsar, K. Christensen, **T. A. Hamlin**,* D. J. Dixon
Chem. Sci. **2021**, *12*, 6064–6072

[63] Lewis Acid-Catalyzed Diels-Alder Reactions: Reactivity Trends Across the Periodic Table
P. Vermeeren, M. Dalla Tiezza, M. van Dongen, I. Fernandez, F. M. Bickelhaupt, **T. A. Hamlin***
Chem. Eur. J. **2021**, *27*, 10610–10620

[62] The Gauche Effect in XCH_2CH_2X Revisited
D. Rodrigues Silva, L. de Azevedo Santos, **T. A. Hamlin**, C. Fonseca Guerra, M. P. Freitas, F. M. Bickelhaupt
ChemPhysChem **2021**, *22*, 641–648

[61] How the Lewis Base F– Catalyzes the 1,3-Dipolar Cycloaddition Between Carbon Dioxide and Nitrilimines
D. Svatunek, T. Hansen, K. N. Houk, **T. A. Hamlin***
J. Org. Chem. **2021**, *86*, 4320–4325

[60] Not Carbon s–p Hybridization, but Coordination Number Determines C–H and C–C Bond Length
P. Vermeeren, W.-J. van Zeist, **T. A. Hamlin**, C. Fonseca Guerra, F. M. Bickelhaupt
Chem. Eur. J. **2021**, *27*, 7074–7079
Highlighted by C2W
Highlighted by Chemistry World

[59] How Metallylenes Activate Small Molecules
P. Vermeeren, M. T. Doppert, F. M. Bickelhaupt, **T. A. Hamlin***
Chem. Sci. **2021**, *12*, 4526–4536

[58] How Lewis Acids Catalyze Ring-Openings of Cyclohexene Oxide
T. Hansen, P. Vermeeren, R. Yoshisada, D. V. Filippov, G. A. van der Marel, J. D. C. Codée, **T. A. Hamlin***
J. Org. Chem. **2021**, *86*, 3565–3573

[57] Chalcogen Bonds: Hierarchical Ab Initio Benchmark and DFT Performance Study
L. de Azevedo Santos, T. C. Ramalho, **T. A. Hamlin**,* F. M. Bickelhaupt
J. Comput. Chem. **2021**, *42*, 688–698

[56] 1,1,4,4-Tetracyanobutadiene-Functionalized Anthracenes: Regioselectivity of Cycloadditions in the Synthesis of Small Near-IR Dyes
C. Philippe, A. T. Bui, S. Batsongo-Boulingui, Z. Pokladek, K. Matczyszyn, O. Mongin, L. Lemiègre, F. Paul, **T. A. Hamlin**,* Y. Trolez
Org. Lett. **2021**, *23*, 2007–2012

[55] A Quantitative MO Perspective of the Chalcogen Bond
L. de Azevedo Santos, S. C. C. van der Lubbe, **T. A. Hamlin**, T. C. Ramalho, F. M. Bickelhaupt
ChemistryOpen **2021**, *10*, 391–401

[54] On the Origin of Regioselectivity in Palladium-Catalyzed Oxidation of Glucosides
I. C. Wan, **T. A. Hamlin**, N. N. H. M. Eisink, N. Marinus, C. de Boer, C. A. Vis, J. D. C. Codée, M. D. Witte, A. J. Minnaard, F. M. Bickelhaupt
Eur. J. Org. Chem. **2021**, 632–636

[53] How Oriented External Electric Fields Modulate Reactivity
S. Yu, P. Vermeeren, **T. A. Hamlin**,* F. M. Bickelhaupt
Chem. Eur. J. **2021**, *27*, 5683–5693

[52] Bifunctional Hydrogen Bond Donor-Catalyzed Diels-Alder Reactions: Origin of Selectivity and Rate Enhancement
P. Vermeeren, **T. A. Hamlin**,* F. M. Bickelhaupt, I. Fernandez
Chem. Eur. J. **2021**, *27*, 5180–5190

[51] Dual Catalytic Enantioselective Desymmetrization of Allene-Tethered Cyclohexanones
L. Zhang, K. Yamazaki, J. A. Leitch, R. Manzano, V. A. M. Atkinson, **T. A. Hamlin**,* D. J. Dixon
Chem. Sci. **2020**, *11*, 7444–7450

[50] Nature and Strength of Lewis Acid/Base Interaction in Boron and Nitrogen Trihalides
D. Rodrigues Silva, L. de Azevedo Santos, M. P. Freitas, C. Fonseca Guerra, **T. A. Hamlin***
Chem. Asian. J. **2020**, *15*, 4043–4054

[49] S_N2 versus E2 Competition of F^- and $PH2^-$ Revisited
P. Vermeeren, Thomas Hansen, M. Grasser, D. Rodrigues Silva, **T. A. Hamlin**,* F. M. Bickelhaupt
J. Org. Chem. **2020**, 85, 14087–14093

[48] A Unified Framework for Understanding Nucleophilicity and Protophilicity in the S_N2/E2 Competition
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