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# Nobel Prize in Chemistry 1981

Kenichi Fukui

Roald Hoffmann

The Nobel Prize in Chemistry 1981 was awarded jointly to Kenichi Fukui and Roald Hoffmann *"for their theories, developed independently, concerning the course of chemical reactions"*

## *Information about winners:*

**Kenichi Fukui**,

Kyoto University, Kyoto, Japan, and the other half to

**Roald Hoffmann**,

Cornell University, Ithaca, NY, USA,

## *RESEARCH INFORMATION:*

### CHEMISTRY PRIZE AWARDED FOR INCREASING OUR UNDERSTANDING OF CHEMICAL REACTIONS

Chemical transformations of the microscopic (atomic) structure of matter have been proceeding on Earth for billions of years. These transformations, or reactions, play a part in the drama of our planet's development. One of the prerequisites for life on Earth is that chemical reactions should be governed by natural laws. For thousands of years man has actively utilized chemical transformation processes for mastering his environment - in

preparing food and drink, in fashioning tools and clothes, and in combatting disease, and so on. This active utilization was initiated by chance discoveries made in the daily round of practical living. The mass of empirical knowledge grew so large in time that theoretical concepts had to be resorted too, so that a meaningful overall view was possible. Theories thus became necessary for the continued conscious and systematic utilization of chemical reactions. The efforts of the Chemistry Prizewinners should be seen as constituting one of the links in this chain of ongoing development.

The Prizewinners' work aims at theoretically anticipating the course of chemical reactions. It is based on quantum mechanics (the theory whose starting point is that the smallest building blocks of matter may be regarded both as particles and as waves), which attempts to explain how atoms behave. The Chemistry Prizewinners' theories developed via close interaction with the empirical findings of experimental chemists. Hoffmann's first really powerful theoretical work carried out in 1965 in collaboration with R.B. Woodward at the University of Harvard. Woodward (died in 1979) was awarded the 1965 Nobel Prize in Chemistry for contributions of a completely different kind - for his outstanding achievements in building up complex organic molecules experimentally. Fukui started his scientific work in experimental chemistry.

More than 25 years ago, Fukui showed that certain properties of the orbits of the most loosely bound electrons and of the "most easily accessible" unoccupied electronic orbits had unexpectedly great significance for the chemical reactivity of molecules. He called these orbits "frontier orbitals". Fukui's earlier **frontier orbital theory** attracted only little attention at first. In the mid-1960s, Fukui and Hoffmann discovered - almost simultaneously and independently of each other - that symmetry properties of frontier orbitals could explain certain reaction courses that had previously been difficult to understand. This gave rise to unusually intensive research activity - both theoretical and practical - in many parts of the world, Fukui and other researchers developed the frontier orbital theory into a highly powerful tool for understanding the reactivity of molecules. Hoffmann and co-workers elaborated the observations he had made together with

Woodward. These observations are collectively termed the theory of **conservation of orbital symmetry** in chemical reactions. Orbital interaction and symmetry relations between molecules or parts of molecules are fundamental concepts in Fukui's and Hoffmann's theories.

A characteristic feature of Fukui's and Hoffmann's method of attacking difficult and complicated problems is that they succeeded in making generalizations through simplifications. In this lies the key to the strength of their theories. The theoretical models that Fukui and Hoffmann introduced have been in many branches of chemistry since the 1970s. Their method of conceiving of the course of chemical reactions is utilized nowadays, for example, by chemists studying life processes and by chemists making new drugs.

Good theoretical models provide guidance for experimental researchers and save them time. Fukui's and Hoffmann's theories are milestones in the development of our understanding of the course of chemical reactions. This development has, however, by no means been brought to a halt by the prizewinning work. This work has provided inspiration for new lines of development. Fukui and Hoffmann are among the most active researchers in these areas today.

***For more details please visit:***

http://www.nobelprize.org/nobel_prizes/chemistry/laureates/1981/press.html