

# TREVOR A. HAMLIN

## PERSONAL DETAILS

**Full Name:** Trevor Alexander Hamlin

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**E-mail:** [t.a.hamlin@vu.nl](mailto:t.a.hamlin@vu.nl)

## PROFESSIONAL EXPERIENCE

**Tenured Assistant Professor**

**Vrije Universiteit Amsterdam**

Research focus: Theory-Driven Experimentation, Physical Organic Chemistry, Computational Chemistry

**2018-Present**  
Amsterdam (NL)

**Postdoctoral Research Fellow**

**Vrije Universiteit Amsterdam**

Principal Investigator: Professor F. M. Bickelhaupt

Research focus: Theory-Driven Experimentation and Computational Chemistry

**2015-2018**  
Amsterdam (NL)

## EDUCATION

**Ph.D. in Physical Organic Chemistry**

**University of Connecticut**

**GPA: 3.88/4.00**

Principal Investigator: Professor Nicholas E. Leadbeater

Research focus: Organofluorine, Oxoammonium Salt Chemistry, Continuous-Flow Processing

**2010-2015**  
Storrs, CT (USA)

**B.S. in Biochemistry**

**Albright College**

**GPA: 3.73/4.00 (cum laude)**

Principal Investigator: Professor Christian S. Hamann

Research focus: Terpene Biosynthesis and Computational Chemistry

**2006-2010**  
Reading, PA (USA)

## AWARDS AND DISTINCTIONS

**Vrije Universiteit Amsterdam**

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

**University of Connecticut**

2014 Doctoral Dissertation Fellowship

2013 Zaiput Flow Technologies Challenge Grant

2011 Chemistry Alumni Outstanding Teaching Assistant Award

**Albright College**

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

**Ph.D. Students (Total = 15)** – 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

**M.Sc. Students (Total = 23)** – Y. Hordijk, T. Gijzen, T. Kaptein, L. Tian, S. Beutick, R. van de Ven, K. Zijdeveld, 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

**B.Sc. 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

## COMMITTEE DUTIES

### Vrije Universiteit Amsterdam

3 <sup>rd</sup> Annual Chemical Bonding Conference	2020
Program Committee Member	2019-Present
23 <sup>rd</sup> International Conference on “Horizons in Hydrogen Bond Research”	2019

## INDUSTRY EXPERIENCE

### Innospec Fuel Specialties

Laboratory Technician	Summer: 2008 & 2009 Newark, DE (USA)
Job description: Analyzed customer fuel samples (Sunoco, CononoPhillips, Valero) to determine ideal fuel additive treatment rates necessary for achieving optimum engine performance.	

**PUBLICATIONS, JOURNAL ARTICLES** (\* denotes corresponding author)

- [81] How Solvation Influences the SN2 versus E2 Competition  
T. Hansen, J. Roozee, F. M. Bickelhaupt,\* **T. A. Hamlin\***  
*J. Org. Chem.* **2021**, *accepted*
- [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\*  
Preprint uploaded to *ChemRxiv* (DOI: 10.33774/chemrxiv-2021-1f3kt)
- [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 y 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*, online
- [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  $\alpha$ -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  $\alpha$ -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  $\alpha$ -Effect in S<sub>N</sub>2 Reactions  
T. Hansen, P. Vermeeren, F. Matthias Bickelhaupt, **T. A. Hamlin**\*  
*Angew. Chem.* **2021**, *133*, 21008-21016; *Angew. Chem. Int. Ed.* **2021**, *60*, 20840-20848
- [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  $\alpha,\beta$ -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<sub>2</sub>CH<sub>2</sub>X 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<sup>-</sup> 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<sub>N</sub>2 versus E2 Competition of F<sup>-</sup> and PH<sub>2</sub><sup>-</sup> 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<sub>N</sub>2/E2 Competition  
P. Vermeeren, Thomas Hansen, P. Janssen, M. Swart, **T. A. Hamlin**,\* F. M. Bickelhaupt\*  
*Chem. Eur. J.* **2020**, *26*, 15538-15548
- [47] Origin of Rate Enhancement and Asynchronicity in Iminium Catalyzed Diels-Alder Reactions  
P. Vermeeren, **T. A. Hamlin**,\* I. Fernandez,\* F. M. Bickelhaupt\*  
*Chem. Sci.* **2020**, *11*, 8105–8112
- [46] Dual Catalytic Enantioselective Desymmetrization of Allene-Tethered Cyclohexanones  
Lin Zhang, Ken Yamazaki, Jamie A. Leitch, Ruben Manzano, Victoria A. M. Atkinson, **T. A. Hamlin**,\*  
Darren J. Dixon\*  
*Chem. Sci.* **2020**, *11*, 7444–7450
- [45] Diastereoselective Synthesis of β-Lactams by Ligand-Controlled Stereodivergent Intramolecular  
Tsuji–Trost Allylation  
M. Faltracco, V. Sukowski, M. van Druenen, **T. A. Hamlin**,\* F. M. Bickelhaupt, E. Ruijter\*  
*J. Org. Chem.* **2020**, *85*, 9566–9584
- [44] Regioselectivity of Epoxide Ring-Openings via S<sub>N</sub>2 Reactions Under Basic and Acidic Conditions  
Thomas Hansen, Pascal Vermeeren, Anissa Haim, Maarten J. H. van Dorp, Jeroen D. C. Codée, F.  
Matthias Bickelhaupt,\* **T. A. Hamlin**\*  
*Eur. J. Org. Chem.* **2020**, 3822–3828
- [43] Understanding the 1,3-Dipolar Cycloadditions of Allenes  
S. Yu, P. Vermeeren, K. van Dommelen, F. M. Bickelhaupt\*, **T. A. Hamlin**\*  
*Chem. Eur. J.* **2020**, *26*, DOI: 10.1002/chem.202000857
- [42] Performance of TDDFT Vertical Excitation Energies of Core-Substituted Naphthalene Diimide  
A. K. Narsaria, J. D. Ruijter, **T. A. Hamlin**, A. W. Ehlers, C. Fonseca Guerra, K. Lammertsma,\* F. M.  
Bickelhaupt\*  
*J. Comput. Chem.* **2020**, *41*, 1448–1455
- [41] How Alkali Cations Catalyze Aromatic Diels-Alder Reactions  
P. Vermeeren, F. Brinkhuis, **T. A. Hamlin**,\* F. M. Bickelhaupt\*  
*Chem. Asian J.* **2020**, *15*, 1167–1174
- [40] Ambident Nucleophilic Substitution: Understanding Non-HSAB Behavior through Activation Strain  
and Conceptual DFT Analyses  
T. Bettens, M. Alonso, F. De Proft,\* **T. A. Hamlin**,\* F. M. Bickelhaupt\*  
*Chem. Eur. J.* **2020**, *26*, 3884–3893
- [39] How Lewis Acids Catalyze Diels-Alder Reactions  
P. Vermeeren, **T. A. Hamlin**, I. Fernandez,\* F. M. Bickelhaupt\*  
*Angew. Chem.* **2020**, *132*, 6260–6265; *Angew. Chem. Int. Ed.* **2020**, *59*, 6201–6206
- [38] Ligand-Mediated Regioselective Rhodium Catalyzed Benzotriazole-Allene Coupling: Mechanistic  
Exploration and Quantum Chemical Analysis  
T. Sergeieva, **T. A. Hamlin**, S. Okovytyy, B. Breit,\* F. M. Bickelhaupt\*  
*Chem. Eur. J.* **2020**, *26*, 2342–2348

- [37] Distortion-Controlled Red-Shift of Organic Dye Molecules  
A. K. Narsaria, J. Poater, C. Fonseca Guerra, A. W. Ehlers, **T. A. Hamlin**,\* K. Lammertsma,\* F. M. Bickelhaupt\*  
*Chem. Eur. J.* **2020**, *26*, 2080–2093
- [36] Understanding Chemical Reactivity Using the Activation Strain Model  
P. Vermeeren, S. C. C. van der Lubbe, C. Fonseca Guerra, F. M. Bickelhaupt,\* **T. A. Hamlin**\*  
*Nature Protocols*, **2020**, *15*, 649–667
- [35] Rapid Assembly of Functionalized Morpholinones and 1,4-Oxazepane-3-ones via [3+3]- and [3+4]-Annulation of Aza-oxyallyl Cation and Amphoteric Compounds  
T. Bera, B. Singh, T. A. Hamlin, S. C. Sahoo, J. Saha\*  
*J. Org. Chem.* **2019**, *84*, 15255–15266
- [34] Computational and Dynamic NMR Studies on the Complexation of Lithium Ion to 8-Crown-4  
A. van der Ham, T. Hansen, G. Lodder, J. D. C. Codée, **T. A. Hamlin**, D. V. Filippov\*  
*ChemPhysChem* **2019**, *20*, 2103–2109
- [33] Dual Activation of Aromatic Diels-Alder Reactions  
A. K. Narsaria, **T. A. Hamlin**,\* K. Lammertsma,\* F. M. Bickelhaupt\*  
*Chem. Eur. J.* **2019**, *25*, 9902–9912  
*Highlighted on the [VU Website](#)*
- [32] Lewis Acid Catalyzed Annulation of Spirocyclic Donor-Acceptor Cyclopropanes with Exo-Heterocyclic Olefins: Access to Highly Functionalized bis-Spirocyclopentane Oxindole Frameworks  
K. Singh, S. Pramanik, **T. A. Hamlin**, B. Mondal, D. Das, J. Saha\*  
*Chem. Commun.* **2019**, *55*, 7069–7072
- [31] PyFrag 2019 — Automating the Exploration and Analysis of Reaction Mechanisms  
X. Sun, T. M. Soini, J. Poater,\* **T. A. Hamlin**,\* F. M. Bickelhaupt\*  
*J. Comput. Chem.* **2019**, *40*, 2227–2233
- [30] How Dihalogens Catalyze Michael Addition Reactions  
**T. A. Hamlin**, I. Fernandez,\* F. M. Bickelhaupt\*  
*Angew. Chem.* **2019**, *131*, 9015–9020; *Angew. Chem. Int. Ed.* **2019**, *58*, 8922–8926  
*Highlighted in [ChemistryWorld](#)*
- [29] Understanding the Differences Between Iron and Palladium in Cross Coupling Reactions  
X. Sun, M. de la Rocha, **T. A. Hamlin**, J. Poater,\* F. M. Bickelhaupt\*  
*Phys. Chem. Chem. Phys.* **2019**, *21*, 9154–9664
- [28] Structural Distortion of Cycloalkynes Influences Cycloaddition Rates by Both Strain and Interaction Energies  
**T. A. Hamlin**, B. J. Levandowski, A. K. Narsaria, K. N. Houk,\* F. M. Bickelhaupt\*  
*Chem. Eur. J.* **2019**, *25*, 6342–6348
- [27] Chemoselectivity of Tertiary Azides in Strain-Promoted Alkyne-Azide Cycloadditions  
D. Svatunek, N. Houszka, **T. A. Hamlin**, F. M. Bickelhaupt,\* H. Mikula\*  
*Chem. Eur. J.* **2019**, *25*, 754–758

- [26] Nucleophilic Substitution at Di- and Triphosphates: Leaving Group Ability of Phosphate vs Diphosphate  
B. van Beek, M. A. van Bochove, **T. A. Hamlin**,\* F. M. Bickelhaupt\*  
*Electr. Stuct.* **2019**, *1*, 024001
- [25] Elucidating the Trends in Reactivity of Aza-1,3-Dipolar Cycloadditions  
**T. A. Hamlin**,\* D. Svatunek, S. Yu, L. Ridder, L. Visscher,\* F. M. Bickelhaupt\*  
*Eur. J. Org. Chem.* **2019**, 378–386
- [24] Diels-Alder Reactivities of Unsaturated Cyclic Diones with Tetrazine  
B. J. Levandowski, **T. A. Hamlin**, H. J. Eckvahl, F. M. Bickelhaupt,\* K. N. Houk\*  
*J. Mol. Model* **2019**, *25*, 33/1–5
- [23] Factors Controlling the Diels-Alder Reactivity of Hetero-1,3-Butadiene  
S. Yu, H. M. de Bruijn, D. Svatunek, **T. A. Hamlin**,\* F. M. Bickelhaupt\*  
*ChemistryOpen* **2018**, *7*, 995–1004
- [22] Nature and Strength of Chalcogen- $\pi$  Bonds  
M. Bortoli, S. M. Ahmad, **T. A. Hamlin**, F. M. Bickelhaupt,\* L. Orian\*  
*Phys. Chem. Chem. Phys.* **2018**, *20*, 27592–27599
- [21] A Methodology for the Photocatalyzed Radical Trifluoromethylation of Indole: A Combined Experimental and Computational Study  
S. A. Miller, B. van Beek, **T. A. Hamlin**,\* F. M. Bickelhaupt, N. E. Leadbeater\*  
*J. Fluorine Chem.* **2018**, *214*, 94–100
- [20] How  $Mg^{2+}$  Ions Lower the  $S_N2@P$  Barrier in Enzymatic Triphosphate Hydrolysis  
M. A. van Bochove, G. Roos, C. Fonseca Guerra, **T. A. Hamlin**,\* F. M. Bickelhaupt\*  
*Chem. Commun.* **2018**, *54*, 3448–3451  
*Highlighted on the VU Website*
- [19] Origins of the *Endo* and *Exo* Selectivities in Cyclopropenone, Iminocyclopropene, and Triafulvene Diels-Alder Cycloadditions  
B. J. Levandowski, **T. A. Hamlin**, R. C. Helgeson, F. M. Bickelhaupt,\* K. N. Houk\*  
*J. Org. Chem.* **2018**, *83*, 3164–3170
- [18] Nucleophilic Substitution ( $S_N2$ ): Dependence on Nucleophile, Leaving Group, Central Atom, Substituents, and Solvent  
**T. A. Hamlin**, M. Swart,\* F. M. Bickelhaupt\*  
*ChemPhysChem* **2018**, *19*, 1315–1330
- [17] Nucleophilic Substitution in Solution: in Solution: Activation Strain Analysis of Weak and Strong Solvent Effects  
**T. A. Hamlin**, B. van Beek, L. Wolters, F. M. Bickelhaupt\*  
*Chem. Eur. J.* **2018**, *24*, 5927–5938
- [16] [(Trifluoromethyl)sulfanyl]ethane: A Key Building Block for the Synthesis of  $CF_3S$ -Containing Isoxanzolidines  
A. Riesco, J. van de Wiel, **T. A. Hamlin**, D. Blanco, B. van Beek, F. M. Bickelhaupt,\* F. P. J. T. Rutjes\*  
*J. Org. Chem.* **2018**, *83*, 1779–1789
- [15] Macrocycles All Aflutter: Substitution at an Allylic Center Reveals Conformational Dynamics of [13]-Macrolactones



- K. M. Rutledge, **T. A. Hamlin**, D. M. Baldisseri, F. M. Bickelhaupt,\* M. W. Peczuł\*  
*Chem. Asian J.* **2017**, *12*, 2623–2633
- [14] The Role of Orbital Interactions and Activation Strain (Distortion Energies) on Reactivities in the Normal and Inverse Electron-Demand Cycloadditions of Strained and Unstrained Cycloalkenes  
B. J. Levandowski, **T. A. Hamlin**, F. M. Bickelhaupt,\* K. N. Houk\*  
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## **REFEREE DUTIES**

Science, Nature, Nature Chemistry, Nature Communications, Angewandte Chemie, Journal of the American Chemical Society, Organic and Inorganic Au, Chemistry - A European Journal, Chemistry - An Asian Journal, Catalysis Science and Technology, Chemical Communications, Journal of Organic Chemistry, European Journal of Organic Chemistry, Physical Chemistry Chemical Physics, Journal of Computational Chemistry, Dalton Transactions, Organic and Biomolecular Chemistry, ChemistryOpen, Journal of Physical Chemistry A, The Journal of Chemical Physics, ChemistrySelect, ACS Omega, Computational and Theoretical Chemistry, International Journal of Chemical Kinetics

## **PRESENTATIONS**

- [30] Pauli Tuning of Reactions - The Role of the Reactants Closed Shells (Invited Talk: The 3rd European Symposium on Chemical Bonding) • Amsterdam, NL • 2020) *\*\*\*postponed due to COVID 19 outbreak\*\*\**
- [29] Pauli Tuning of Reactions - The Role of the Reactants Closed Shells (Invited Talk: European Meeting on Physical Organic Chemistry) • University of Wrocław, PL • 2020) *\*\*\*postponed due to COVID 19 outbreak\*\*\**
- [28] Understanding Chemical Reactivity Using the Activation Strain Model (Invited Talk: Université de Rennes) • Rennes, FR • 2019)
- [27] 1,3-Dipolar Cycloaddition Reactivity of Cycloalkynes (Invited Talk: 23rd International Conference on "Horizons in Hydrogen Bond Research" • Amsterdam, NL • 2019)
- [26] How Dihalogenes Catalyze Michael Addition Reactions (Invited Talk: Chemistry as Innovating Science (Chains) • Veldhoven, NL • 2019)
- [26] 1,3-Dipolar Cycloaddition Reactivity of Cycloalkynes (Talk: 17th European Symposium on Organic Reactivity • Dubrovnik, HR • 2019)
- [25] 1,3-Dipolar Cycloaddition Reactivity of Cycloalkynes (Invited Talk: 1st Annual Symposium of the Division of Computational and Theoretical Chemistry (CTC) of the Royal Netherlands Chemical Society (KNCV) • Amsterdam, NL • 2019)
- [24] Predicting and Understanding Vinyl-SCF<sub>3</sub> Reactivity in 1,3-Dipolar Cycloadditions (Poster: Oriëntatiemarkt Scheikunde ACD • University of Amsterdam • Amsterdam, NL • 2017)
- [23] Nucleophilic Substitution in Solution: Activation Strain Analysis of Weak and Strong Solvent Effects (Poster: Chemistry as Innovating Science (Chains) • Veldhoven, NL • 2018)
- [22] How do (Exo)Planetary Environments Affect Chemistry? (Talk: PEPSci Evaluation Meeting • Leiden, NL • 2018)
- [21] Diels-Alder Reactivity of Strained Cycloalkenes (Talk: Second European Symposium on Chemistry Bonding • Oviedo, ES • 2018)
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- [18] B-DNA Stability and Replication in Non-Terran Bio-Solvents (Poster: DNA Damage and Repair: Computations Meet Experiments • Lorentz Center • Leiden, NL • 2017)
- [17] B-DNA Replication in Exotic Solvents: Focus on Archetypical Nucleophilic Substitution Reactions (Talk: Chemistry as Innovating Science (Chains) • Veldhoven, NL • 2016)
- [16] B-DNA Stability and Replication in Non-Terran Bio-Solvents (Poster: First European Symposium on Chemical Bonding • Rouen, FR • 2016)
- [15] B-DNA Stability and Replication: Interplay of Solvation, Stacking, and H-bonding (Invited Talk: PEPsci Meeting Netherlands Institute for Space Research • University of Groningen • Groningen, NL • 2016)
- [14] Using Borane, Ammonium, and Methylene Substitutions to Characterize Stabilizing Features of a Macrocyclic Sesquiterpene Cation (Poster: 249<sup>th</sup> National American Chemical Society Meeting • Denver, CO • 2015; *this poster was also selected for presentation at the Sci-Mix*)
- [13] Quantum Chemical Calculations for the Elucidation of Reaction Mechanism (Poster: 48<sup>th</sup> Annual RT Major Conference • University of Connecticut • Storrs, CT • 2015)
- [12] A Continuous-Flow Approach to 3,3,3-Trifluoromethylpropenes (Poster: 48<sup>th</sup> Annual RT Major Conference • University of Connecticut • Storrs, CT • 2015)
- [11] 1,3- $\gamma$ -Silyl-Elimination in Electron-Deficient Cationic Systems (Invited Talk: Tantillo Group Meeting • University of California at Davis • Davis, CA • 2015)

- [10] Monitoring Continuous-Flow Reactions Using Raman Spectroscopy. (**Talk:** Northeast Regional Meeting of the ACS • New Haven, CT • 2013)
- [9] Raman Spectroscopy as a Tool for Monitoring Mesoscale Continuous-Flow Organic Synthesis: Equipment Interface and Assessment in Four Medicinally-Relevant Reactions (Poster: 47<sup>th</sup> Annual RT Major Conference • University of Connecticut • Storrs, CT • 2013)
- [8] Raman Spectroscopy as a Tool for Monitoring Mesoscale Continuous-Flow Organic Synthesis: Equipment Interface and Assessment in Four Medicinally-Relevant Reactions (Poster: Zing Conference on Microwave and Flow Chemistry • Napa, CA • 2013) (**Poster Award**)
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- [5] Using Borane, Ammonium, and Methylene Substitution to Characterize the Stabilizing Features of a Macrocyclic Sesquiterpene Cation (Talk: 239<sup>th</sup> National American Chemical Society Meeting • San Francisco, CA • 2010)
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