

Roald Hoffmann
Career-in-Review (CIR)

David Wang (Danishefsky Group)
June 29, 2007

Synthesis Literacy Group
Columbia University Chemistry

Roald Hoffmann
Frank H. T. Rhodes Professor of Human Letters
Cornell University

Born: 1937, Zloczow, Poland
Arrived in US at 12, attended Stuyvesant

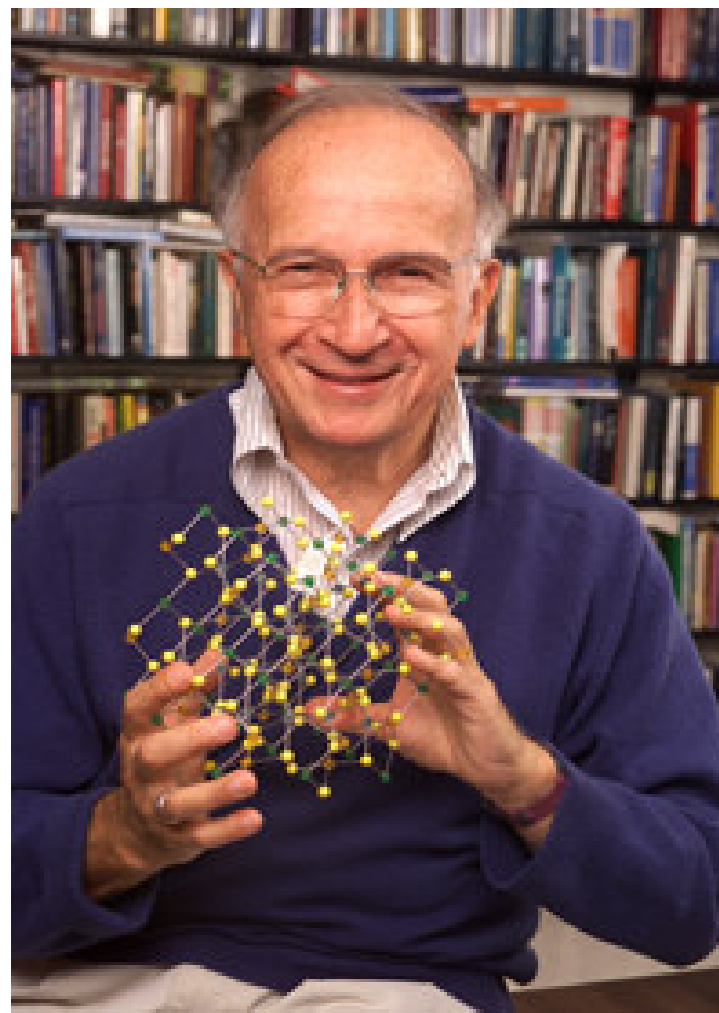
B.A. Columbia University (1958)
M.A. Harvard University (1960)
Ph.D. Harvard University (1962)

His Science:

Nobel Prize (1981), shared with K. Fukui
National Medal of Science (1983)
Priestly Medal (1990)

His Art:

The Metamict State (1987)
Gaps and Verges (1990)
Memory Effects (1998)
Oxygen (2001), with C. Dejarassi



AMMETER JH, BURGI HB, THIBEAULT JC, et al.

COUNTERINTUITIVE ORBITAL MIXING IN SEMI-EMPIRICAL AND ABINITIO MOLECULAR-ORBITAL CALCULATIONS

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 100 (12): 3686-3692 1978

Times Cited: 1407

LAUHER JW, **HOFFMANN R**

STRUCTURE AND CHEMISTRY OF BIS(CYCLOPENTADIENYL)-MLN COMPLEXES

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 98 (7): 1729-1742 1976

Times Cited: 1237

HAY PJ, THIBEAULT JC, **HOFFMANN R**

ORBITAL INTERACTIONS IN METAL DIMER COMPLEXES

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 97 (17): 4884-4899 1975

Times Cited: 1191

HOFFMANN R

BUILDING BRIDGES BETWEEN INORGANIC AND ORGANIC-CHEMISTRY (NOBEL LECTURE)

ANGEWANDTE CHEMIE-INTERNATIONAL EDITION IN ENGLISH 21 (10): 711-724 1982

Times Cited: 1042

Professor Hoffmann claims he is an “Applied Theoretical Chemist”

His main research interests are:

Role of orbital symmetry in chemical reaction courses

Inorganic-organic chemistry reactivity connection: Isolobal analogy

Interaction of small molecules with surfaces

Electronic structures of cluster compounds

New metallic forms of carbon

Our group looks at the electronic structure of molecules of any complexity, whether organic or inorganic, discrete molecular structures, or extended arrays in one, two, or three dimensions.

----- Hoffmann group webpage

The Year of 1965

1958-1962: Ph.D. with Professors W. Lipscomb & M. Gouterman

1962-1965: Harvard Junior Fellow in the Society of Fellows

Three landmark papers co-authored with Woodward:

“Stereochemistry of electrocyclic reactions”,

J. Am. Chem. Soc. 1965, 87, 395.

“Selection rules for concerted cycloaddition reactions”

J. Am. Chem. Soc. 1965, 87, 2046

“Selection rules for sigmatropic reactions”

J. Am. Chem. Soc. 1965, 87, 2511

*The success on such a theory depends on
critical collaboration of the two!*

Did Corey play a role in the development of orbital conservation theory!?

Corey's claim:

Chem & Eng News, 2004, March 29 issue, pp 42-44

Hoffmann refuted immediately:

Angew. Chem. Int. Ed. 2004, 43, 6586-90

What was the history!?

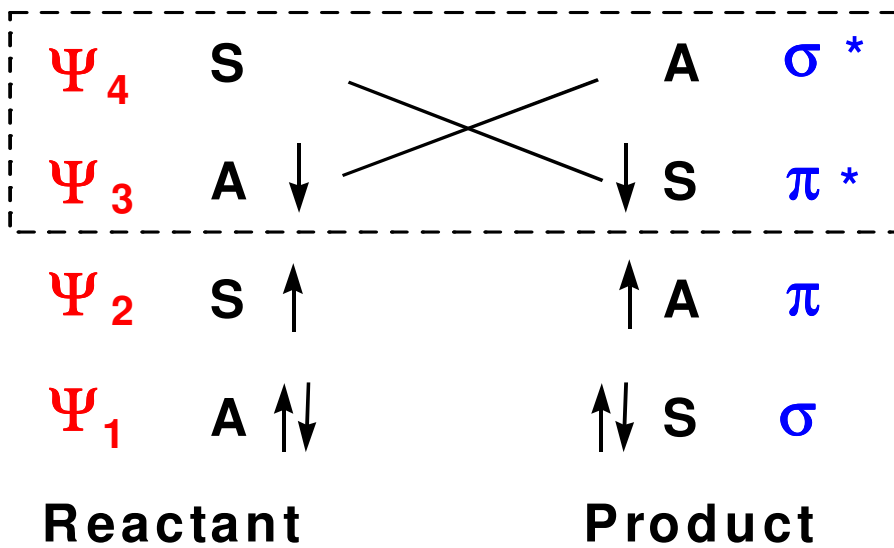
The Dutch chemist Oosterhoff's Idea:

“....Those differences in stereochemical courses may have an origin in the symmetry property of the highest occupied π -orbital of the triene system”

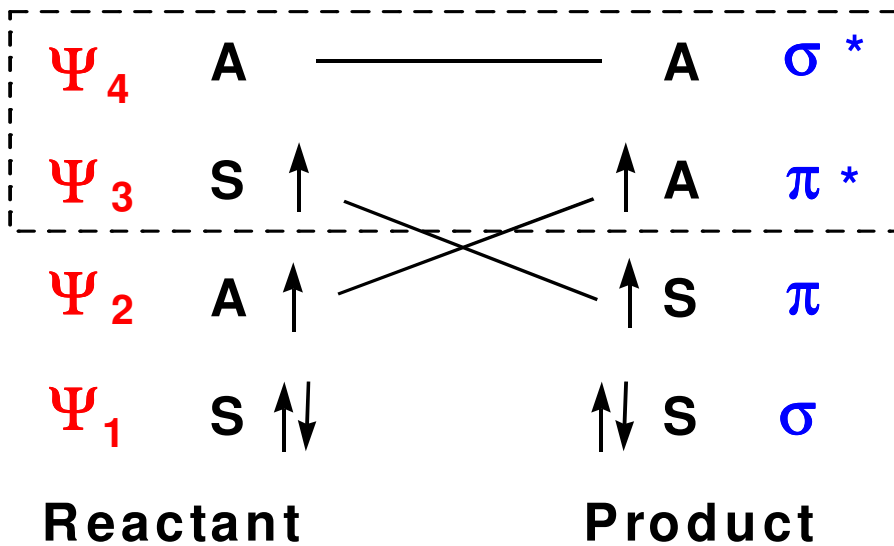
Too bad, he did not pursue this idea further!

***“Speculate as widely as possible, people will remember you only when you are right*”**

R. B. Woodward



⇒ forbidden



⇒ allowed

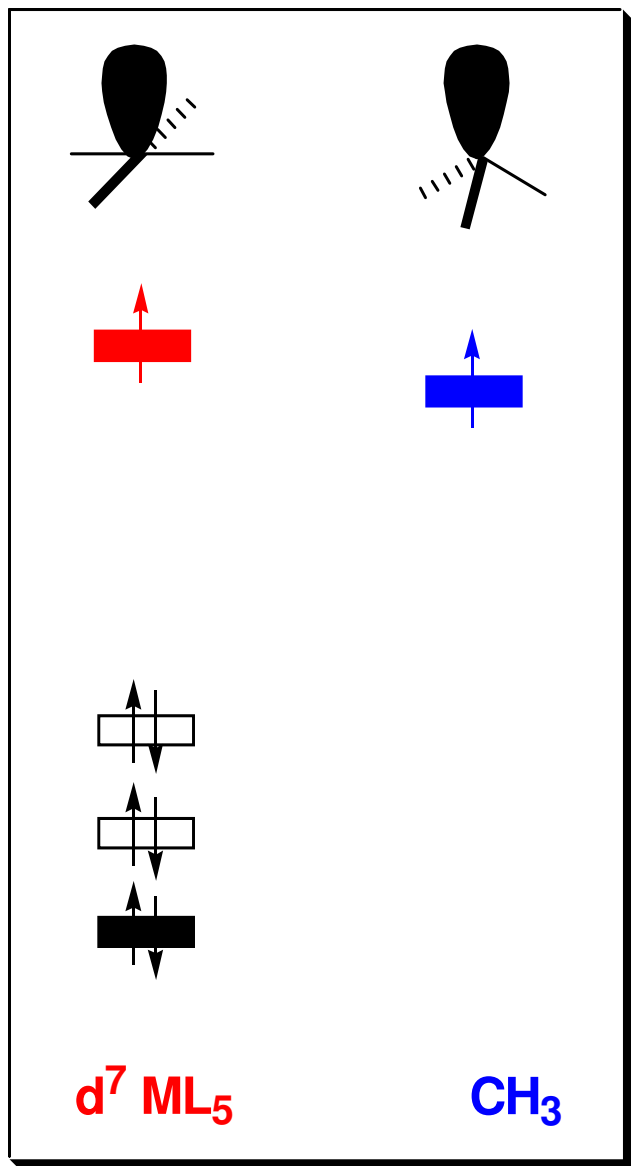
The concept of Isolobal Analogy:

“Building Bridges Between Inorganic and Organic Chemistry”

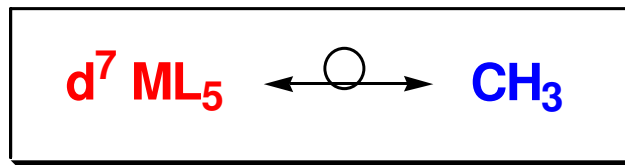
Nobel Lecture, 1981

Key Point:

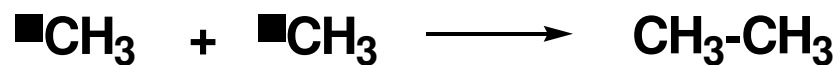
*Molecular species having similar frontier orbital pictures
would behave similarly in their reactivities.*



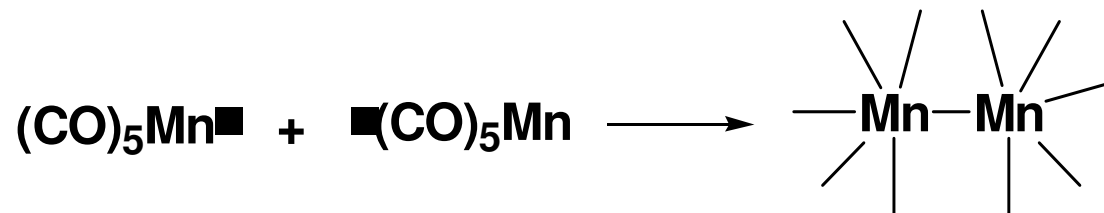
$d^7 ML_5$: $Mn(CO)_5$, $Co(CN)_5^{3-}$, etc



Because:



Therefore:



Thank You!