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Arthur C. Cope Award: Kendall N. Houk

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The most sophisticated calculations **Kendall N. Houk** did as a graduate student were Hückel calculations, and his fanciest computational tools were graph paper and a pencil. These days, his research group at the University of California, Los Angeles, logs millions of hours of computer time each year as it teases out a deeper understanding of reactions in organic chemistry.

Proving that one can do cutting-edge organic chemistry with a computer rather than a condenser, Houk, 67, garnered this year's Arthur C. Cope Award "for achievements in the understanding of organic reactivity and selectivity and development of theoretical models for predictions of products of complex organic and biological reactions."

"There is continuing skepticism about computational theory, but I've always felt that experimental organic chemists were eager to have a deeper understanding about the theoretical origin of what they are doing," Houk notes. Winning the Cope Award, he says, "really is validation from my respected peers and colleagues of this approach and the impact we've had on organic chemistry."

Houk vividly recalls attending his first ACS national meeting in 1973 and seeing the inaugural Cope Award given jointly to Harvard University's R. B. Woodward—whom Houk calls his hero—and Roald Hoffmann, now at Cornell University. The following year, UCLA's Donald Cram, who would be very influential in Houk's career, took the prize. "Then, Elias J. Corey, for whom I was a teaching assistant at Harvard, and Orville L. Chapman, another influential colleague at UCLA, were awarded the Cope Award. In fact, I have met and admired all 32 previous recipients. Not to mention that the Cope rearrangement is one that I have studied extensively. To be receiving that award is really amazing for me," Houk says.

"Houk is the leader of the new era of theoretical organic chemistry, where state-of-the-art quantum mechanics is used to discern the principles that govern organic reactivity and selectivity," Hoffmann says.

A child of the Sputnik era, Houk remembers growing up with the idea that science was an important and glamorous field to get into. But mostly, he says, he was "just very curious, and science was the way to learn how things work." He also recalls wanting to be an inventor, which, he says, he more or less is these days—just an inventor of conceptual principles about chemistry.

Houk earned his bachelor's degree in chemistry from Harvard in 1964, and working with Woodward, he earned a doctoral degree from the school in 1968. Houk then took an assistant professor position at Louisiana State University. It was good place to get into computational studies, he says. The university had good computer resources, and his colleagues were helpful in guiding him through theory and computations.

He began working with John Pople's Gaussian 70—the first program, Houk says, that made it possible for anybody to do computations easily in a standardized way. Since then, he explains, "I've just gradually learned about every state-of-the-art method as it was developed and applied that to organic chemistry." In 1980, he moved to the University of Pittsburgh, and in 1986, he moved again to UCLA, where he currently holds the Saul Winstein Chair in Organic Chemistry.

"Houk has uniquely wide-ranging interests in chemistry," Yale University's Kenneth B. Wiberg notes, as is evidenced by his 764 publications. "He has made many important contributions to the way chemists think about their work."

Over the years, Houk and his students have tackled all types of organic reactions, trying to develop a deeper knowledge of stereoselectivity, regioselectivity, and reactivity, as well as working to establish a quantitative understanding of the transition states in organic reactions. For example, he created a frontier molecular orbital theory of regioselectivity in cycloadditions.

"His classic series of papers showed for the first time how the regioselectivity of 1,3-dipolar cycloadditions could be understood and predicted, based upon frontier molecular orbital theory," Hoffmann says. "His generalizations about the shapes and energies of frontier molecular orbitals of alkenes, dienes, and 1,3-dipoles are in common use today."

Houk is also well-known for his study of pericyclic reactions. He "discovered a powerful and unanticipated substituent effect in electrocyclic reactions of substituted cyclobutenes," Hoffmann notes, which led to the theory of 'torquoselectivity,' as Houk dubbed it. The theory describes a stereoselectivity that arises from preferential rotation of terminal substituents accompanied by a torque on the breaking bond. "The better the donor, the greater the preference for outward rotation," Hoffmann explains. "And," Houk adds, "we predicted —correctly—that a strong acceptor would rotate inward."

"Houk has created a new level of understanding of the role of electronic effects in reactivity and selectivity and has excelled in designing and executing theoretical tests of models proposed to understand organic reactivity," Hoffmann says. "His accomplishments have formed our modern view of transition states of organic reactions and of chemical reactivity."

"For many years I have admired Professor Houk, who has made a number of truly outstanding contributions to theoretical and computational organic chemistry," says Ryoji Noyori, president of RIKEN, a research institute in Japan. "The synthetic organic chemistry community deeply appreciates his theoretical contributions to the practically significant chemical world."

The Houk group just might hold the record for numbers of published organic reaction transition states. For example, they extended the Felkin staggered transition-state model beyond nucleophilic reactions to include electrophilic and radical additions as well. "Whenever additions to unsaturated systems occur," Houk says, "the allylic bonds rotate into a staggered arrangement." Models for stereoselectivity in all kinds of additions and cycloadditions have resulted from these computations.

"We are now going beyond mapping out transition states and intermediates to study the dynamics of reactions," Houk notes. Another new direction for the Houk group's research involves the use of computational methods to design novel enzymes to catalyze reactions for which there are no natural enzymes. "Success in this project will have profound applications, but it is the most challenging thing we have ever undertaken," Houk says. "The

collaboration with many other computational and experimental chemists and biologists will make it possible."

When he isn't doing chemistry, Houk is involved in athletics, art, and music. He runs, bikes, or swims almost every day, and he wants to finish a triathlon this year. "Robin Garrell, my wife and accomplished chemist who is also a professor and Senate Chair at UCLA, and I are fans of the LA Philharmonic, the many LA-area galleries, and we like to dabble in art, too," he says. Visitors to their home can find his brushstrokes in an abstract mural on the wall.

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