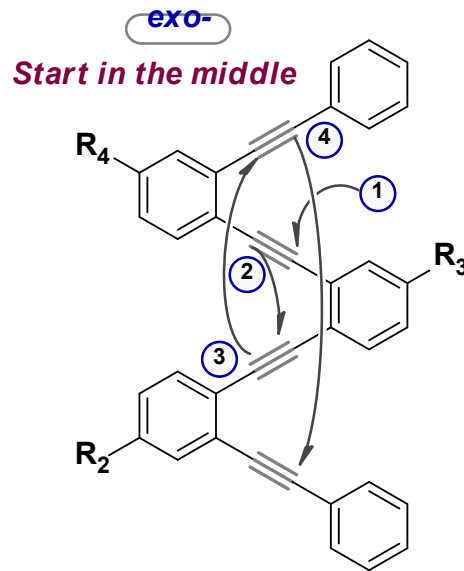
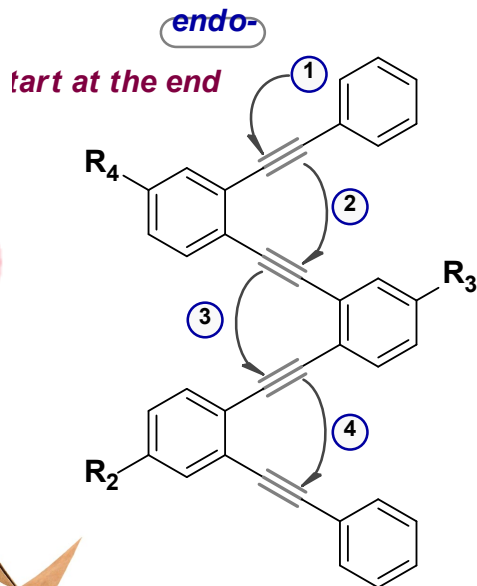
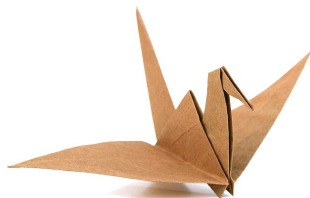
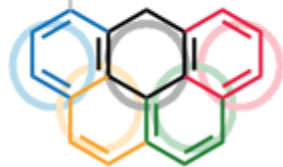


# How to Become Famous (with Organic Chemistry)

Alternative Folding Patterns:

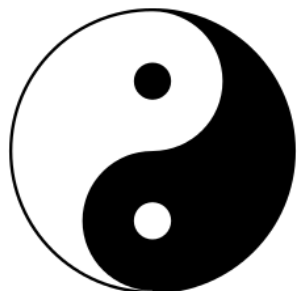
2 0 1 8



$$2 + ? = 4$$

*Igor Alabugin,  
Florida State University,*

*July 23, 2024*



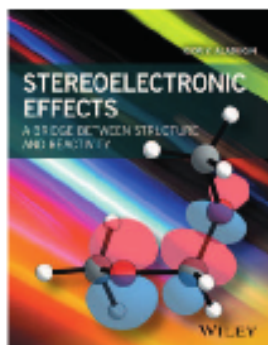
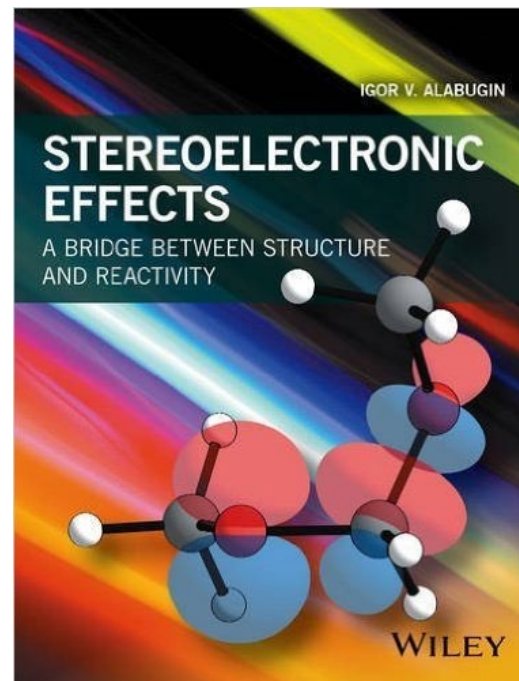
# The main questions of chemistry:

How to **make** a bond?

How to **break** a bond?

GDCh

Books



**StereoElectronic Effects**  
A Bridge between Structure and Reactivity  
By Igor V. Alabugin. John Wiley and Sons, Hoboken  
2016 392 pp. softcover

*StereoElectronic Effects*

Obviously, a profound knowledge of structures, energies, and reactivities of chemical compounds is essential for every chemist, and stereoelectronic effects have a significant influence on these factors. In this book, Igor Alabugin, a widely acknowledged expert in this field, gives an up-to-date and comprehensive overview of this topic with a strong focus on organic chemistry. The relevance of these stabilizing effects,

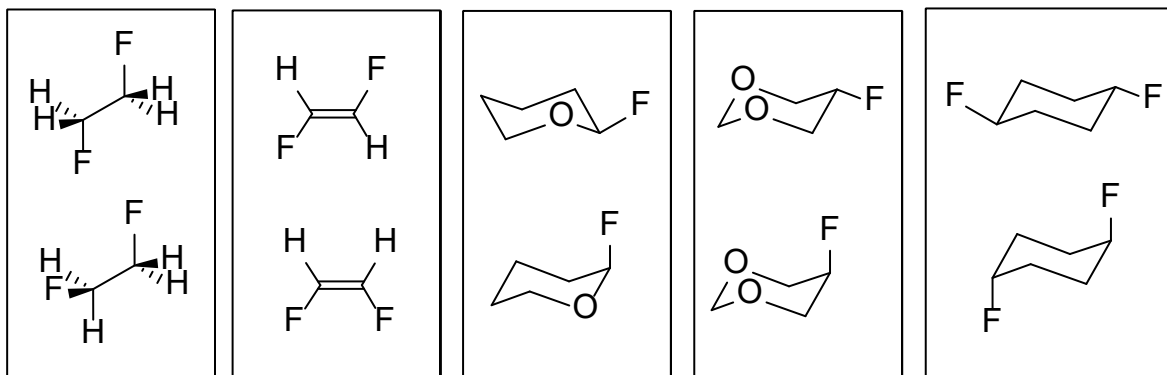
“This book is highly recommended to every chemist and **particularly to every student...**” *Angew. Chem. Int. Ed.* **2017**, 56, 2.



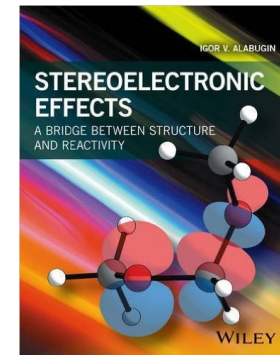
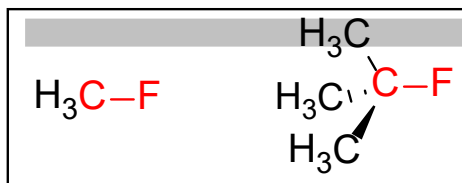
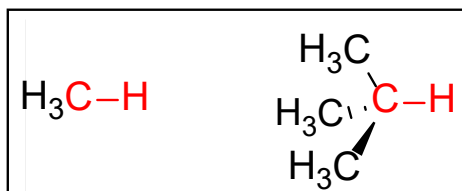
# How not to be wrong

## Let's take a quiz!

Circle the more stable structure in these pairs

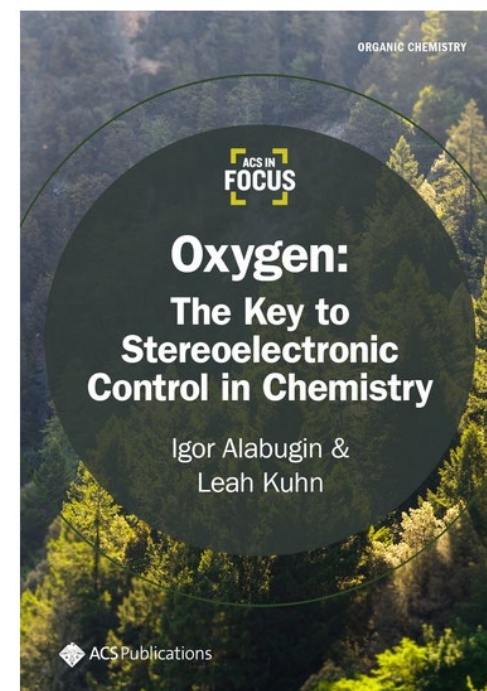
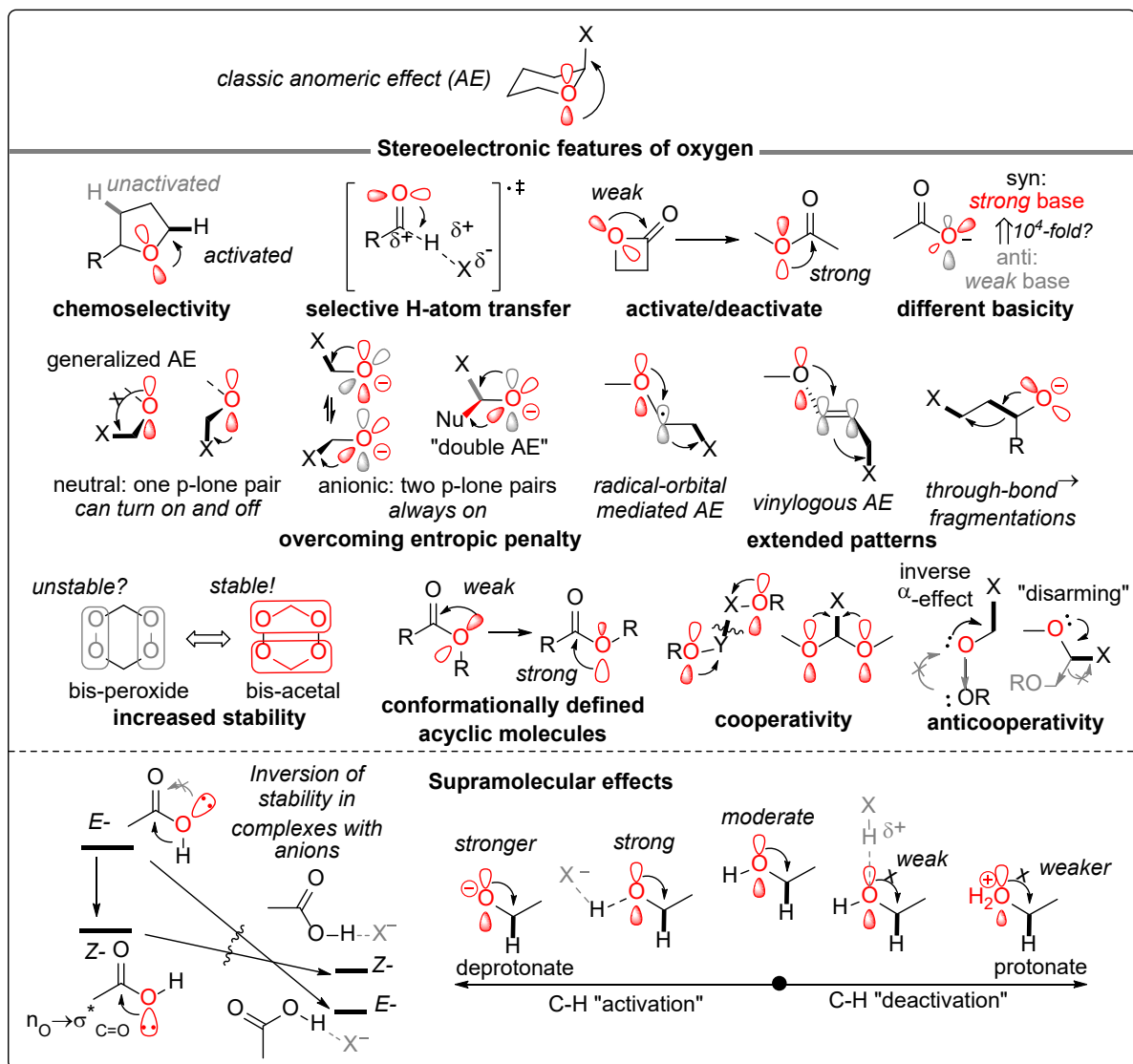
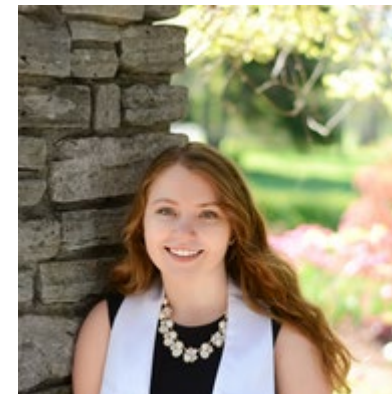


Circle the stronger bond in the two pairs



# Everything you need to know about oxygen in organic molecules

Leah Kuhn

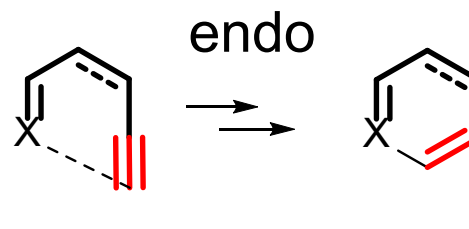
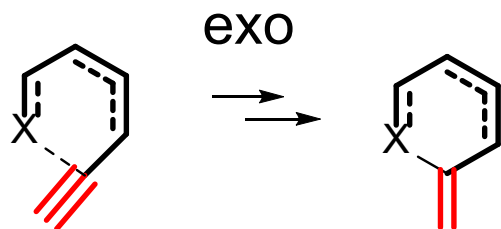


Back-to-back 2021 papers in Chem. Soc. Reviews (impact factor =55):

1. Anomeric Effect, Hyperconjugation and Electrostatics: Lessons from Complexity in a Classic Stereoelectronic Phenomenon.
2. Stereoelectronic Power of Oxygen in Control of Chemical Reactivity: the Anomeric Effect is not Alone

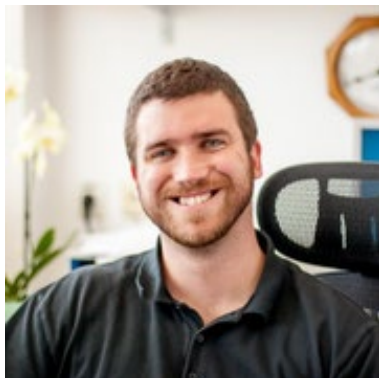
# Choosing the right path for alkyne cyclizations

solved



**Stereoelectronic analysis supports exo-selectivity for radical cyclizations**

**For “endo” cyclizations, stereoelectronic requirements need to be reversed (e.g., “LUMO umpolung” in EPNCs etc)**



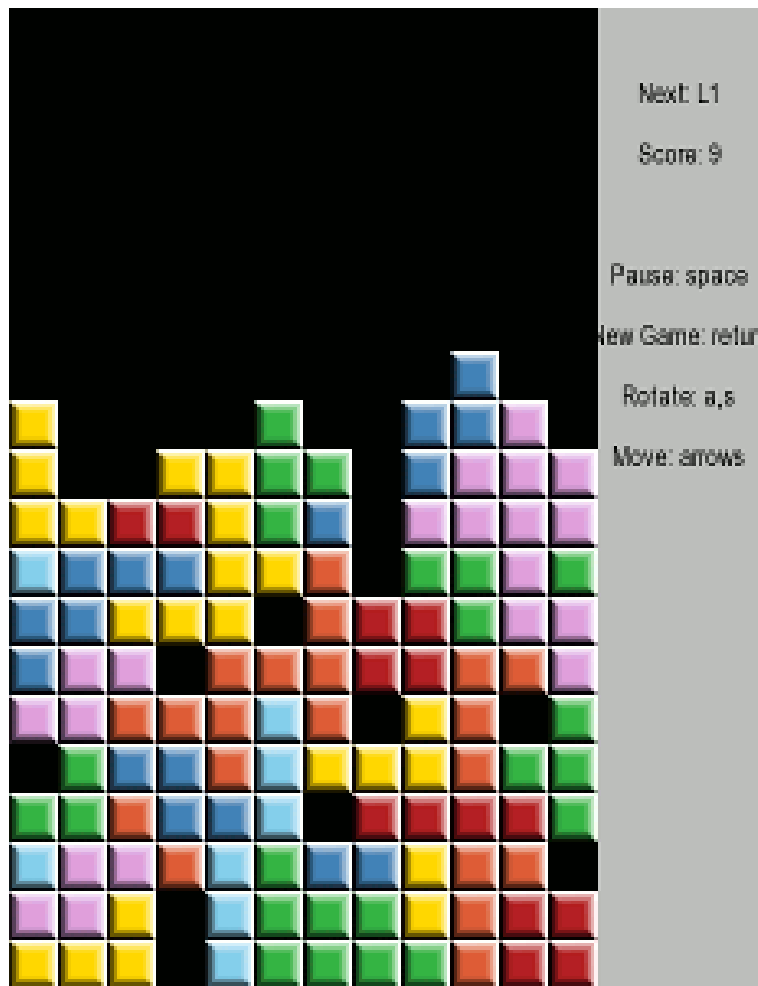
Kerry Gilmore,  
University of Connecticut  
(2020 ACS Green  
Chemistry Award)

TITLE

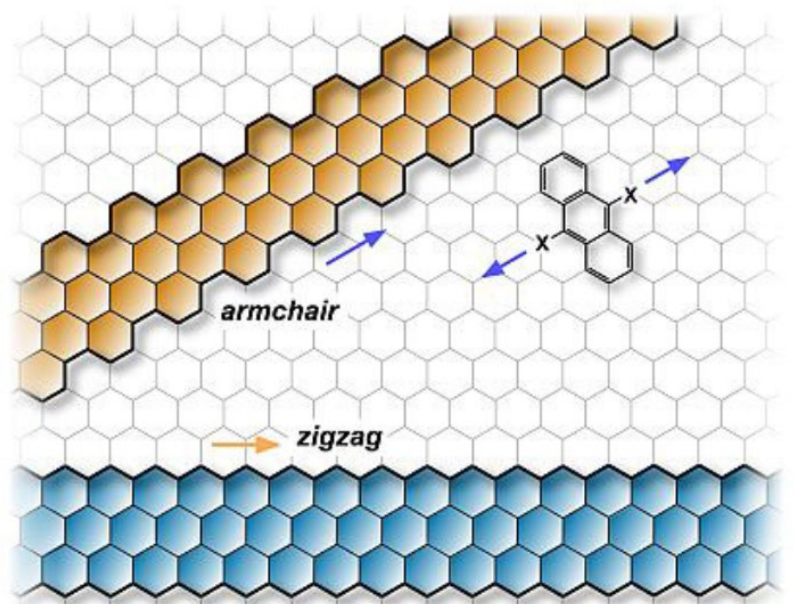
CITED BY YEAR

- |                                                                                                                                                                                                 |     |      |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|------|
| <input type="checkbox"/> <a href="#">Cyclizations of alkynes: revisiting Baldwin's rules for ring closure</a><br>K Gilmore, IV Alabugin<br>Chemical Reviews 111 (11), 6513-6556                 | 554 | 2011 |
| <a href="#">Rules for anionic and radical ring closure of alkynes</a><br>IV Alabugin, K Gilmore, M Manoharan<br>Journal of the American chemical society 133 (32), 12608-12623                  | 181 | 2011 |
| <a href="#">Finding the right path: Baldwin “Rules for Ring Closure” and stereoelectronic control of cyclizations</a><br>IV Alabugin, K Gilmore<br>Chemical Communications 49 (96), 11246-11250 | 171 | 2013 |

# Playing Molecular Tetris - mostly with hexagons



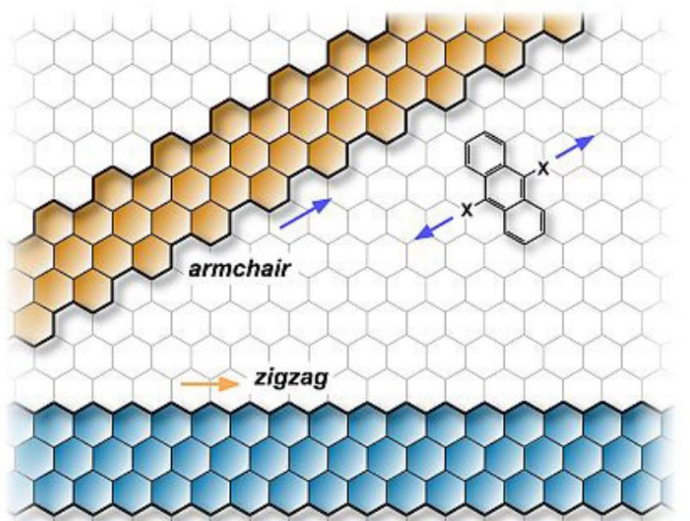
Cyclic molecules can force desired electron delocalization patterns: by organizing space, we can organize energy



Müllen, Fasel and coworkers.  
*Nature*, 531, 489–492, **2016**

There is more than one way to “cut” graphene into interesting substructures. This can be useful as long as we can make these substructures with precise control of shapes and sizes

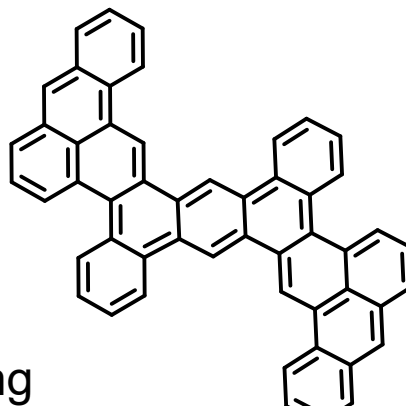
# What can we make with hexagons?



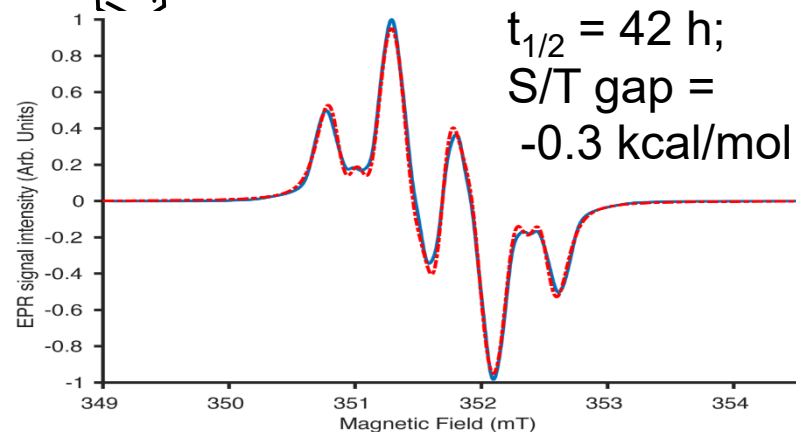
No need to go far to find something unusual

Has no NMR signals

... but shows an EPR signal



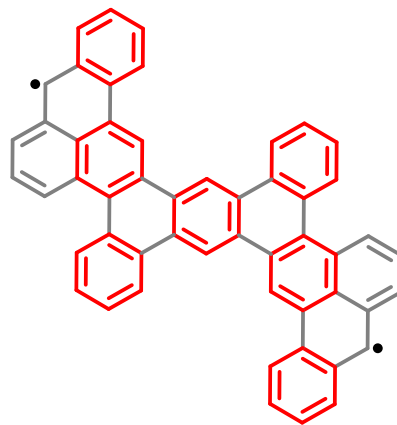
Beginning of new technologies – as long as we can make these structures with precise control of shapes and sizes



Febin  
Kuriakose



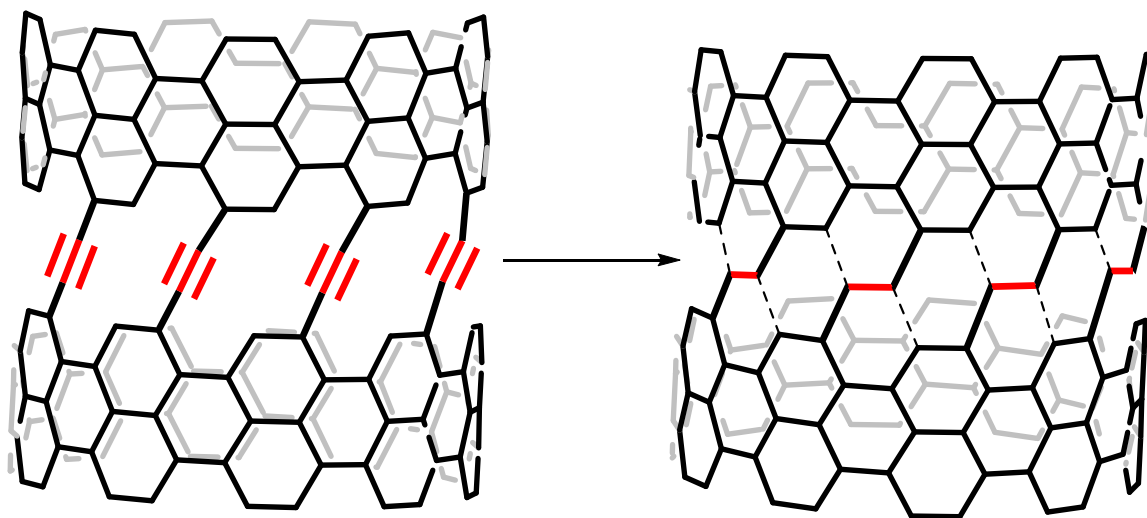
Michael  
Commodore



Kuriöse, Commodore et al. *J. Amer. Chem. Soc.* **2022**, 23448. <https://pubs.acs.org/doi/10.1021/jacs.2c09637>

# Radicals and alkynes – a perfect combination?

Neutral reactive intermediates + carbon-rich high-energy functionality = fewer problems with overoxidation/ fewer hydrogens to remove

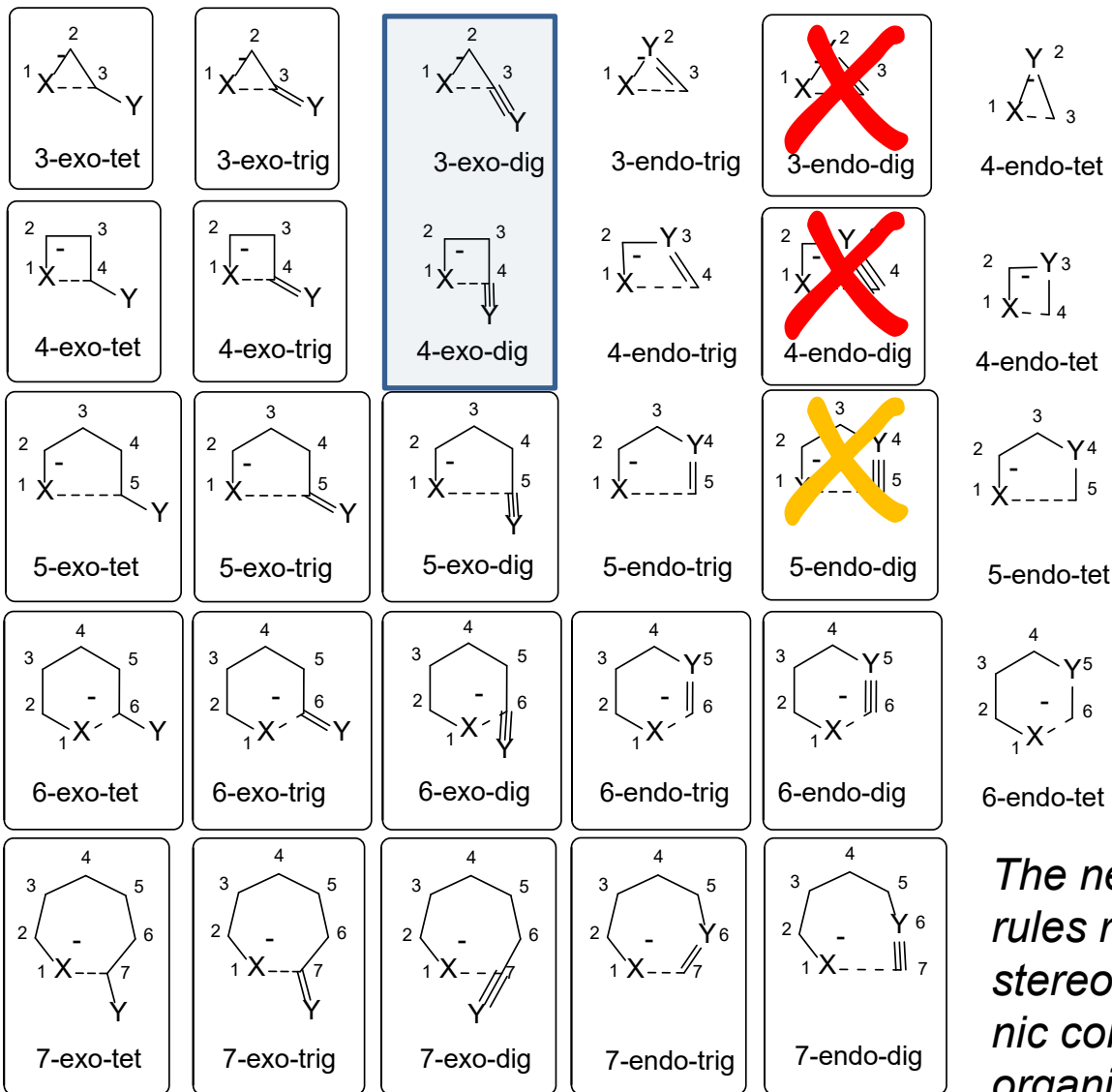


Two challenges –

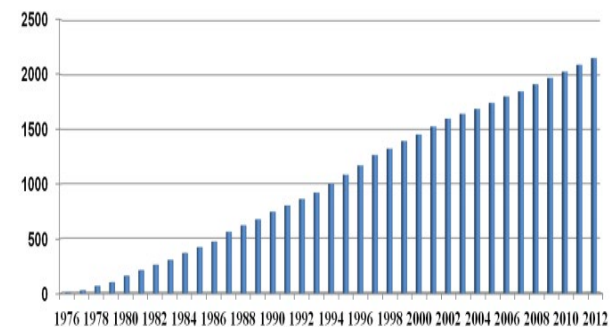
- 1) understanding how alkynes can be used to form a cycle
- 2) understanding how radicals can be used efficiently and selectively in alkyne reactions



# Refined cyclization rules (Baldwin rules)

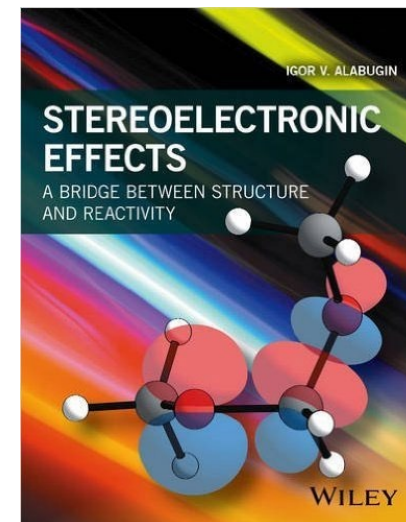


Citations for the “Rules for Ring Closure” (1976-2012) – *the most cited paper in the first 40 years of ChemComm*



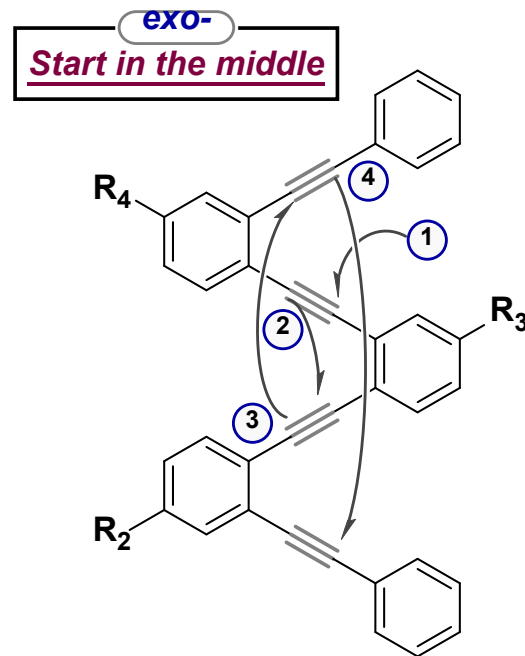
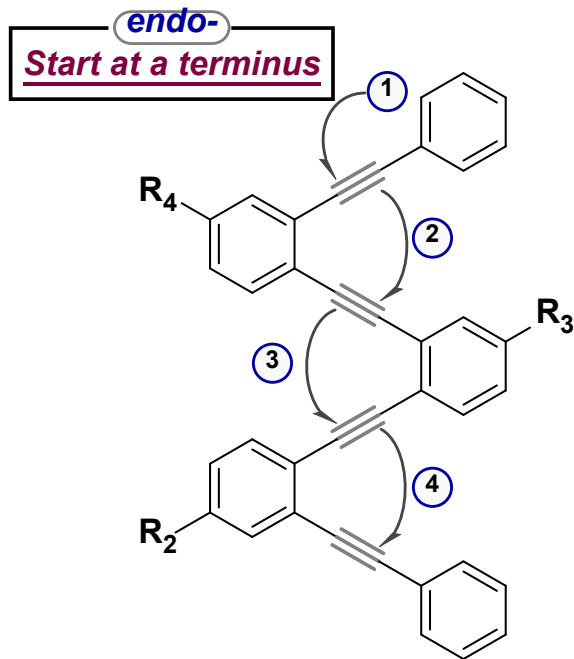
Baldwin, *Chem. Commun.* **1976**, 734

*The new rules reflect stereoelectronic control of organic reactivity*



# Let's add aromatic spacers to oligoalkynes

## Alternative Folding Patterns:



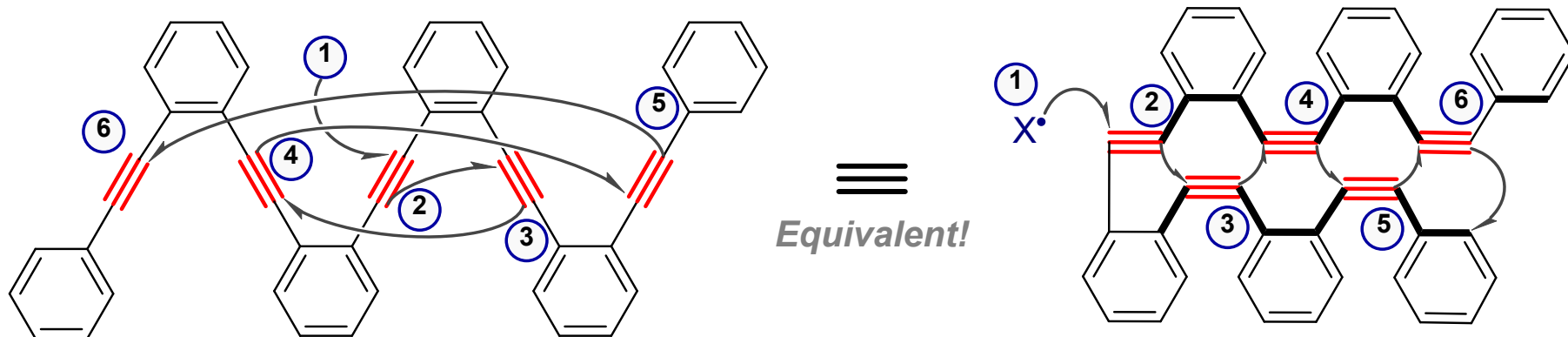
Which of the two “alkyne origami” patterns to choose?

**Topogically:**  
**endo is preferred**

**Stereoelectronically:**  
**Exo is preferred**

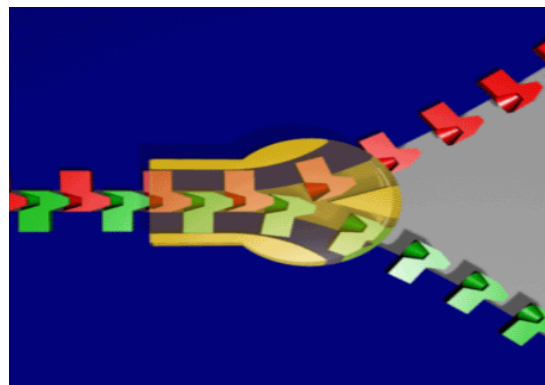
# “To bend or not to bend”: Simplifying the analysis of alkyne folding

The “all-exo” cascade

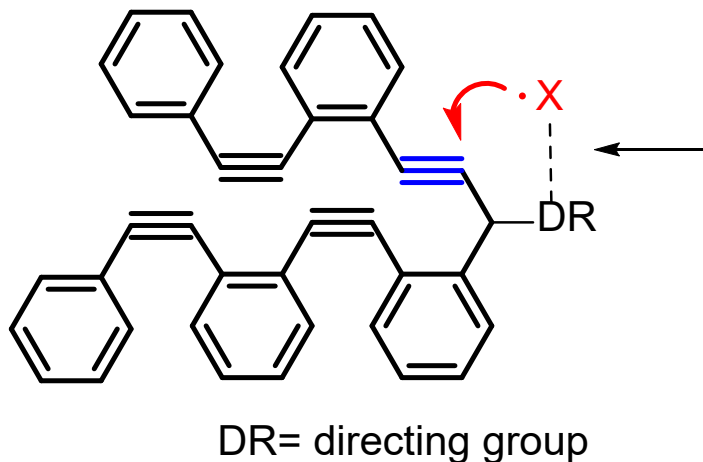


*The “bent alkyne” representation simplifies analysis of oligoalkyne folding into an aromatic ribbon*

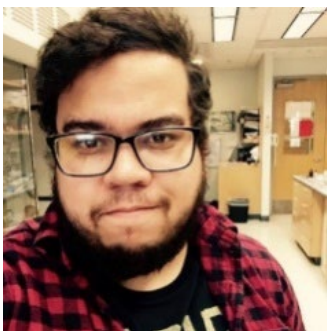
Can we make a  
polyacetylene chain between  
two rows of benzenes with  
this radical “polymerization”?



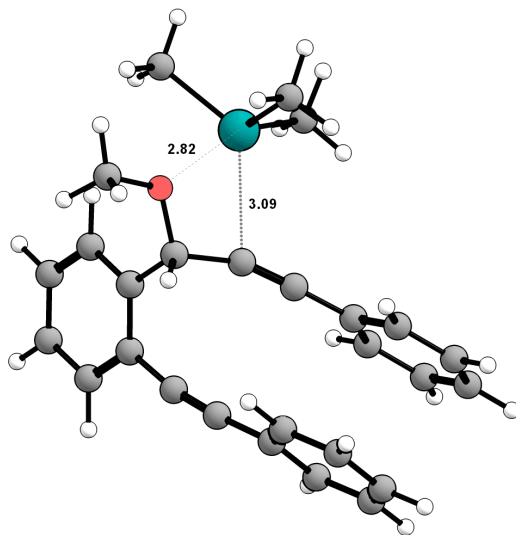
# “Directing groups” for intermolecular control of reactivity?



What is the right combination that will create a transient but effective supramolecular X...DR “bond”?



Gabriel dos Passos Gomes



***O...Sn interaction***

K. Pati, **G. Gomes**, T. Harris, A. Hughes, H. Phan, T. Banerjee, K. Hanson, I. Alabugin, *J. Am. Chem. Soc.*, **2015**, 1165.

# How many papers will you publish in grad school?

- F S. Umedu, **G. P. Gomes**, M. Sakae, T. Yoshinaga, K. Matsumoto, T. Iwata, I. Alabugin, M. Shindo "Regioselective One-pot Synthesis of Triptycenes via Triple-Cycloadditions of Arynes to Ynolates" [\*Angew. Chem. Int. Ed.\*, \*\*2016\*\*, 56, 1298](#) (featured on: • [Synfacts 2017, 13 \(03\), 253](#) "Three Benzynes and the Ynolate", doi: [10.1055/s-0036-1590046](#))
- F S. Z. Vatsadze, Y. Loginova, **G. P. Gomes**, I. V. Alabugin "Stereoelectronic Chameleons: The Reversal of Donor-Acceptor Properties of Common Functional Groups by a Geometric Change" [\*Chem. Eur. J.\*, \*\*2016\*\*, 23, 3225](#) ([Frontpiece of Chemistry – A European Journal](#), doi: [10.1002/chem.201781461](#))
- F K. Pati, **G. P. Gomes**, I. V. Alabugin "Combining Traceless Directing Groups with Hybridization Control of Radical Reactivity: from Skipped Enynes to Defect-Free Hexagonal Frameworks" [\*Angew. Chem. Int. Ed.\*, \*\*2016\*\*, 55, 11633](#)
- F T. Harris, **G. P. Gomes**, R. Clark, I. V. Alabugin, "Domino Fragmentations in Traceless Directing Groups of Radical Cascades: Evidence for the Formation of Alkoxy Radicals via C-O Scission" [\*J. Org. Chem.\*, \*\*2016\*\*, 81 \(14\), 6007](#) (featured on: • [sciencing.net](#))
- F K. Pati, **G. P. Gomes**, T. Harris, I. V. Alabugin "Fused Catechol Ethers from Gold (I)-Catalyzed Intramolecular Reaction of Propargyl Ethers with Acetals" [\*Org. Lett.\*, \*\*2016\*\*, 18 \(5\), 928](#)
- F **G. P. Gomes**, V. A. Vil', A. Terent'ev and I. V. Alabugin, "Stereoelectronic Source of the Anomalous Stability of Bis-peroxides", [\*Chem. Sci.\*, \*\*2015\*\*, 6, 6783](#) (featured on: • [Chemistry World](#); • NBO's features [website](#); • [chem.fsu.edu/News](#))
- F K. Pati, **G. P. Gomes**, T. Harris, A. Hughes, H. Phan, T. Banerjee, K. Hanson, I. V. Alabugin "Traceless Directing Groups in Radical Cascades: From Oligoalkynes to Fused Helicenes without Tethered Initiators" [\*J. Am. Chem. Soc.\*, \*\*2015\*\*, 137, 1165](#)
- F I. V. Alabugin, S. Bresch, **G. P. Gomes** "Orbital Hybridization: A Key Electronic Factor in Control of Structure And Reactivity" [\*J. Phys. Org. Chem.\*, \*\*2014\*\*, 28, 147](#) (one of the [most accessed](#) papers on: • *JPOC* between 10/2015-09/2016 & 02/2016-08/2017 • department's most read paper on *ResearchGate* in October–November 2017; featured on: • [amphoterios.com](#))

# How many papers will you publish in grad school?

- F 11. S. Umedu, **G. P. Gomes**, M. Sakae, T. Yoshinaga, K. Matsumoto, T. Iwata, I. Alabugin, M. Shindo "Regioselective One-pot Synthesis of Triptycenes via Triple-Cycloadditions of Arynes to Ynolates" [\*Angew. Chem. Int. Ed.\*, 2016, 56, 1298](#) (featured on: • [Synfacts 2017, 13 \(03\), 253](#) "Three Benzynes and the Ynolate", doi: [10.1055/s-0036-1590046](#))
- F 10. S. Z. Vatsadze, Y. Loginova, **G. P. Gomes**, I. V. Alabugin "Stereolectronic Chameleons: The Reversal of Donor-Acceptor Properties of Common Functional Groups by a Geometric Change" [\*Chem. Eur. J.\*, 2016, 23, 3225](#) ([Frontpiece of Chemistry – A European Journal](#), doi: [10.1002/chem.201781461](#))
- F 9. K. Pati, **G. P. Gomes**, I. V. Alabugin "Combining Traceless Directing Groups with Hybridization Control of Radical Reactivity: from Skipped Enynes to Defect-Free Hexagonal Frameworks" [\*Angew. Chem. Int. Ed.\*, 2016, 55, 11633](#)
- F 8. T. Harris, **G. P. Gomes**, R. Clark, I. V. Alabugin, "Domino Fragmentations in Traceless Directing Groups of Radical Cascades: Evidence for the Formation of Alkoxy Radicals via C-O Scission" [\*J. Org. Chem.\*, 2016, 81 \(14\), 6007](#) (featured on: • [sciencing.net](#))
- F 6. K. Pati, **G. P. Gomes**, T. Harris, I. V. Alabugin "Fused Catechol Ethers from Gold (I)-Catalyzed Intramolecular Reaction of Propargyl Ethers with Acetals" [\*Org. Lett.\*, 2016, 18 \(5\), 928](#)
- F 5. **G. P. Gomes**, V. A. Vil', A. Terent'ev and I. V. Alabugin, "Stereolectronic Source of the Anomalous Stability of Bis-peroxides", [\*Chem. Sci.\*, 2015, 6, 6783](#) (featured on: • [Chemistry World](#); • NBO's features [website](#); • [chem.fsu.edu/News](#))
- F 2. K. Pati, **G. P. Gomes**, T. Harris, A. Hughes, H. Phan, T. Banerjee, K. Hanson, I. V. Alabugin "Traceless Directing Groups in Radical Cascades: From Oligoalkynes to Fused Helicenes without Tethered Initiators" [\*J. Am. Chem. Soc.\*, 2015, 137, 1165](#)
- F 1. I. V. Alabugin, S. Bresch, **G. P. Gomes** "Orbital Hybridization: A Key Electronic Factor in Control of Structure And Reactivity" [\*J. Phys. Org. Chem.\*, 2014, 28, 147](#) (one of the [most accessed](#) papers on: • *JPOC* between 10/2015-09/2016 & 02/2016-08/2017 • department's most read paper on *ResearchGate* in October–November 2017; featured on: • [amphoteris.com](#))

# How many papers will you publish in grad school?

- F 25. **G. P. Gomes** & I. V. Alabugin "Stereolectronic Effects: Analysis by Computational and Theoretical Methods", chapter 15 for the book "Applied Theoretical Organic Chemistry" Editor: Prof. Dean Tantillo (UC-Irvine), [2018](#).
- F 23. N. P. Tsvetkov, E. Gonzalez-Rodriguez, A. Hughes, **G. P. Gomes**, F. D. White, I. V. Alabugin "Radical Alkyne Peri-annulations for Synthesis of Functionalized Phenalenes, Benzanthrenes, and Olympicene", *Angew. Chem. Int. Ed.*, **2018**, *in print*, [doi: 10.1002/anie.201712783](#) (• [Top 5% of ACIE's output](#). Featured on [FSU News](#), reproduced on: • [phys.org](#); • [nsf.gov/news](#); • [sciencedaily.com](#); • [EurekAlert!](#))
- F 22. V. A. Vil', **G. P. Gomes**, O. V. Bityukov, M. A. Syroeshkin, K. A. Lyssenko, G. I. Nikishin, I. V. Alabugin. A. O. Terent'ev "Interrupted Baeyer-Villiger Rearrangement: Building A Stereolectronic Trap for the Criegee Intermediate", *Angew. Chem. Int. Ed.*, **2018**, *in print*, [doi: 10.1002/anie.201712651](#). (• [Top 5% of ACIE's output](#). Featured on: • [Chemical & Engineering News](#))
- F 20. C. J. Evoniuk, **G. P. Gomes**, S. Hill, F. Satoshi, I. V. Alabugin "Coupling C-H activation, N-H deprotonation and Oxidation: metal-free C(sp<sup>3</sup>)-H aminations with unprotected anilines" *J. Am. Chem. Soc.*, **2017**, *139* (45), 16210 (featured on: • [Synfacts 2018, 14 \(02\), 144 "Expanded N-Heterocycles through C\(sp<sup>3</sup>\)-H Amination"](#); • in the top 20 most-read JACS papers in [Oct-Nov 2017](#))
- F 19. T. Harris, **G. P. Gomes**, R. Clark, S. Ayad, V. V. Lobodin, K. Hanson, I. V. Alabugin "Twisted chiral cyclodecynes and remote activation of click reactivity" *Chem.*, **2017**, *3* (4), 629 (• [video-summary of the paper](#). Featured on: • [FSU News](#))
- F 18. N. H. Park, **G. P. Gomes**, M. Fevre, G. O. Jones, I. V. Alabugin, J. L. Hedrick, "Organocatalyzed Synthesis of Fluorinated Poly(aryl thioethers)" *Nature Communications*, **2017**, *8*, 166; (a collaboration with IBM Research, San Jose, CA. Featured on: • [Plastic News](#); • [Synfacts 2017, 13 \(10\), 1035 "Salt-Free Polymerization Yields Fluorinated Poly\(aryl thioether\)s"](#))
- F 17. E. Juaristi, **G. P. Gomes**, A. O. Terent'ev, R. Notario, I. V. Alabugin "Stereolectronic Interactions as a Probe for the Existence of the Intramolecular  $\alpha$ -Effect", *J. Am. Chem. Soc.*, **2017**, *139* (31), 10799
- F 15. **G. P. Gomes**<sup>§</sup>, C. J. Evoniuk<sup>§</sup>, M. Ly, I. V. Alabugin "Changing the path of least resistance, or access to *endo*-dig products *via* a sequence of three *exo*-trig transition states: electronic effects in homoallylic ring expansion cascades of alkenyl isonitriles" *Org. Biom. Chem.*, **2017**, *15*, 4135
- F 13. **G. P. Gomes**<sup>§</sup>, Y. A. Yaremenko<sup>§</sup>, P. S. Radulov, R. A. Novikov, V. V. Chernyshev, A. A. Korlyukov, G. I. Nikishin, A. O. Terent'ev, I. V. Alabugin "Stereolectronic Control in the Ozone-Free Synthesis of Ozonides" *Angew. Chem. Int. Ed.*, **2017**, *56*, 4955
- F 12. **G. P. Gomes** & I. V. Alabugin "Drawing Catalytic Power from Charge Separation: Stereolectronic and Zwitterionic Assistance in the Au(I)-Catalyzed Bergman Cyclization" *J. Am. Chem. Soc.*, **2017**, *139* (9), 3406

Less than four years since starting his PhD

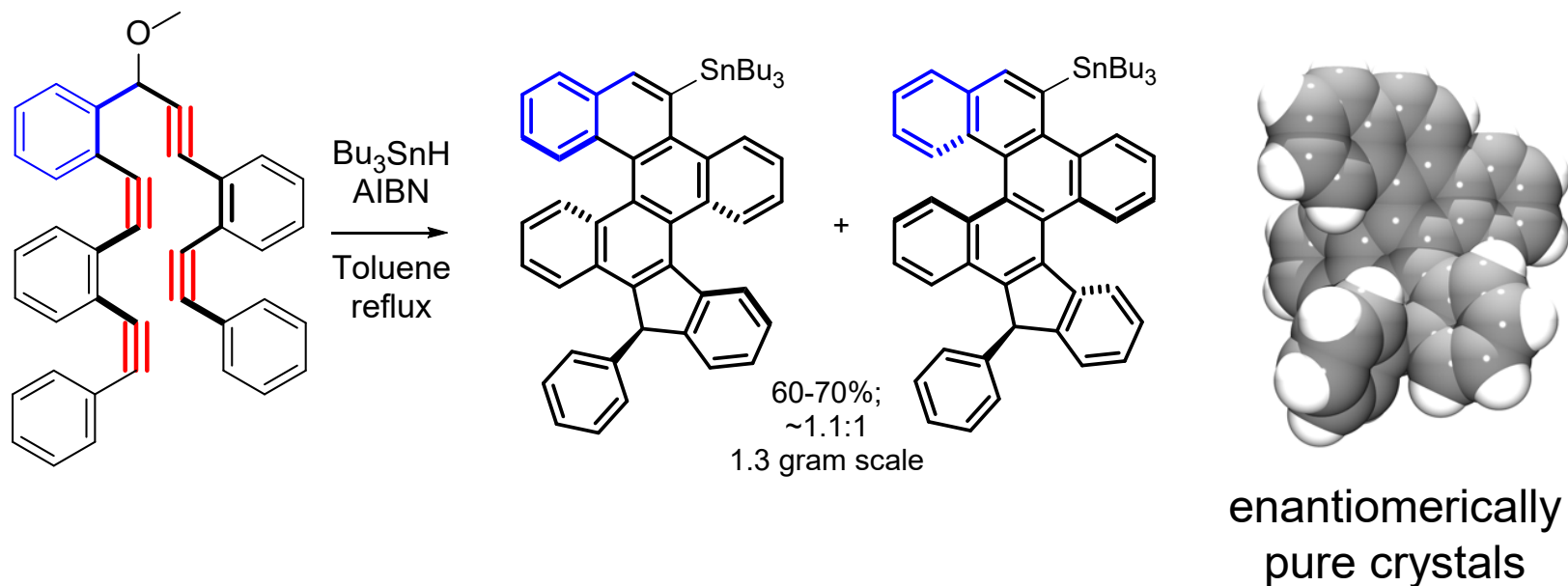
# How many papers will you publish in grad school?

## 32-42...Were also published (one more is under review)

- 31.** A. Hughes, **G. P. Gomes**, I. V. Alabugin, Stereoelectronic Influence of a “Spectator” Propargylic Substituent Can Override Aromaticity Effects in Radical Peri-cyclizations on Route to Expanded Polyaromatics, *J. Org. Chem.*, **2019**, *84*, 1853
- 30.** CO<sub>2</sub> or SO<sub>2</sub>: Should it stay or should it go? Gomes, G.; Wimmer, A.; Smith, J.; König, B.; Alabugin, I.V. *J. Org. Chem.*, **2019**, *84*, 6232-6243.
- 29.** V. A. Vil', **G. P. Gomes**, M. V. Ekimova, K. A. Lyssenko, G. I. Nikishin, I. V. Alabugin, A. O. Terent'ev “From transient Bayer-Villiger (Criegee) intermediate to stable peroxides: BF<sub>3</sub>-catalyzed synthesis of β-hydroperoxy-β-peroxylactones from five different types of substrates”, *J. Org. Chem.*, **2018**, *83*, 13427–13445
- 28.** **G. P. Gomes**, Y. Loginova, S. Z. Vatsadze, I. V. Alabugin "Isocyanides as Stereoelectronic Chameleons: The Donor-Acceptor Dichotomy in Radical Additions", *J. Am. Chem. Soc.* **2018**, *140*, 14272-14288.
- 27.** **G. P. Gomes**, A. E. Morrison, G. B. Dudley, I. V. Alabugin "Optimizing amine-mediated alkyne-allene isomerization to improve benzannulation cascades: synergy between theory and experiments", *Eur. J. Org. Chem.*, **2019**, 512-518.
- 26.** I. V. Alabugin, **G. P. Gomes**, M. Abdo, "Hyperconjugation", *WIREs Comput. Mol. Sci.*, **2019**, doi/full/10.1002/wcms.1389.



# Non-planar aromatics from skipped alkynes

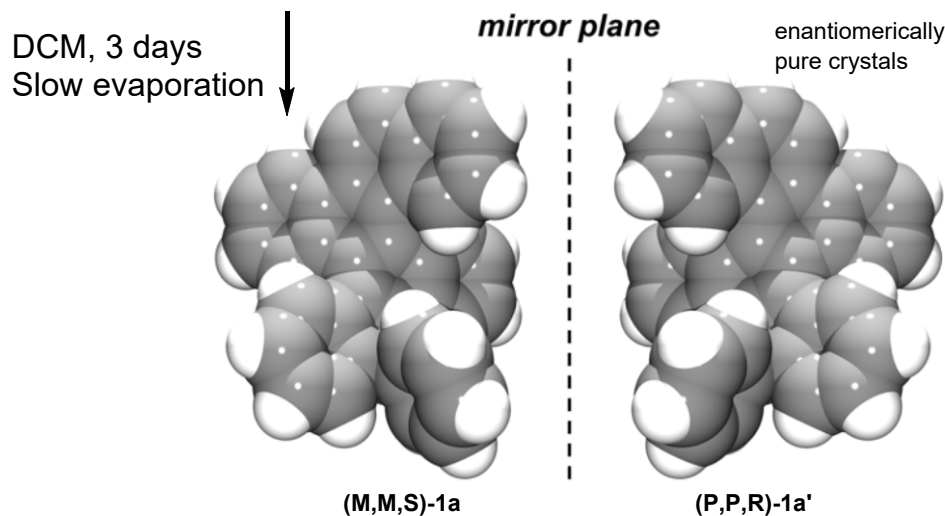
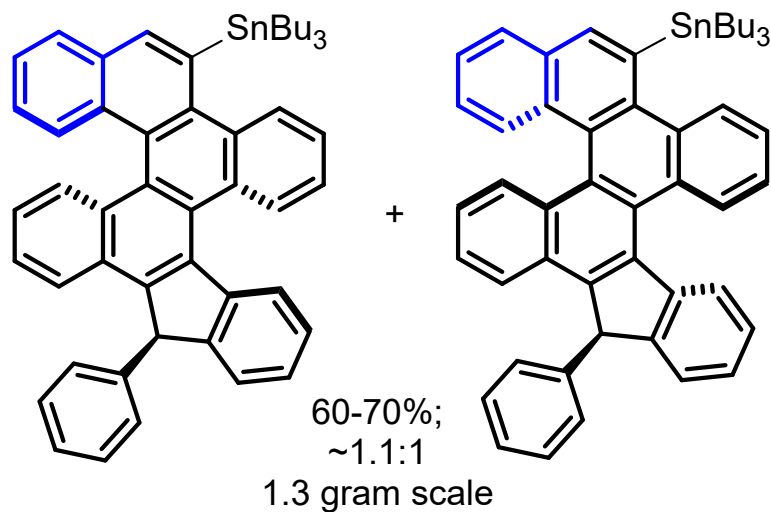


Pati, K.; Gomes, G. P.; Harris, T.; Hughes, A.; Phan, H.; Banerjee, T.; Hanson, K.; Alabugin, I. V. *JACS*, **2015**, 1165.

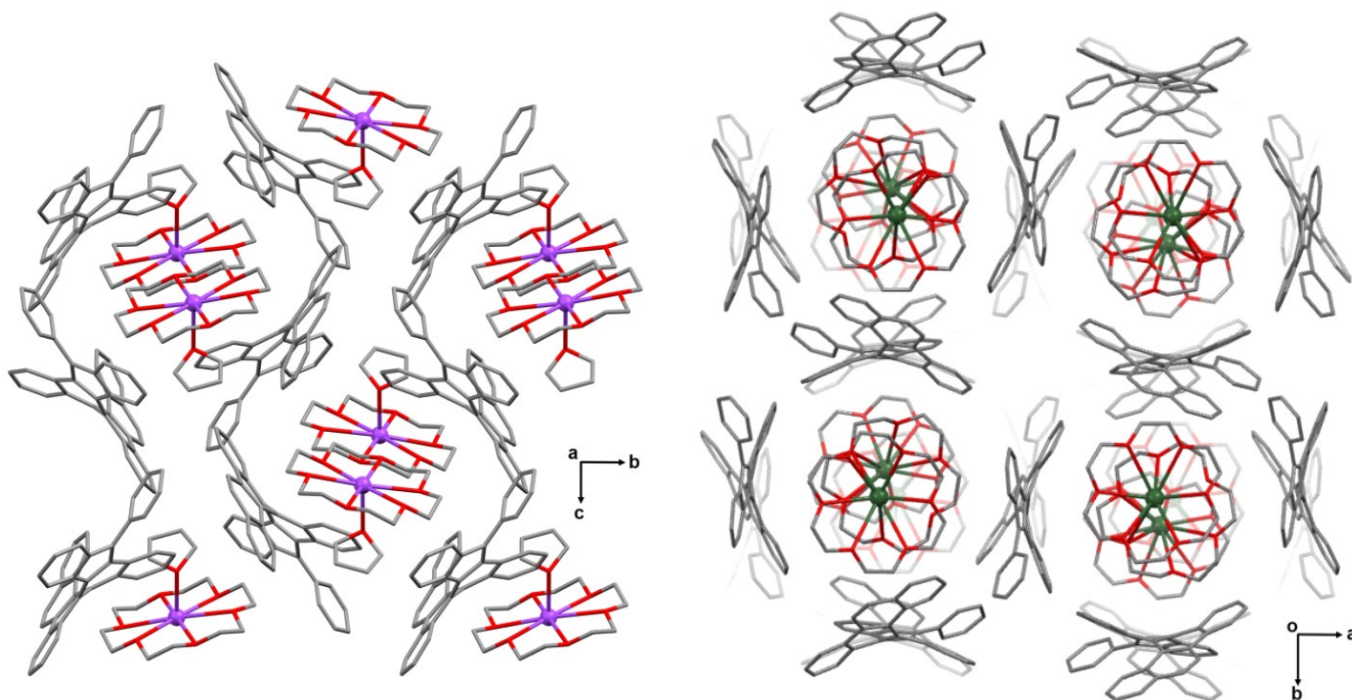
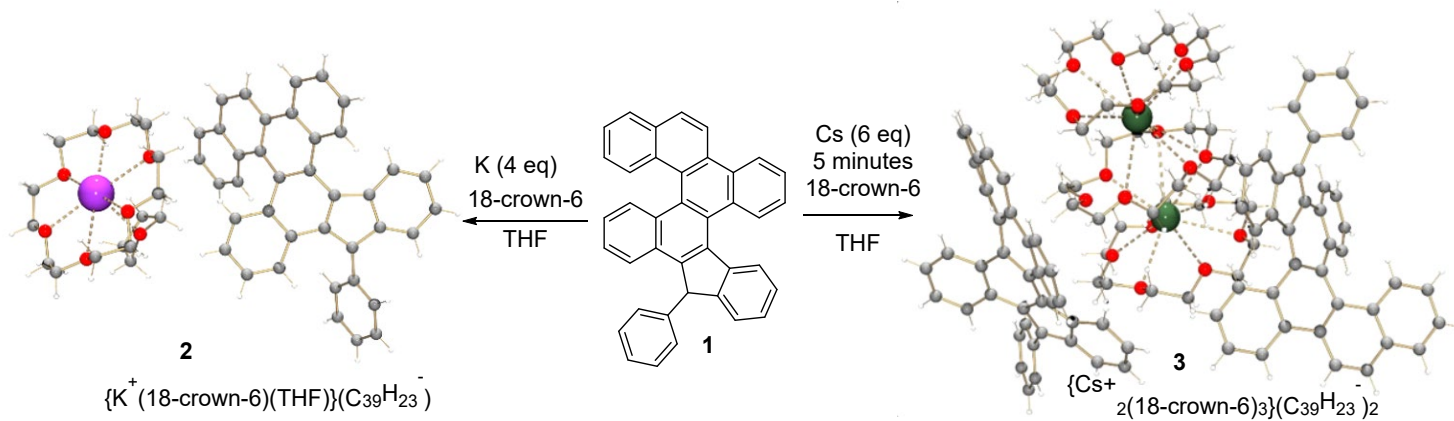
## More on why this cascade works so well:

Design principles of the use of alkynes in radical cascades. C. Hu, J. Mena, I.V. Alabugin, *Nature Reviews Chemistry*, **2023**, <https://www.nature.com/articles/s41570-023-00479-w>.

# Fun with helicenes: how to make graphene chiral?

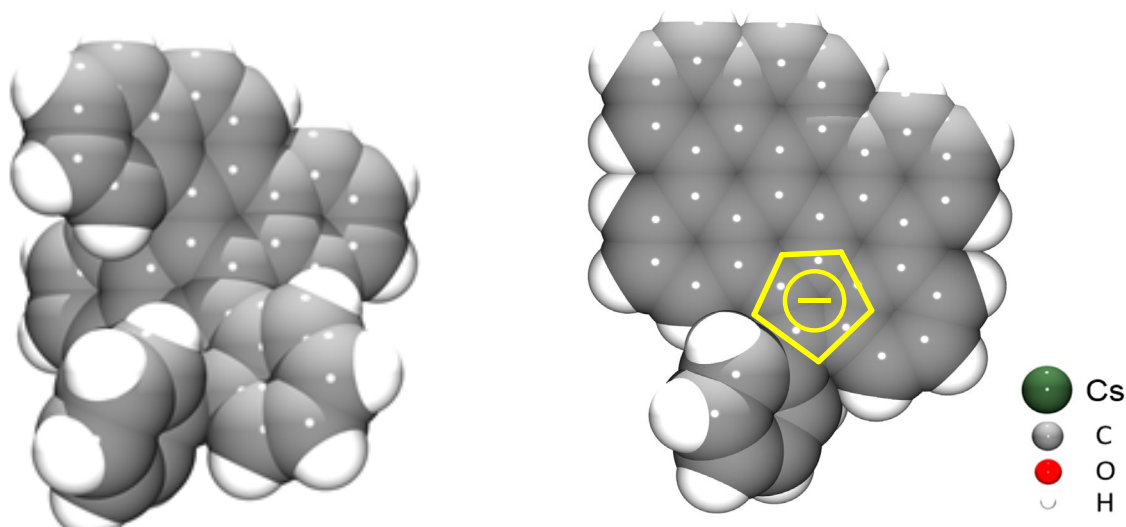
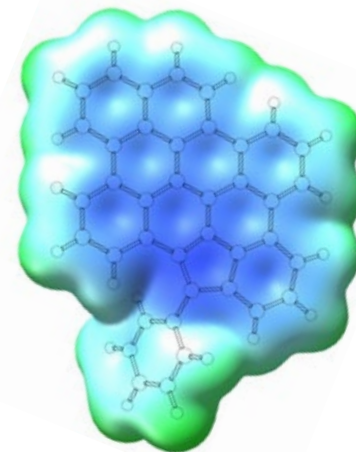
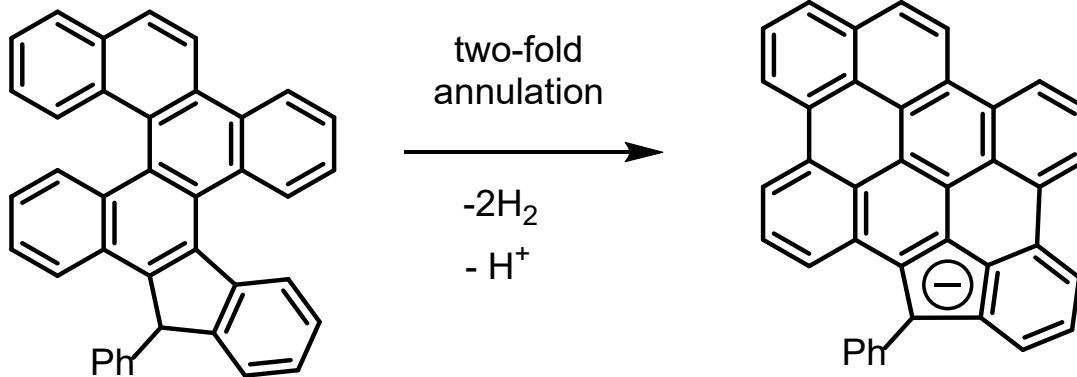


# Fun with helicenes: how to make graphene anionic?



Zheng Zhou, Rahul Kisan Kawade, Renana Gershoni-Poranne, Zheng Wei, Febin Kuriakose, Marina A. Petrukhina, and Igor V. Alabugin, *Angew.Chem.*, 2020

# Towards a new form of carbon?



**X-ray structures**

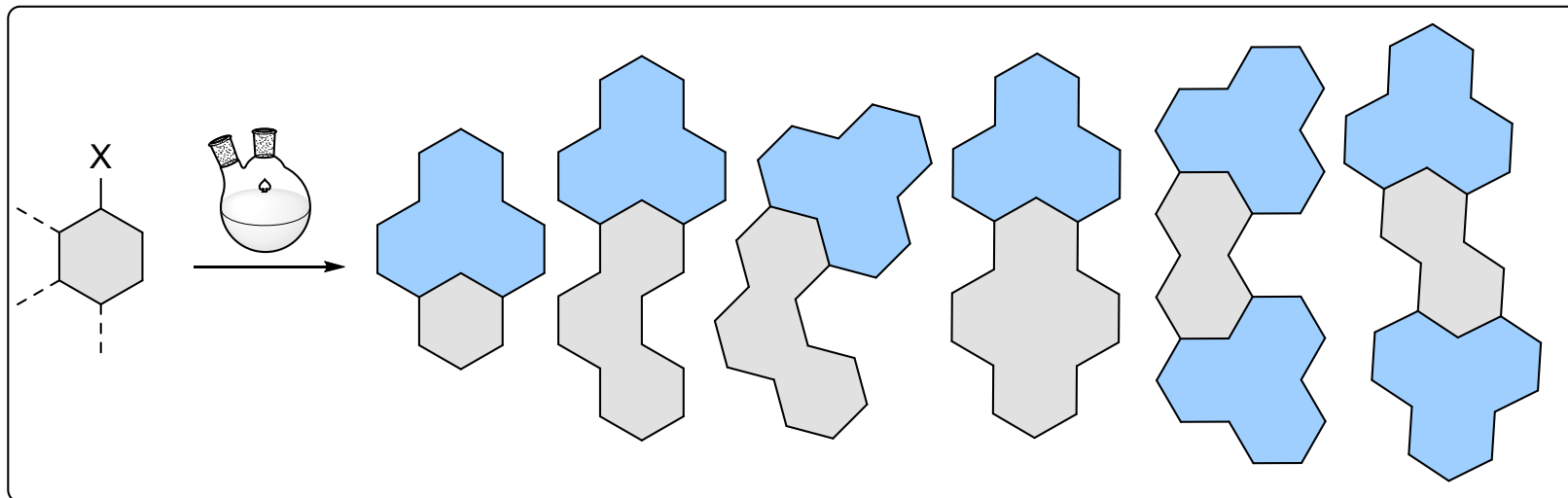
July 11, 2022  
Volume 144  
Number 27  
pubs.acs.org/JACS

# J | A | C | S

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

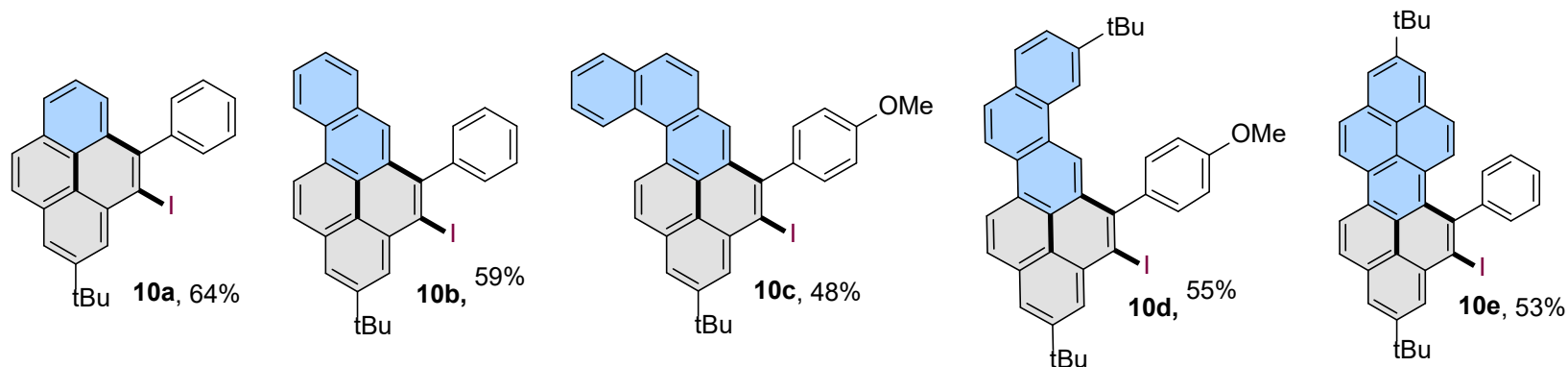
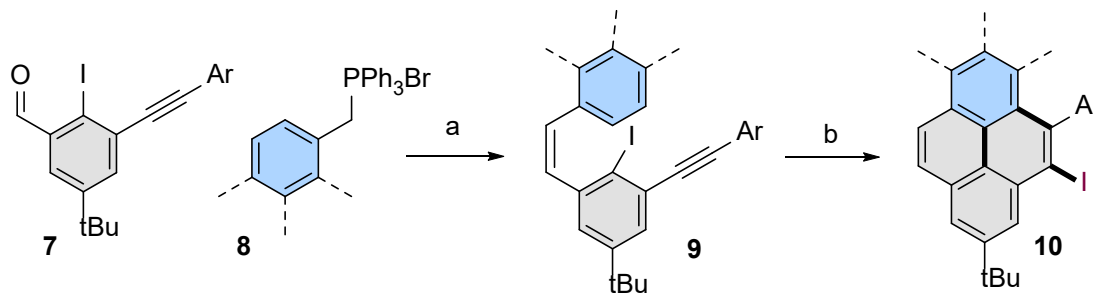


# Phenalenannulations: “three-point” double annulation reactions that convert benzenes into pyrenes



How to build polycyclic structures faster?

# Scope of 3-point double annulations: design #2



a) KOtBu (1.4 equiv.), THF; b) i) [9a] 0.02 M, Bu<sub>3</sub>SnH (1.3 equiv.), AIBN (0.3 equiv.), toluene, 90°C, ii) Bu<sub>3</sub>SnH (3.0 equiv.), AIBN (2.0 equiv.), 110°C iii) I<sub>2</sub> (5.0 equiv.), DCM; isolated yields are reported from 9 to 10

**Ask Nik Dos Santos how to do it without Bu<sub>3</sub>SnH, AIBN and any other chemicals!**



Kawade, R. K., Hu, C. W.; Dos Santos N. R., Watson, N., Lin, X., Hanson, K.; Alabugin, I. V. *Angew.Chem. Int. Ed.* **2020**, 59, 14352-14357

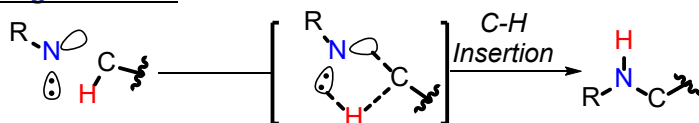
**Tired of carbon?  
How about a new way to make  
C-N bonds?**

# Reinventing C-H aminations

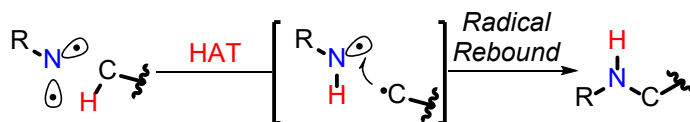
## a) Direct Activation

- Nitrogen is responsible for C-H activation
- Nitrogen is responsible for C-N and N-H bond formation

### Singlet Nitrene



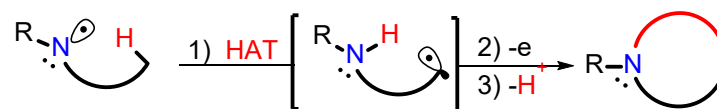
### Triplet Nitrene



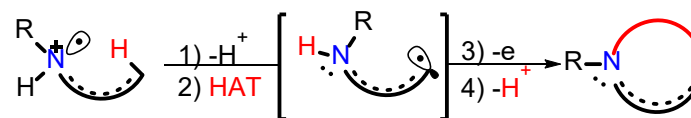
## b) C-H Activation with Delayed C-N Bond Formation

- Nitrogen is responsible for C-H activation
- Additional reagent needed for C-N bond formation
- Usually, remote intramolecular activation

### Nitrogen Centered Radical



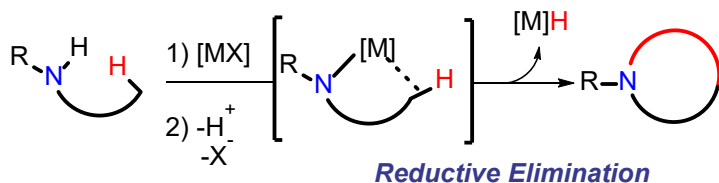
### Conjugated Nitrogen Centered Radical Cation



## c) Nitrogen-Assisted C-H Activation

- Nitrogen is not directly involved in C-H activation
- Nitrogen may play a secondary role as directing group

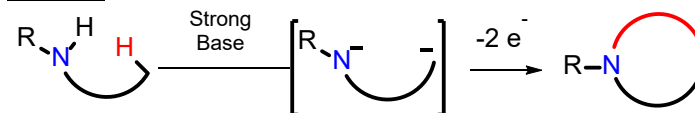
### Transition Metal C-H activation



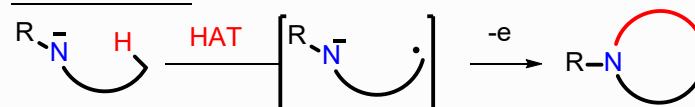
## d) Independent N-H/C-H activation

- Two independently formed reactive intermediates: N- and C-centered

### 4iii Dianion "Reductive Elimination without a metal"

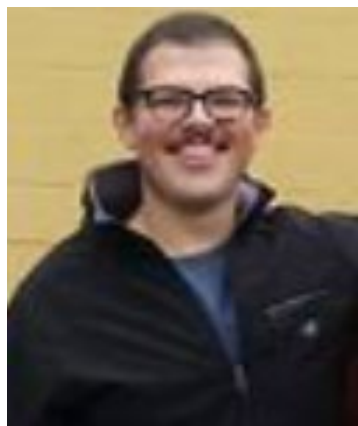


### 4ii Radical-anion This work





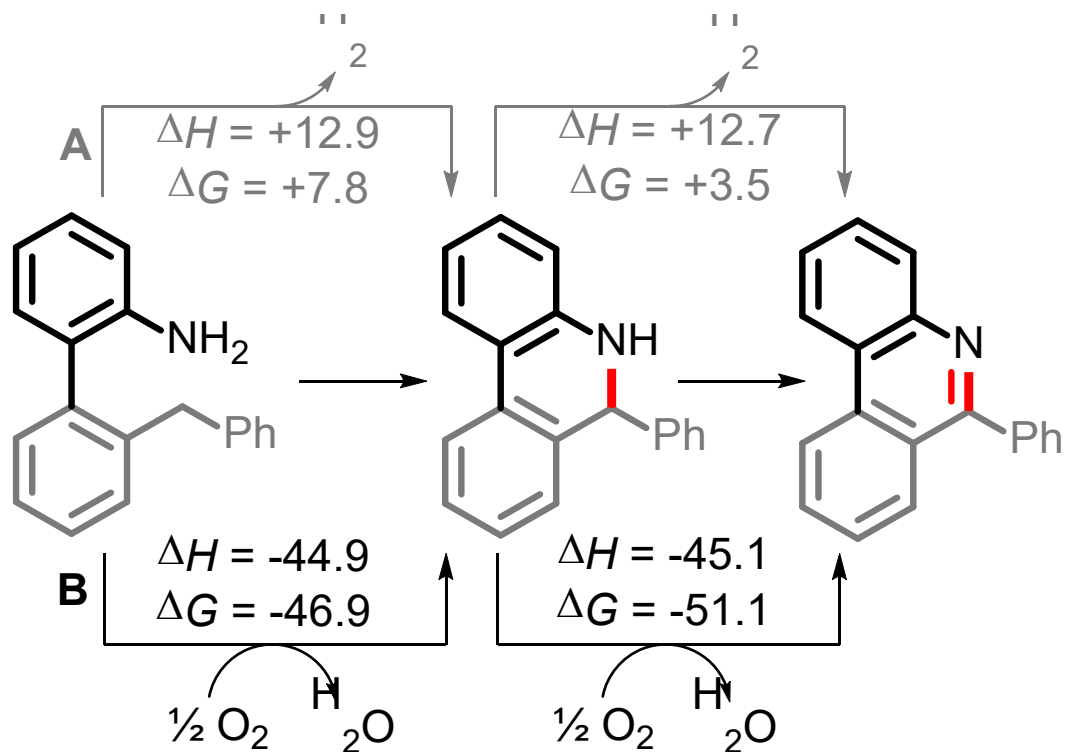
# How to fix thermodynamics of C-H aminations



Experiments:  
Chris Evoniuk



Calculations:  
Gabe Gomes

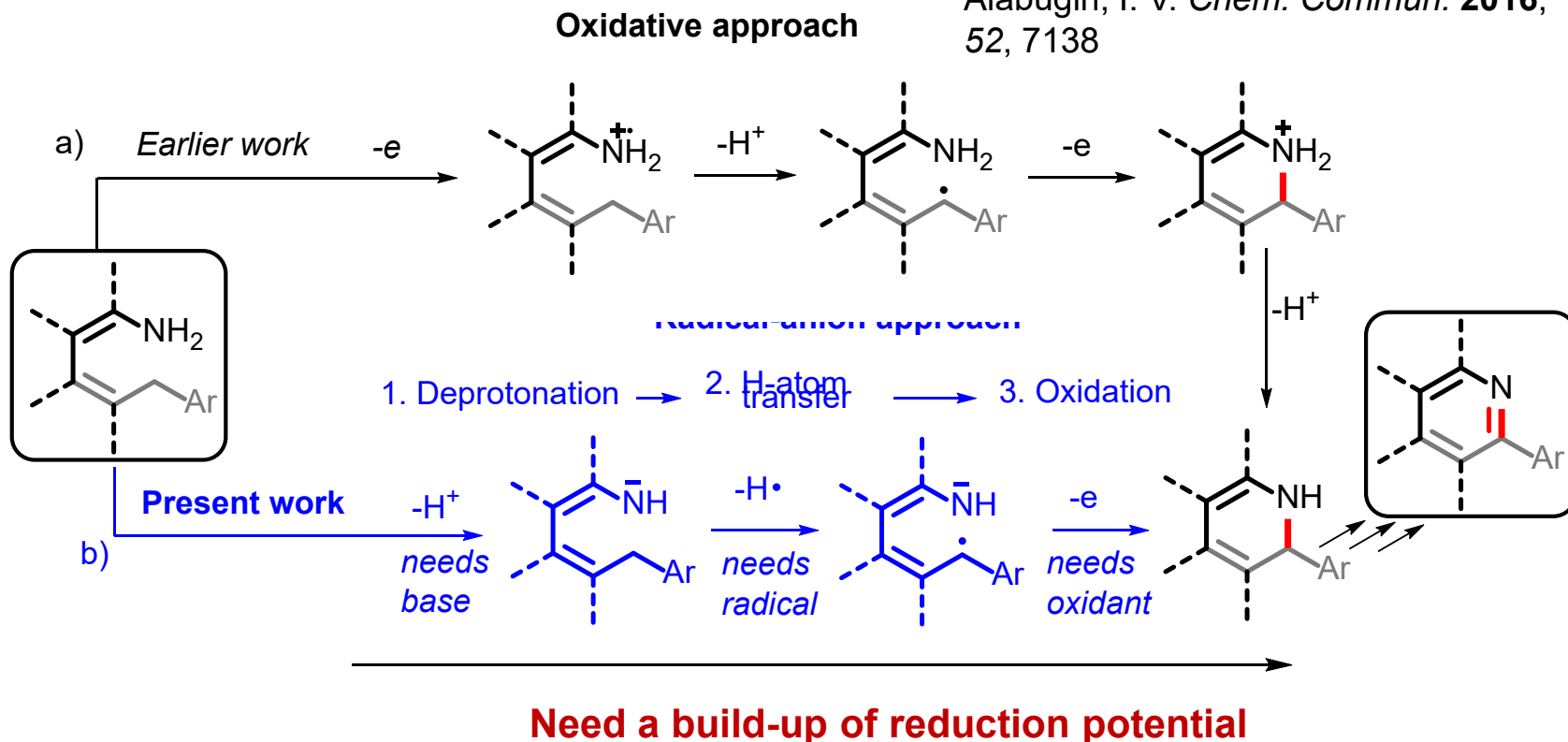


Evoniuk, C. J.; Gomes, G. dos P.; Hill, S. P.; Fujita, S.; Hanson, K.; Alabugin, I.V. *J. Am. Chem. Soc.* **2017**, *139*, 16210

(SMD=DMF)/(U)M06-2X(D3)/6-31+G(d,p)/int=ufine, kcal/mol

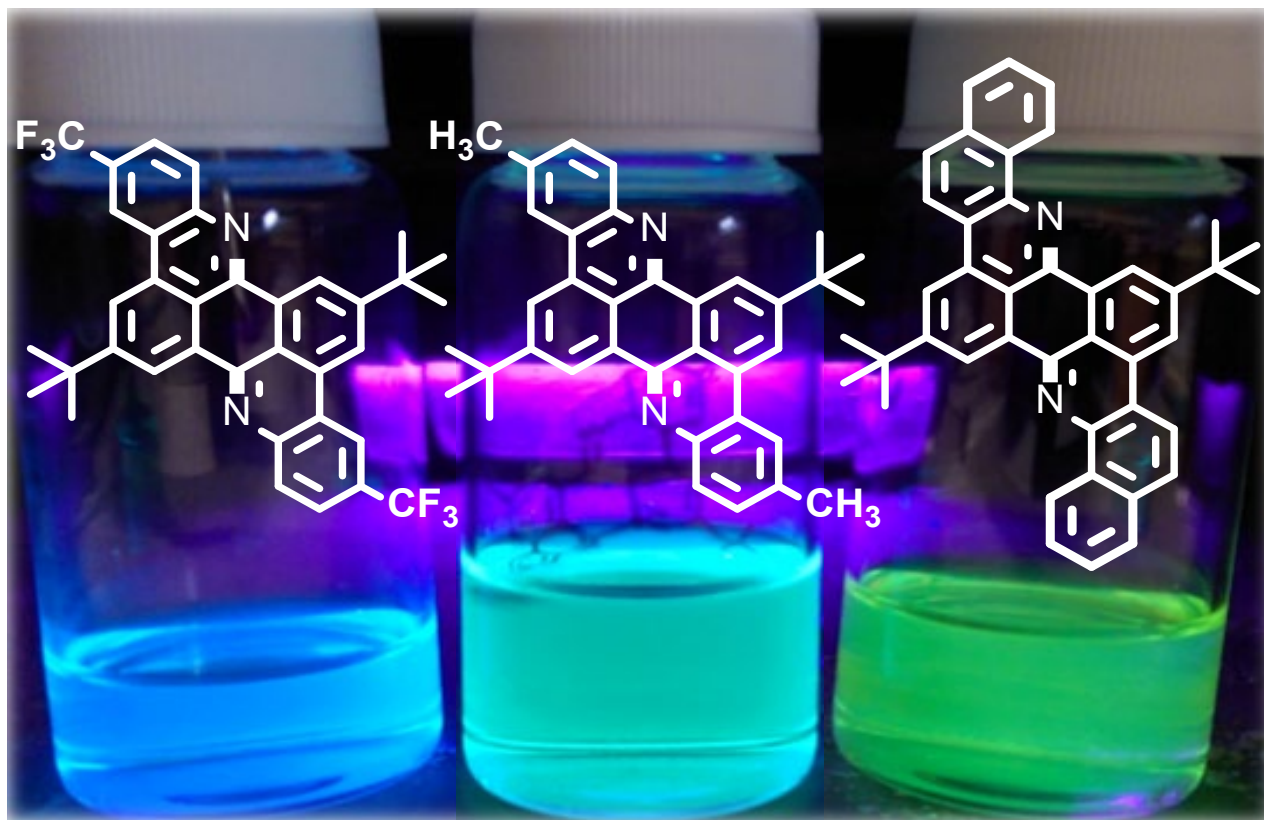
# A milder approach to C-H aminations: the base/radical/oxidant trio

Evoniuk, C. J.; Hill, S. P.; Hanson, K.;  
Alabugin, I. V. *Chem. Commun.* **2016**,  
52, 7138



Evoniuk, C. J.; Gomes, G. dos P.; Hill, S. P.; Fujita, S.; Hanson, K.; Alabugin, I. V.  
*J. Am. Chem. Soc.* **2017**, 139, 16210

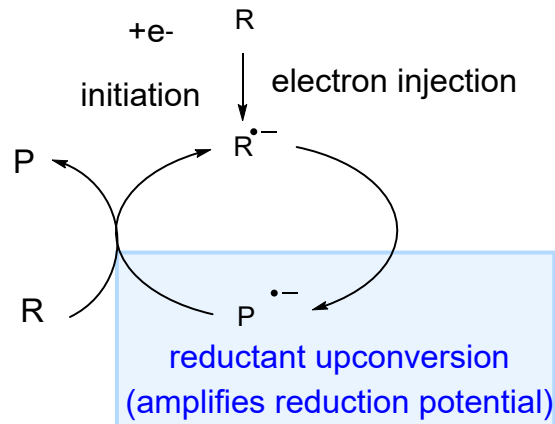
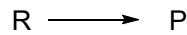
# N-heterocycles twist and bend



Evoniuk, C. J.; Gomes, G. dos P.; Hill, S. P.; Fujita, S.; Hanson, K.; Alabugin, I.V.  
*J. Am. Chem. Soc.* **2017**, *139*, 16210

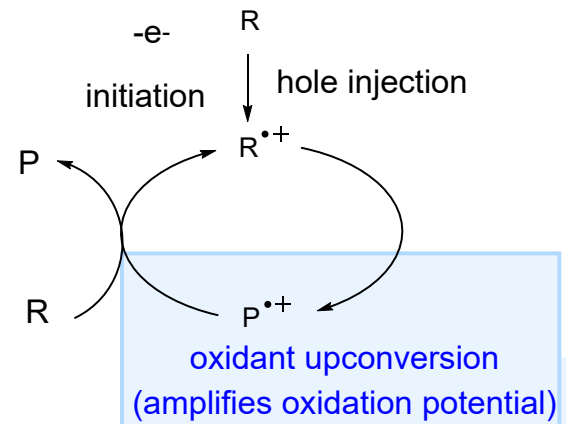
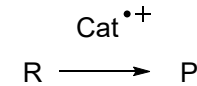
# What is the smallest possible catalyst?

## Electron?



Electrocatalytic chain process is possible  
if  $P^{\bullet-}$  is stronger oxidant than  $R^{\bullet-}$

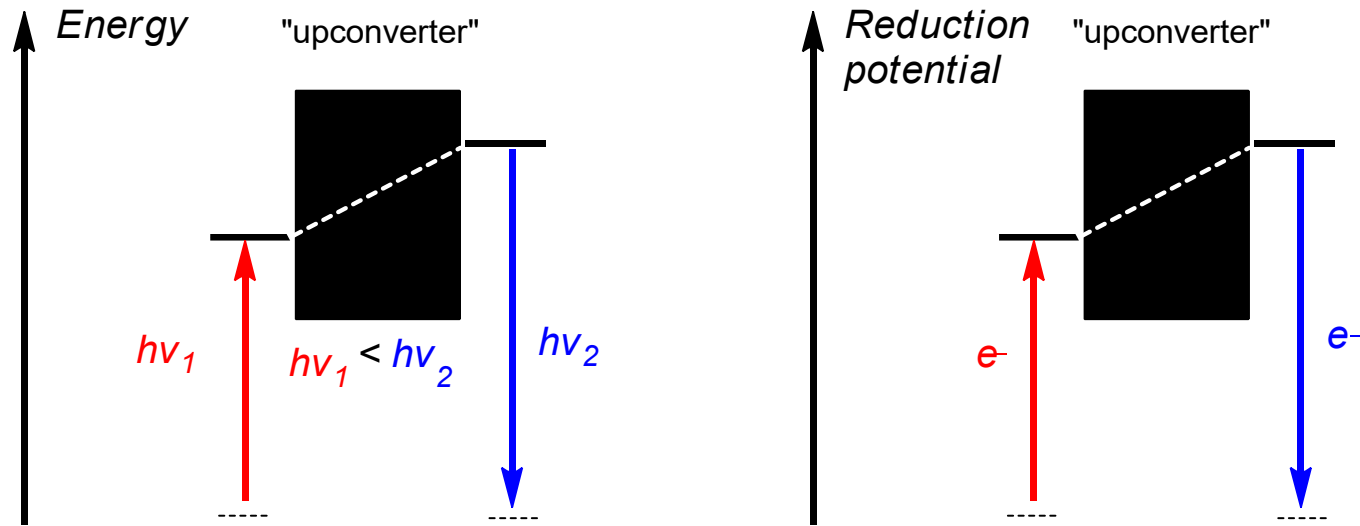
## Or hole?



Electrocatalytic chain process is possible  
if  $P^{\bullet+}$  is stronger oxidant than  $R^{\bullet+}$

# A new concept

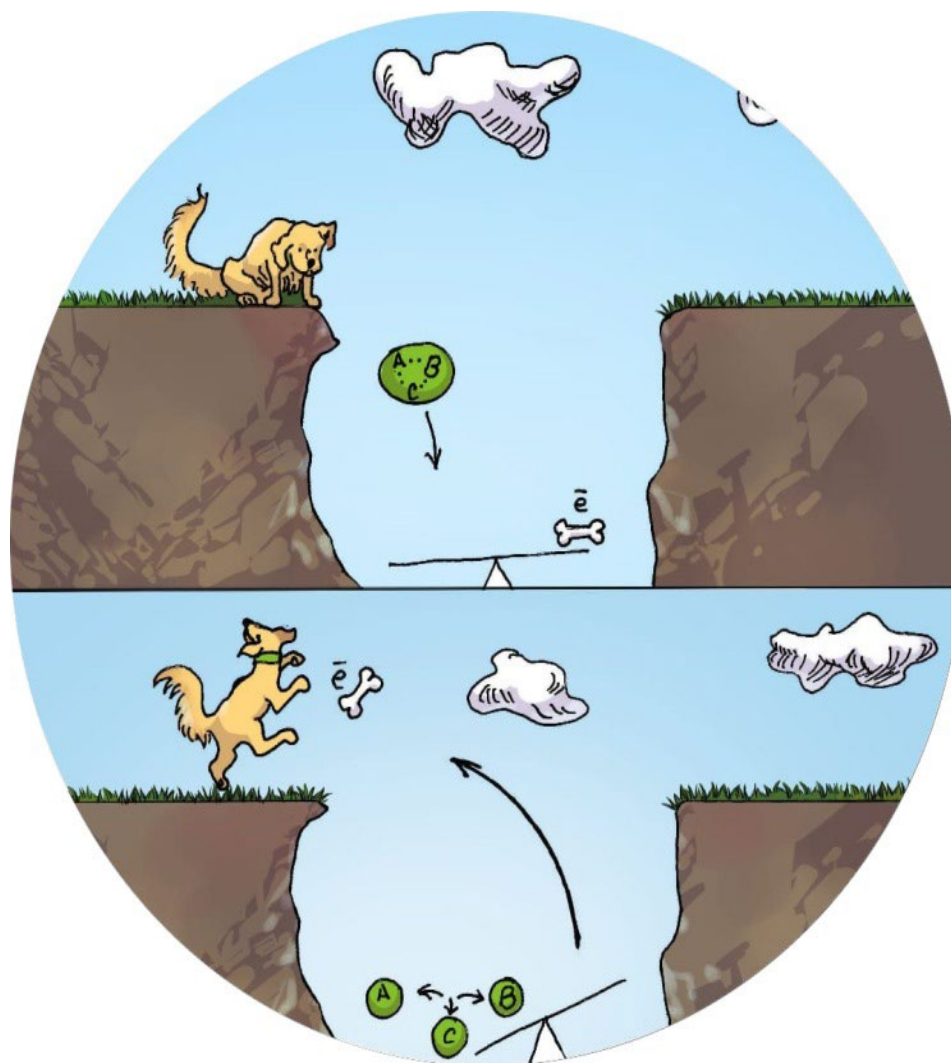
## Electron upconversion



*Can we figure out how to build this black box?*

# Electron upconversion is possible

...and you can be  
find a way to make it  
useful!

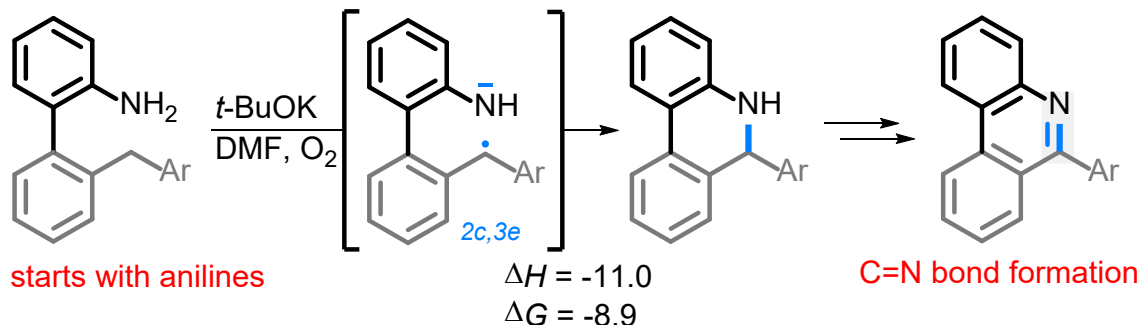


# Expanding the scope of three-electron approach to C-N bond formation



Previous work:

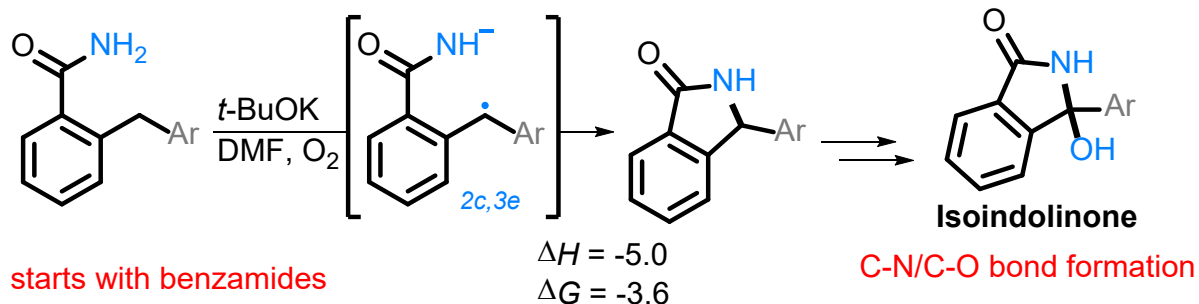
6-membered aromatic heterocycles



Chris Evoniuk

Current work:

5-membered non-aromatic heterocycles



Quintin Elliott

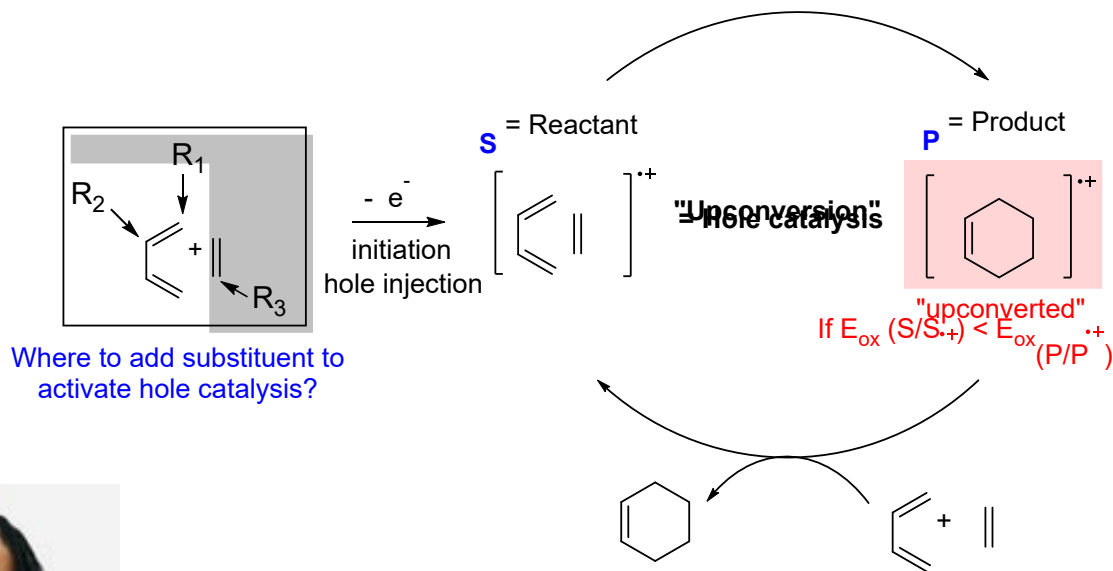
a 10-million-fold decrease in basicity of N-anion

Why is it interesting?

Because it hides a paradox

Evoniuk, C. J.; Gomes, G. dos P.; Hill, S. P.; Fujita, S.; Hanson, K.; Alabugin, I.V. *J. Am. Chem. Soc.* **2017**, *139*, 16210. Q. Elliott, G. Gomes, C. J. Evoniuk, I. V. Alabugin, *Chem. Science*, **2020**, *11*, 6539

# The smallest catalyst for the Diels-Alder reaction



Beauty Chabuka

*ACM SIGHPC Computational and  
Data Science Fellowship (2023)*

Hole Catalysis of Pericyclic Reactions: How to Activate and Control Oxidant Upconversion in Radical-Cationic Diels-Alder Cycloaddition. Beauty Chabuka, Igor Alabugin, *JACS*, *in print*



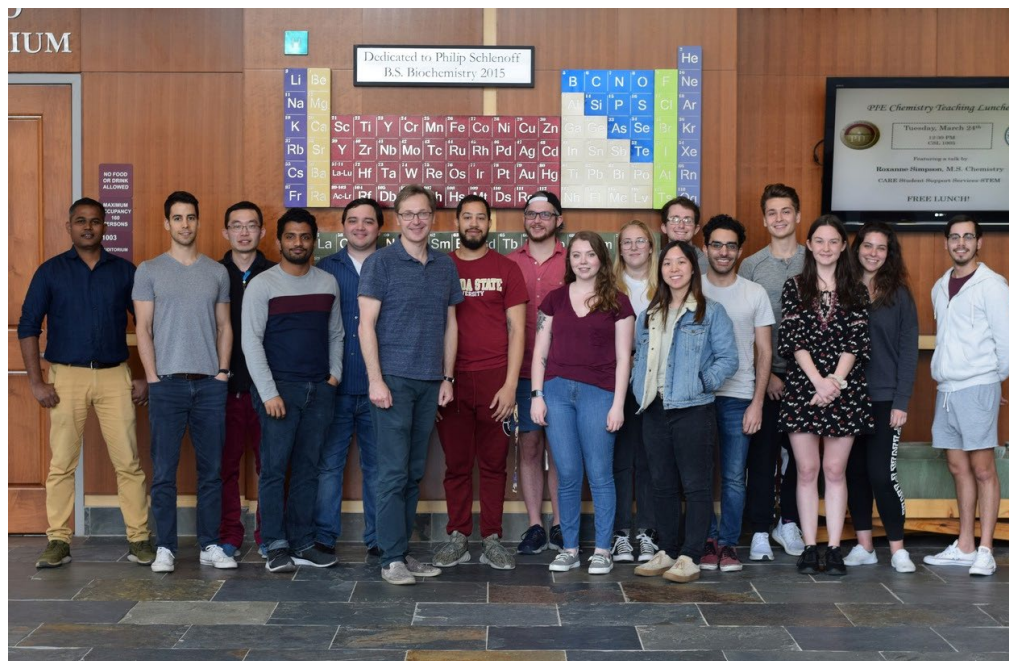
# Collaborations

- 2016-2023:

Visiting students: Sweden, Germany, Mexico, Brazil, Russia, Spain

Coauthors in published papers: Sweden, Japan, Australia, Germany, Russia, Mexico, Spain, Iran, India, Czech Republic, Wales, France

# The A-Group



**Alumni:** Dr. Kerry Gilmore, Dr. Phil Byers, Dr. Paul Peerson, Dr. Brian Gold, Dr. Sayantan Mondal, Dr. Kishore Pati, Dr. Nikolay Tsvetkov, Dr. Rana Mohamed, Dr. Stefan Bresch, Dr. Dinesh Vidhani, Dr. Trevor Harris, Dr. Chris Evonyuk, Dr. Audrey Hughes, Dr. Gabriel dos Passos Gomes, Dr. Edgar Rodriguez-Gonzalez, Dr. Rahul Kawade, Dr. Febin Kuriakose, Dr. Quintin Elliott, Dr. Chaowei Hu, Dr. Daria Tonkoglazova, Dr. Antony Sekar, Dr. Leah Kuhn

**Graduate students/Postdocs:** Nik Dos Santos, Beauty Chabuka, Michael Commodore, Favour Makurvet, Kimberley Christopher

**Undergrads (out of >180):** Jahbari Bowen, Joshua Loewenstern, Ian Vallari, Christopher Rincon, Devon Nobrega, Gage Bayliss, Thomas Suarez, Airionna Fordham

**\$\$\$:** *NSF, FSU, ACS Cope Scholar Fund*