Jeehiun Katherine Lee - Curriculum Vitae
Department of Chemistry and Chemical Biology, Wright-Rieman Laboratories
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EDUCATION

National Institutes of Health Postdoctoral Fellow, Univ. of California, Los Angeles (1995-1997)
Ph.D., Organic Chemistry, Harvard University, Cambridge, MA (1995)
B.A., Chemistry (Summa Cum Laude), Cornell University, Ithaca, NY (1990)

CURRENT POSITIONS

Professor, Department of Chemistry, Rutgers University
Member, Environmental and Occupational Health Sciences Institute (EOHSI)
Member, Molecular Biophysics Graduate Program
Member, Molecular Biosciences Graduate Program

SCHOLARSHIP
Selected Publications

Hinz, D. J.; Krajewski, A. E.; Lee, J. K. "Carbon−Fluorine Activation in the Gas Phase: The Reactions of Benzyl C−F Bonds and Silyl Cations," *J. Org. Chem.*, **2024**, *89*, 13595−13600.

Zhang, L.; Ding, X.; Kratka, C. R.; Levine, A.; Lee, J. K. "Gas Phase Experimental and Computational Studies of AlkB Substrates: Intrinsic Properties and Biological Implications," *J. Org. Chem.*, **2023**, *88,* 13115-13124.

Zhang, L.; Kiruba, G. S. M.; Lee, J. K. "Gas Phase Studies of Hypoxanthine-Guanine-(Xanthine) Phosphoribosyltransferase (HG(X)PRT) Substrates," *J. Org. Chem.*, **2023**, *88*, 6816-6826.

Krajewski, A. E.; Lee, J. K. "Nucleophilicity and Electrophilicity in the Gas Phase: Silane Hydricity," *J. Org. Chem., special issue, "Solvation Effects in Organic Chemistry,"* **2022**, *87*, 1840-1849.

Zhang, L.; Hinz, D. J.; Kiruba, G. S. M.; Ding, X.; Lee, J. K. "Gas-Phase Experimental and Computational Studies of Human Hypoxanthine-Guanine Phosphoribosyltransferase Substrates: Intrinsic Properties and Biological Implications," *J. Phys. Org, special issue honoring Barry Carpenter,* **2022**, e4343.

Hinz, D. J.; Zhang, L.; Lee, J. K. "Mass Spectrometry in Organic and Bio-organic Catalysis: Using Thermochemical Properties to Lend Insight into Mechanism," *Mass Spectrom. Rev.*, **2022**, 1-19.

Lotsof, E. R.; Krajewski, A. E.; Anderson-Steele, B.; Rogers, J. P.; Zhang, L.; Yeo, J.; Conlon, S.; Manlove, A. H.; Lee, J. K.; David, S. S. "NEIL1 Recoding due to RNA Editing Impacts Lesion-Specific Recognition and Excision," *J. Am. Chem. Soc.*, **2022**, *144*, 14578–14589.

Krajewski, A. E.; Lee, J. K. "Gas-Phase Experimental and Computational Studies of 5-Halouracils: Intrinsic Properties and Biological Implications," *J. Org. Chem.*, **2021***, 86*, 6361-6370.

Lee, J. K. "Gas Phase Models for Biocatalysis," in "Gas Phase Models for Catalysis: Atoms, Molecules, Clusters, and Complexes/Physical Chemistry in Action," Lang, S.; Bernhardt, T.. Eds. Springer, **2021**.

Majumdar, C.; McKibbin, P. L.; Krajewski, A. E.; Manlove, A. H.; Lee, J. K.; David, S. S. "Unique Hydrogen Bonding of Adenine with the Oxidatively Damaged Base 8-Oxoguanine Enables Specific Recognition and Repair by DNA Glycosylase MutY," *J. Am. Chem. Soc.,* **2020**, *142*, 20340-20350.

Wang, N.; Lee, J. K. "Gas-Phase and Ionic Liquid Experimental and Computational Studies of Imidazole Acidity and Carbon Dioxide Capture," *J. Org. Chem.*, **2019**, *84*, 14593-14601.

Xu, J.; Krajewski, A. E.; Niu, Y.; Kiruba, G. S. M.; Lee, J. K. "Kinetic Hydricity of Silane Hydrides in the Gas Phase," *Chemical Science*, **2019**, *10*, 8002-8008.

Xu, J.; Mieres-Perez, J.; Sanchez-Garcia, E.; Lee, J.K. "Gas-Phase Deprotonation of Benzhydryl Cations: Carbene Basicity, Multiplicity, and Rearrangements," *J. Org. Chem.*, **2019**, *84*, 7685-7693. *Also highlighted as journal issue cover.*

Wang, N.; Xu, J.; Lee, J. K. "The Importance of *N*-Heterocyclic Carbene Basicity in Organocatalysis," *Org. Biomol. Chem*., **2018**, *16*, 6852-6866.

Lee, J. K.; Niu, Y. "pK_a Prediction," in "Applied Theoretical Organic Chemistry," World Scientific, **2018**, 503-518.

Niu, Y.; Wang, N.; Munoz, A.; Xu, J.; Zeng, H.; Rovis, T.; Lee, J. K. "Experimental and Computational Gas Phase Acidities of Conjugate Acids of Triazolylidene Carbenes: Rationalizing Subtle Electronic Effects," *J. Am. Chem. Soc.,* **2017**, *139,* 14917-14930.

Bird, J. G.; Zhang, Y.; Tian, Y.; Greene, L.; Liu, M.; Buckley, B.; Lee, J. K.; Kaplan, C. D.; Ebright, R. H.; Nickels, B. E. "The Mechanism of RNA 5' Capping with NAD+, NADH, and CoA," *Nature,* **2016**, *535*, 444-447.

Kiruba, G. S. M.; Xu, J.; Zelikson, V.; Lee, J. K. "Gas Phase Studies of Formamidopyrimidine Glycosylase (Fpg) Substrates," *Chem. Eur. J.*, **2016**, *22*, 3881-3890 *(special issue "Women in Chemistry":* http://bit.ly/CEJ_Women2016).

Tian, Y.; Lee, J. K. "Gas Phase Studies of *N*-Heterocyclic Carbene-Catalyzed Condensation Reactions," *J. Org. Chem.* **2015**, *80*, 6831-6838. *Selected by "Organic Process Research & Development" as a "Highlight from the Literature"*

Teator, A. J.; Tian, Y.; Chen, M.; Lee, J. K.; Bielawski, C. W. "An Isolable, Photoswitchable N-Heterocyclic Carbene: On-Demand Reversible Ammonia Activation," *Angew. Chem. Int. Ed.*, **2015**, *54*, 11559-11563. *Selected by "Advances in Engineering" as a "Featured Article"*

Chen, M.; Lee, J. K. "Computational Studies of the Gas-Phase Thermochemical Properties of Modified Nucleobases," *J. Org. Chem.*, **2014**, *79*, 11295-11300. *Selected by JOC as "Highlighted Article"*

Zeng, H.; Wang, K.; Tian, Y.; Niu, Y.; Greene, L.; Hu, Z.; Lee, J. K. "The Benzoin Condensation: Charge Tagging of the Catalyst Allows for Tracking by Mass

Spectrometry," *Int. J. Mass. Spectrom.* **2014**, *369*, 92-97*(special issue to honor Veronica Bierbaum)*

Wang, K.; Chen, M.; Wang, Q.; Shi, X.; Lee, J. K. "1,2,3-Triazoles: Gas Phase Properties," *J. Org. Chem.*, **2013**, *78*, 7249-7258.

Chen, M.; Moerdyk, J. P.; Blake, G. A.; Bielawski, C. W.; Lee, J. K. "Assessing the Proton Affinities of *N,N'*-Diamidocarbenes," *J. Org. Chem.* **2013**, *78*, 10452–10458 *Selected by JOC as a "Highlighted Article"*

Maiti, A.; Michelson, A. Z.; Hwang, B.-J.; Armwood, C. J.; Lu, A.-L.; Lee, J. K.; Drohat, A. C. "Divergent Mechanisms for TDG Excision of 5-Formylcytosine and 5-Carboxylcytosine from DNA," *J. Am. Chem. Soc.*, **2013**, *135* (42), pp 15813–15822.

Michelson, A. Z.; Rozenberg, A.; Tian, Y.; Sun, X.; Davis, J.; Francis, A. W.; O'Shea, V. L.; Halasyam, M.: Manlove, A. H.; David, S. S.; Lee, J. K. "Gas-Phase Studies of Substrates for the DNA Mismatch Repair Enzyme MutY," *J. Am. Chem. Soc.*, **2012**, *134*, 19839-19850.

Michelson, A. Z.; Chen, M.; Wang, K.; Lee, J. K. "Gas-Phase Studies of Purine 3-Methyladenine DNA Glycosylase II (AlkA) Substrates," *J. Am. Chem. Soc.*, **2012**, *134*, 9622-9633.

Michelson, A. Z.; Petronico, A. "2-Pyridone and Derivatives: Gas Phase Acidity, Proton Affinity, Tautomer Preference and Leaving Group Ability," *J. Org. Chem.*, **2012**, *77,* 1623-1631.

Liu, M.; Chen, M.; Zhang, S.; Yang, I.; Buckley, B.; Lee, J. K. "Reactivity of Carbene•Phosphine Dimers: Proton Affinity Revisited," *J. Phys. Org. Chem.* **2011**, *24*, 929-936.

Tantillo, D. J.; Lee, J. K. "Reaction Mechanisms: Pericyclic Reactions," *Annu. Rep. Prog. Chem., Sect. B* **2011**, *107*, 266-286.

Liu, M.; Tran, N. T.; Franz, A. K.; Lee, J. K. "Gas-Phase Acidity Studies of Dual Hydrogen-Bonding Organic Silanols and Organocatalysts," *J. Org. Chem.* **2011**, *76*, 7186-7194.

Liu, M.; Yang, I.; Buckley, B.; Lee, J. K. "Proton Affinities of Phosphines versus N-Heterocyclic Carbenes," *Org. Lett.* **2010**, *21*, pp 4764–4767

Tantillo, D. J.; Lee, J. K. "Reaction Mechanisms: Pericyclic Reactions," *Annu. Rep. Prog. Chem.*, *Sect. B,* **2010**, *106*, 283-303.

Sun, X.; Lee, J. K. "The Stability of DNA Duplexes Containing Hypoxanthine (Inosine): Gas versus Solution Phase and Biological Implications," *J. Org. Chem.*, **2010**, *75*, 1848-1854.

Zhachkina, A.; Lee, J. K. "Uracil and Thymine Reactivity in the Gas Phase: The S_N2 Reaction and Implications for Electron Delocalization in Leaving Groups," *J. Am. Chem. Soc.* **2009**, *131*, 18376-18385.

Zhachkina, A.; Liu, M.; Sun, X.; Amegayibor, F. S.; Lee, J. K. "Gas-Phase Thermochemical Properties of the Damaged Base O-Methylguanine versus Adenine and Guanine," *J. Org. Chem.* **2009**, *74*, 7429-7440.

Tantillo, D. J.; Lee, J. K. "Reaction Mechanisms: Pericyclic Reactions," *Annu. Rep. Prog. Chem., Sect. B,* **2009**, *105*, 285-309.

Liu, M.; Li, T.; Amegayibor, F. S.; Cardoso, D. S.; Fu, Y.; Lee, J. K. "Gas-Phase Thermochemical Properties of Pyrimidine Nucleobases," *J. Org. Chem.*, **2008**, *73*, 9283-9291.

Rozenberg, A; Lee, J. K. "Theoretical Studies of the Quinolinic Acid to Nicotinic Acid Mononucleotide Transformation," *J. Org. Chem.*, **2008**, *73*, 9314-9319.

Wepukhulu, W. O.; Smiley, V. L.; Vemulapalli, B.; Smiley, J. A.; Phillips, L. M.; Lee, J. K. "Evidence for Pre-Protonation in the Catalytic Reaction of OMP Decarboxylase: Kinetic Isotope Effects using the Remote Double Label Method," *Organic and Biomolecular Chemistry*, **2008**, *6*, 4533-4541 (ALSO FEATURED ON COVER).

Tantillo, D. J.; Lee, J. K. "Reaction Mechanisms: Pericyclic Reactions," *Annu. Rep. Prog. Chem., Sect. B,* **2008**, *104*, 260-283.

Liu, M.; Xu, M.; Lee, J. K. "The Intrinsic Reactivity of Ethenoadenine and Mechanism for Excision from DNA," *J. Org. Chem.,* **2008**, *73*, 5907-5914.

Sun, X.; Lee, J. K. "The Acidity and Proton Affinity of Hypoxanthine in the Gas Phase versus in Solution: Intrinsic Reactivity and Biological Implications," *J. Org. Chem.*, **2007**, *72*, 6548-6555.

Tantillo, D. J.; Lee, J. K. "Reaction Mechanisms: Pericyclic Reactions," *Annu. Rep. Prog. Chem., Sect. B,* **2007**, *103*, 272-293.

Current and Past

National Science Foundation
NSF, 2025-2028, pending
NSF, 2021-2025. CHE 2054395
NSF, 2020-2021. CHE 2027221
NSF, 2018-2023. CHE 1761151
NSF, 2014-2019. CHE 1361462
NSF, **2010-2015.** CHE 0954364
NSF, 2006-2010. CHE 0543038
NSF, 2001-2007. NSF CAREER Award, CHE 0092215

Other
ACS Petroleum Research Fund, **2011-2014.** "Gas Phase Studies of Stable Carbenes and Triazoles"
NIH, 2011. "Triple Quadrupole Mass Spectrometer" (co-PI)
Rutgers Busch Foundation 2003-2005. "Novel MS Studies of DNA Duplexes"
Alfred P. Sloan Foundation, **2002-2006.** "Foundation Fellow"
ACS Petroleum Research Fund, 1998-2001. "Method to Simultaneously Quantitate DNA Duplex Stability in the Gas Phase and in Solution"
Rutgers Busch Foundation, 1999-2001. "Novel DNA Binding Studies"
Rutgers Strategic Resources and Opportunity Analysis, **2001.** "A Mass Spectrometric Facility for Rutgers University" (co-PI)

Research Corporation, 1998-2001. "DNA Duplex Stability"
National Institutes of Environmental Health Sciences, 1998-1999, "Mass Spectrometric Studies of DNA Duplexes and Adducts"
NSF, 1998-1999. "Purchase of a 300 MHz NMR Spectrometer" (co-PI)

Selected External Presentations (all are invited addresses)
since 2007 (as P1)

Gordon Research Conference, Physical Organic Chemistry, June 2025, Discussion Leader.
Reaction Mechanisms Conference, Albuquerque, New Mexico, June 2024, Discussion Leader
International Symposium on Reactive Intermediates and Unusual Molecules, Bad Honnef, Germany, September 2023
American Chemical Society, A Symposium in Honor of the 80th Birthday of Prof. Kendall N. Houk: Pushing Back the Frontiers of Computational Organic Chemistry and Chemical Biology, August 2023
Gordon Research Conference, Gaseous Ions GRC, February 2023
Houk Research Symposium, Los Angeles, California, August 2022
International Symposium on Reactive Intermediates and Unusual Molecules, Hiroshima, Japan, July 2022
Radical in the Rockies Conference, Telluride, Colorado, June 6-10, 2022
Reaction Mechanisms Conference, Boulder, Colorado, co-organizer, June 13-16, 2022
RESOLV Summer School Solvation Science, German Cluster of Excellence, Bochum, Germany, June 2022
Barnard College, Department of Chemistry, March 2021
James Flack Norris Award Symposium, ACS Philadelphia, March 2020 *delayed by COVID*, invited speaker (by honoree, Professor Herbert Mayr)
University of Colorado, Boulder, Colorado, December 2019
New Jersey Institute of Technology, Newark, New Jersey, October 2019
Reaction Mechanisms Conference, Vancouver, Canada, June 2018.
Isolated Biomolecules Biomolecular Interactions Meeting, Texel Island, The Netherlands, April 2018.
Catalysis and Computation Symposium, ACS Washington DC, August 2017.
International Symposium on Reactive Intermediates and Unusual Molecules, Sorrento, Italy, June 2017.
James Flack Norris Award Symposium, ACS San Francisco, April 2017, organizer and speaker.
Gordon Research Conference on Gaseous Ions: Structures, Energetics and Reactions, Ventura, California, February 2017, discussion leader+short talk.
ACS Pacifichem, Honolulu, Hawaii, December 2015.
Rutgers University Newark, Newark, New Jersey, October 2015.
Princeton ACS Symposium - Houk Symposium + presenter for Ken Houk, Princeton, New Jersey, October 2015.
International Bunsen Discussion Meeting on Gas Phase Model Systems for Catalysis, Ulm, Germany, April 2014.
International Symposium on Reactive Intermediates and Unusual Molecules (ISRIUM), Hiroshima, Japan, April 2014.
City College of New York, New York, New York, March 2014
Radicals in the Rockies Conference, Telluride, Colorado, July 2013.
Gordon Research Conference on Gaseous Ions, Galveston, Texas, February 2013.
Accelerating Reaction Discovery Conference, Telluride, Colorado, August 2012.
Reaction Mechanisms Conference, Columbia, Missouri, June 2012.
American Chemical Society Pacifichem Meeting, Honolulu, Hawaii, December 2010.

NSF Workshop on Physical Organic Chemistry, Austin, Texas January 2010 (invited but could not attend).
Wake Forest University, North Carolina, April 2009.
University of California, Davis, Department of Chemistry, Davis, California, February 2009.
Swarthmore College, Pennsylvania, February 2009
10th International Symposium on Organic Free Radicals (ISOFR 10) and 3rd Pacific Symposium on Radical Chemistry (PSRC 3), Heron Island, Australia, August 2008 (invited but could not attend)
Houk 65th Birthday Symposium, UCLA, June 2008
Georgia Institute of Technology, Department of Chemistry, Atlanta, Georgia, May 2008.
International Symposium on Reactive Intermediates and Unusual Molecules (ISRIUM), Heron Island, Australia, August 2007.
Gordon Research Conference on Physical Organic Chemistry, Plymouth, New Hampshire, June 2007.
Gordon Research Conference on Gas Phase Ion Energetics and Structure, Ventura, California, February 2007.

Awards and Honors

ACS PROGRESS/Dreyfus Lectureship Award	2006
Alfred P. Sloan Fellowship	2002-2006
NSF CAREER Award	2001-2006
Rutgers Faculty of the Arts and Sciences Undergraduate Teaching Award	2003
National Institutes of Health Postdoctoral Fellowship	1995-1997
Sigma Xi Scientific Honor Society	1994-present
Division of Organic Chemistry ACS Graduate Research Fellowship	1993-1994
Department of Defense Graduate Research Fellowship	1990-1993
National Science Foundation Graduate Research Fellowship (declined)	1990
National Physical Science Consortium Top 80 Woman Scholar	1990
Merrill Presidential Scholar, Outstanding Senior, Cornell University	1990
George Caldwell Prize, Outstanding Senior Chemistry Major	1990
American Institute of Chemists Award, Outstanding Graduating Senior in Chemistry	1990
NSF-REU Fellow	1988, 1989
Phi Beta Kappa National Honor Society	1989
Mortar Board Honor Society	1989
A.W. Laubengayer Award, Outstanding Student in Freshman Chemistry, Cornell U.	1987