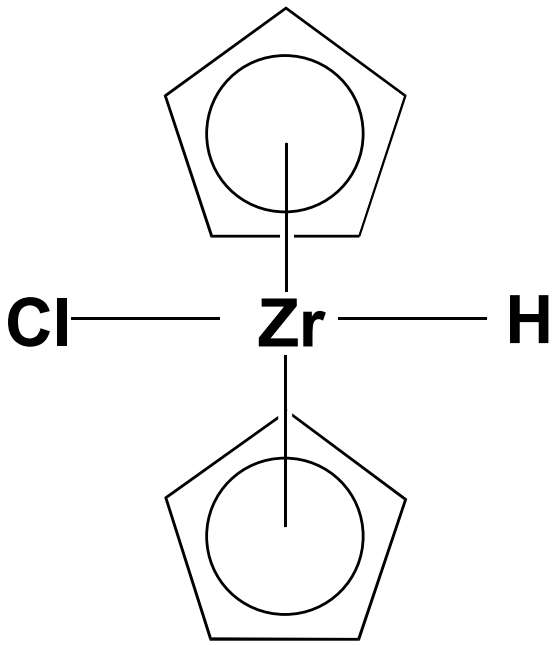
Zirconocene Chloride Hydride (Schwartz Reagent)

Technical Data



NICHIA CORPORATION

1. Product Guide

Physical and Chemical Properties:

Chemical Name: Bis-Cyclopentadienyl Zirconium (IV) Chloride Hydride Zirconocene Chloride Hydride

Molecular Formula: $(C_5H_5)_2ZrHCl$

Molecular Weight: 257.87

Appearance: White powder

Decomposability: Zirconocene Chloride Hydride easily decomposes from the moisture in air forming $(C_{p2}ZrCl)_2O$ and it also gradually decomposes when exposed to light.

Assay and Impurities:

Analytical data of Zirconocene Chloride Hydride:

	Specifications	Typical Data	Theoretical Value
Zr	≥33.60%	34.4%	35.38%

Comparison with reagent products:

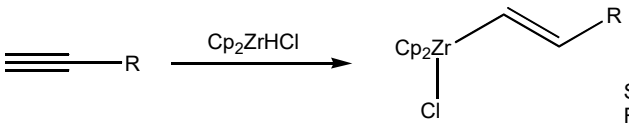
Suppliers		Zr(%)[1]	Cl(%)[1]	Cl/Zr (Molar Ratio)	Notes	Reaction Time of Hydrizirconation with 3-Hexyne (min)@28°C[2]	State of the Acid-hydrolyzed Solution
Nichia		34.4	13.1	1.02	White Powder	26	Clear
Reagent	A	35.2	12.5	1.09	Pale Pink Powder	88	Insoluble Solid Remains
	B	35.3	12.7	1.08	White Powder	45	Insoluble Solid Remains
	C	36.1	12.7	1.10	White Powder	53	Insoluble Solid Remains
	D	35.4	13.3	1.03	White Powder	72	Cloudy, Insoluble Solid Remains
Thoretical Value		35.38	13.75	1.00			

[1] Zr and Cl contents were analyzed by Nichia.
[2] The time at which the reaction solution turned into a clear liquid was used as the hydrozirconation reaction endpoint.

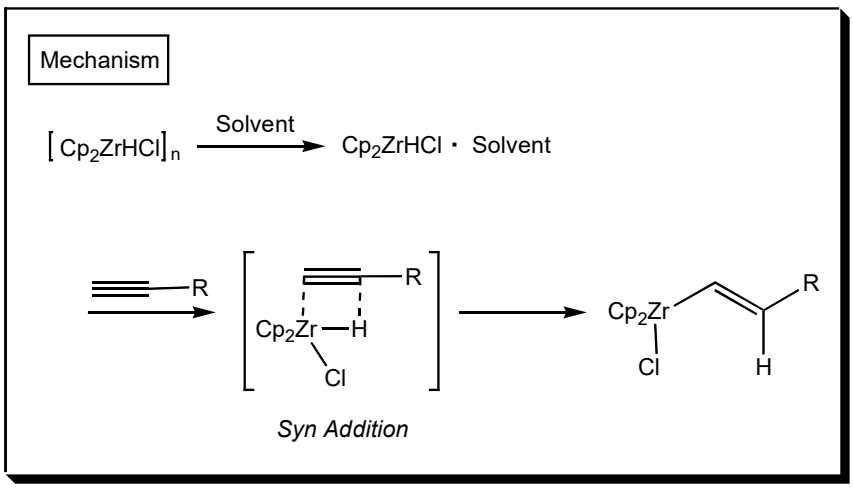
2. Application in Organic Synthesis

A. Hydrozirconation

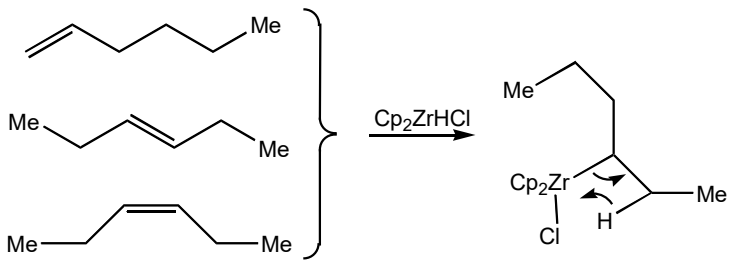
- Hydrozirconation of Alkyne

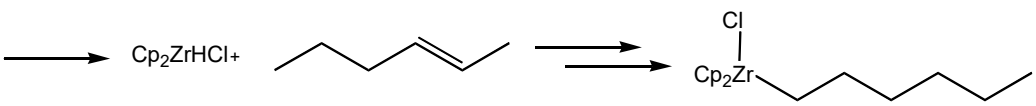


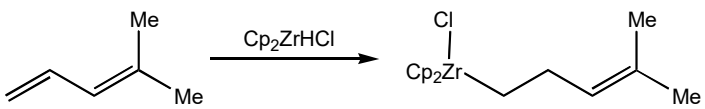
Stereo Selectivity : >98%
Regio Selectivity : >98%



- Hydrozirconation of Alkene

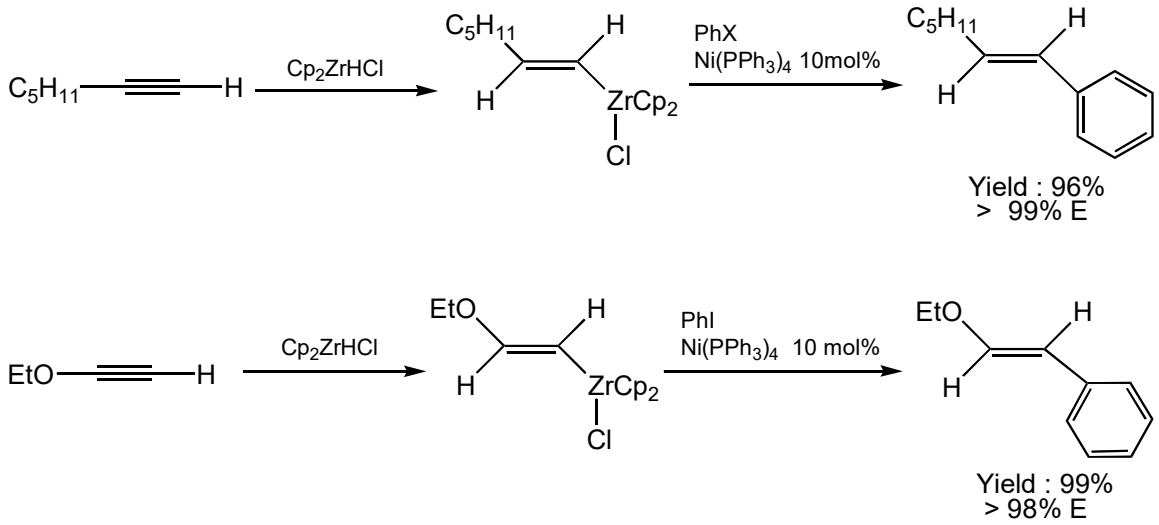




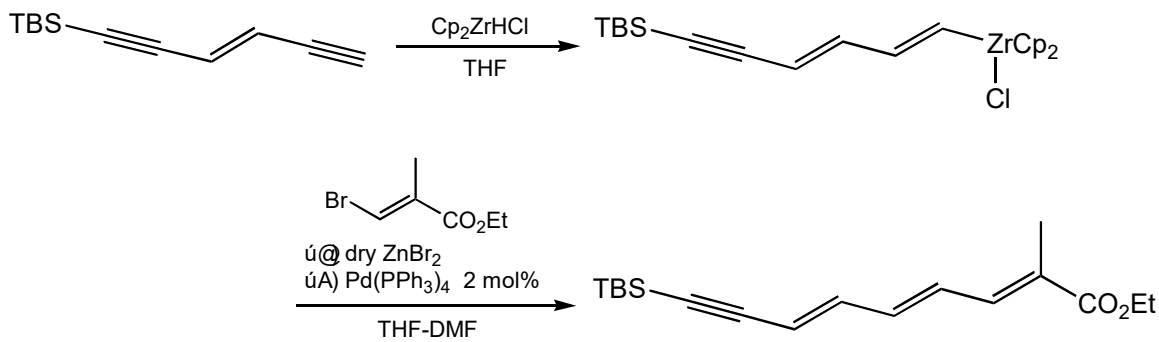


The 5th Series of Experimental Chemistry., 18, 254 (2004)

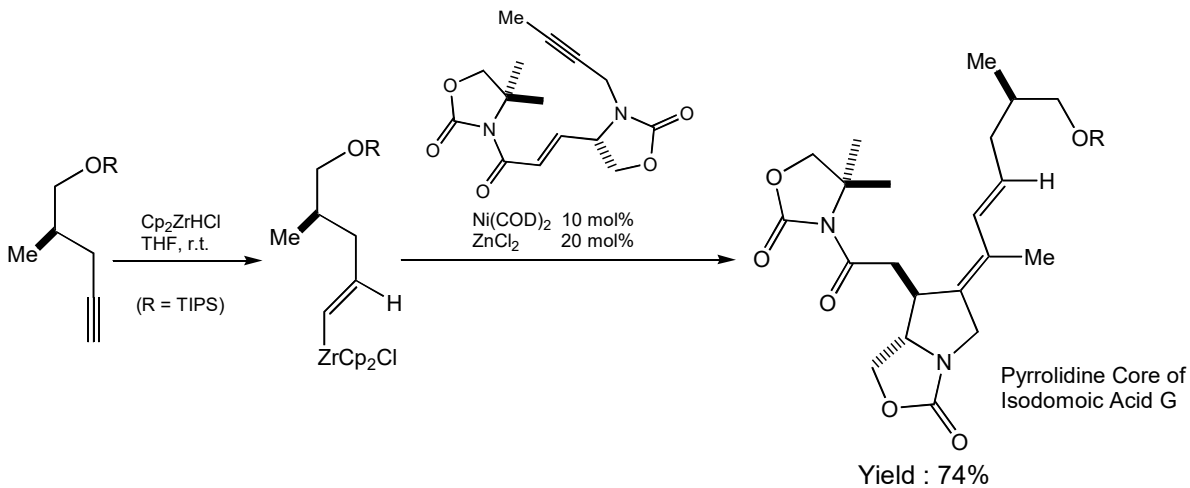
B. Cross Coupling via Hydrozirconation



J. Am. Chem. Soc., 99, (9), 3168 (1977)



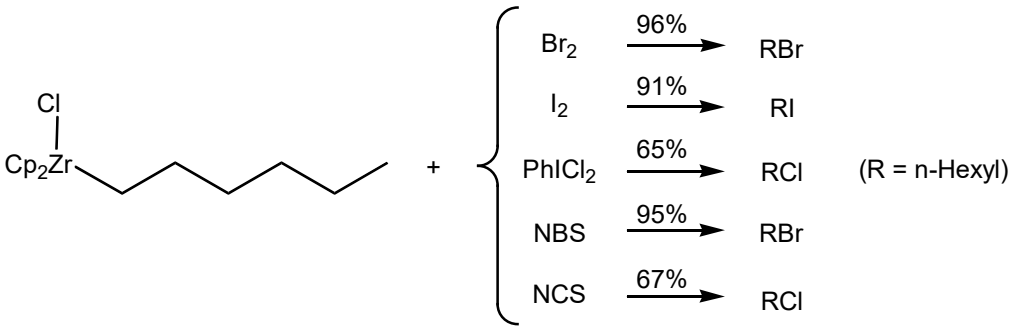
Org. Lett., 8, (17), 3675 (2006)

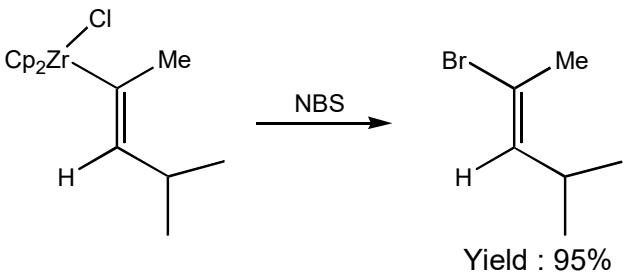


Org. Lett., 5, (20), 3771 (2003)

C. Reaction of Alkyl- and Alkenylzirconium Compounds

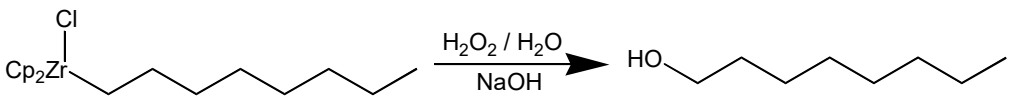
- Synthesis of Alkyl and Alkenyl Halides





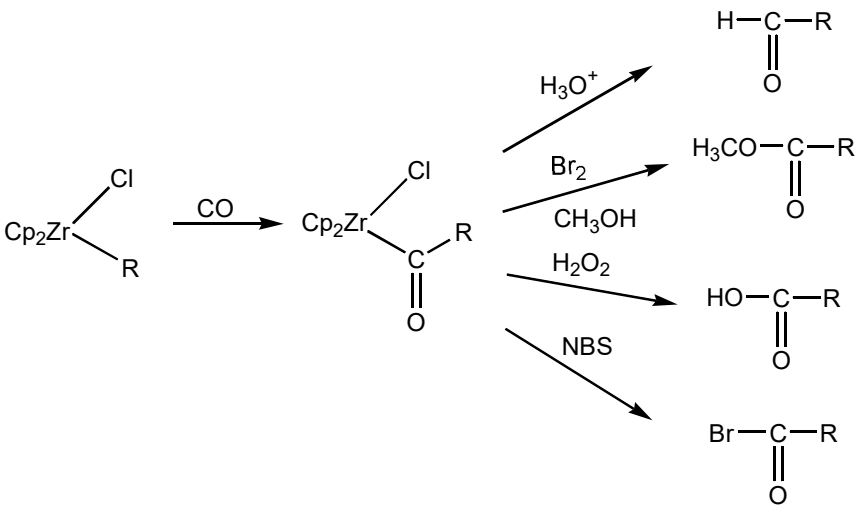
Yield : 95%

- Synthesis of Alcohols



Yield : 68%

- Insertion Reactions



Angew. Chem. Int. Ed. Eng., 15, 333 (1976)

■ The information in this document is as of December 2023.

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