



K. N. Houk

The author presented on this page has published more than **10 articles** in *Angewandte Chemie* in the last 10 years, most recently: "Rapid Catalyst Identification for the Synthesis of the Pyrimidinone Core of HIV Integrase Inhibitors": A. Bellomo, N. Celebi-Olcum, X. Bu, N. Rivera, R. T. Ruck, C. J. Welch, K. N. Houk, S. D. Dreher, *Angew. Chem.* **2012**, 124, 7018–7021; *Angew. Chem. Int. Ed.* **2012**, 51, 6912–6915.



The work of K. N. Houk has been featured on the cover of *Angewandte Chemie*: "Spirodiporphyrins—As Binuclear Metal Complexes": E. Vogel, M. Michels, L. Zander, J. Lex, N. S. Tuzun, K. N. Houk, *Angew. Chem.* **2003**, 115, 2964–2969; *Angew. Chem. Int. Ed.* **2003**, 42, 2857–2862.

Kendall N. Houk

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Position: Saul Winstein Chair in Organic Chemistry, University of California, Los Angeles
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Education: **1964** AB, Harvard College
1968 PhD with R. B. Woodward, Harvard University
Awards: **2002** Fellow of the American Academy of Arts and Sciences; **2003** ACS Award for Computers in Chemical and Pharmaceutical Research; **2003** Member of the International Academy of Quantum Molecular Science; **2009** Arthur C. Cope Award, American Chemical Society; **2010** Member of the National Academy of Sciences; **2012** Robert Robinson Award, Royal Society of Chemistry
Current research interests: Theoretical and computational organic chemistry: rules to understand reactivity, computer modeling of complex organic reactions, and experimental tests of the predictions of theory; theoretical investigations and design of enzyme-catalyzed reactions, quantitative modeling of asymmetric reactions used in synthesis, and mechanisms and dynamics of pericyclic reactions and competing diradical processes
Hobbies: Running, biking, swimming, art, music

What I look for first in a publication is ... a memorable discovery leading to a new idea.

The most important thing I learned from my parents is ... keep working for your goals and enjoy life (no matter what happens).

The best advice I have ever been given is ... eschew obfuscation.

The most significant scientific advance of the last 100 years has been ... quantum mechanics.

If I could have dinner with three famous scientists from history, they would be ... P. A. M. Dirac, Emil Fischer, and R. B. Woodward.

I chose chemistry as a career because ... I get a thrill from making things for the first time. Now I mostly make ideas.

My favorite place on earth is ... Hawaii (Big Island).

My best investment was ... my Porsche.

If I were not a scientist, I would be ... a musician (I played trumpet, classical, and jazz).

My most exciting discovery to date has been ... torquoselectivity!

My greatest achievement has been ... mentoring many great young computational organic chemists.

The most exciting thing about my research is ... the rush that comes from understanding something for the first time.

Guaranteed to make me laugh is ... the Hawaii Five-O dance.

I would have liked to have discovered ... the Woodward–Hoffmann rules.

The downside of my job is ... each day ends too soon.

A good work day begins with ... waking up with a fresh brain and a great idea.

The most amazing chemistry adventure in my career was ... hosting R. B. Woodward in my apartment in 1967 to watch the Boston Red Sox play in the World Series on TV.

Has your approach to publishing your results changed since the start of your career?

I have always been eager to publish discoveries that my group has made. That is why I have so many papers! I still feel that eagerness; the publications of my group are our announcements to the world of our discoveries and are our contribution to scientific knowledge.

My 5 top papers:

1. “The frontier molecular orbital theory of cycloaddition reactions”: K. N. Houk, *Acc. Chem. Res.* **1975**, *8*, 361–369.
This account summarizes our early discoveries on the use of frontier molecular theory to understand reactivity and regioselectivity in Diels–Alder and 1,3-dipolar cycloadditions. The generalities about the shapes of the molecular orbitals of typical 1,3-dipoles and substituted dienes and dienophiles have been widely used since that time.
2. “Theory of stereoselection in conrotatory electrocyclic reactions of substituted cyclobutenes”: N. G. Rondan, K. N. Houk, *J. Am. Chem. Soc.* **1985**, *107*, 2099–2111.
This article describes the discovery of the molecular orbital basis of “torquoselectivity”, the selective formation of only one of the Woodward–Hoffmann-allowed products in electrocyclic reactions. Many examples have been explored in the last 27 years, and unintuitive predictions were made and verified experimentally.
3. “Transition Structures of Hydrocarbon Pericyclic Reactions”: K. N. Houk, Y. Li, J. D. Evanseck, *Angew. Chem.* **1992**, *104*, 711–739; *Angew. Chem. Int. Ed. Engl.* **1992**, *31*, 682–708.
This article is a mixture of a review and new results. My two co-authors are both great computational chemists

What do you think the future holds for your field of research?

Computational chemistry and simulation have a limitless future. As mathematical chemists improve algorithms, and as computers are made faster, the accuracy and size of reactions that can be studied will steadily increase. Predictions will become more commonplace and more useful to experimentalists.

- and graphic artists. This work documents the shapes and energies of pericyclic reaction transition states.
4. “Kemp elimination catalysts by computational enzyme design”: D. Röthlisberger, O. Khersonsky, A. M. Wolcott, L. Jiang, J. DeChancie, J. Betker, J. L. Gallaher, E. A. Althoff, A. Zanghellini, O. Dym, S. Albeck, K. N. Houk, D. S. Tawfik, D. Baker, *Nature* **2008**, *453*, 190–195.
The first paper that combines my group’s active-site design and ranking methods and the Baker group’s protein design methods as well as experiments. Successful designs of proteins that act as catalysts are reported. We continue to collaborate with Baker, Mayo, Tawfik, Hilvert, and others to develop methods for enzyme design and to make catalysts for nonnatural reactions.
 5. “Theory of 1,3-Dipolar Cycloadditions: Distortion/Interaction and Frontier Molecular Orbital Models”: D. H. Ess, K. N. Houk, *J. Am. Chem. Soc.* **2008**, *130*, 10187–10198.
The first of many papers from my group describing how distortion energies influence activation barriers of cycloaddition reactions. This continues to be an active area of research and a powerful model to understand reactivity. Together with FMO theory, this provides a comprehensive way to understand cycloaddition reactivity.

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