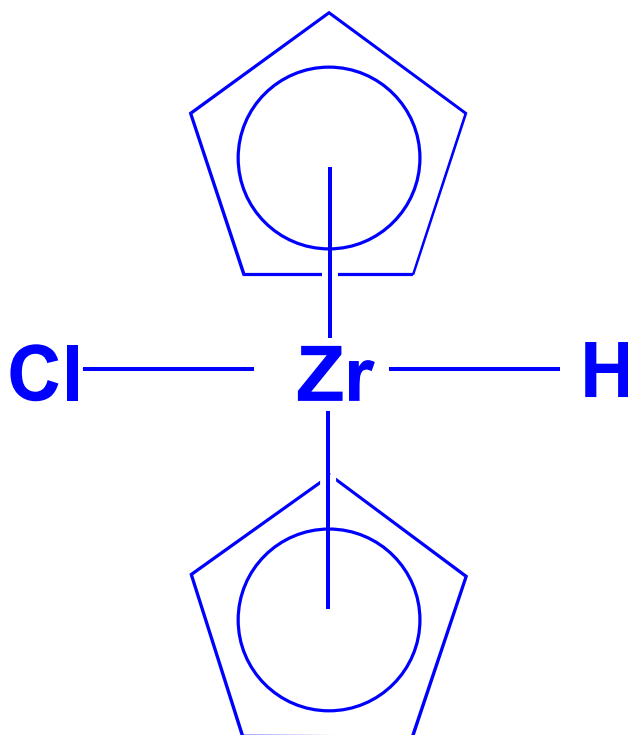


Zirconocene Chloride Hydride (Schwartz Reagent)

Technical Data



NICHIA CORPORATION

1. Product Guide

1-1. 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

Melting Point : No data available

Sublimation Point : No data available

Solubility : No data available

Decomposability : Zirconocene Chloride Hydride easily decomposes by the moisture in air to give $(Cp_2ZrCl)_2O$ and also gradually decomposes by the light.

1-2. Assay and Impurities

	Specifications	Typical data	Theoretical value
Zirconium (Zr)	$\geq 33.6\%$	34.4%	35.38%

Analytical data of Zirconocene Chloride Hydride

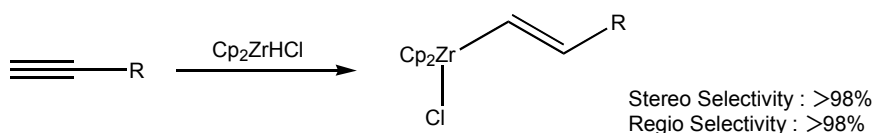
Suppliers	Zr(%) ^{*1}	Cl(%) ^{*1}	Zr/Cl (Molar ratio)	Notes	A reaction time of hydrozirconation with 3-Hexyne (min) @28 °C ^{*2}	A state of acid-hydrolyzed solution
Nichia	34.4	13.10	1.02	White powder	26	Clear
Reagent A	35.2	12.50	1.09	Pale pink powder	88	Insoluble solid remains
Reagent B	35.3	12.70	1.08	White powder	45	Insoluble solid remains
Reagent C	36.1	12.70	1.10	White powder	53	Insoluble solid remains
Reagent D	35.4	13.30	1.03	White powder	72	Insoluble solid remains Cloudy
Theoretical value	35.38	13.75	1.00			

*1 Zr and Cl contents were determined in Nichia.

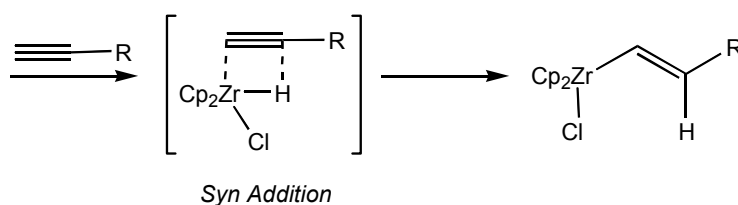
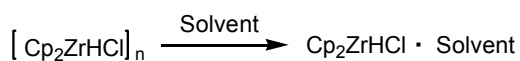
*2 The endpoint of the hydrozirconation reaction is signaled when the heterogeneous reaction mixture turns clear.

2. Application in Organic Synthesis

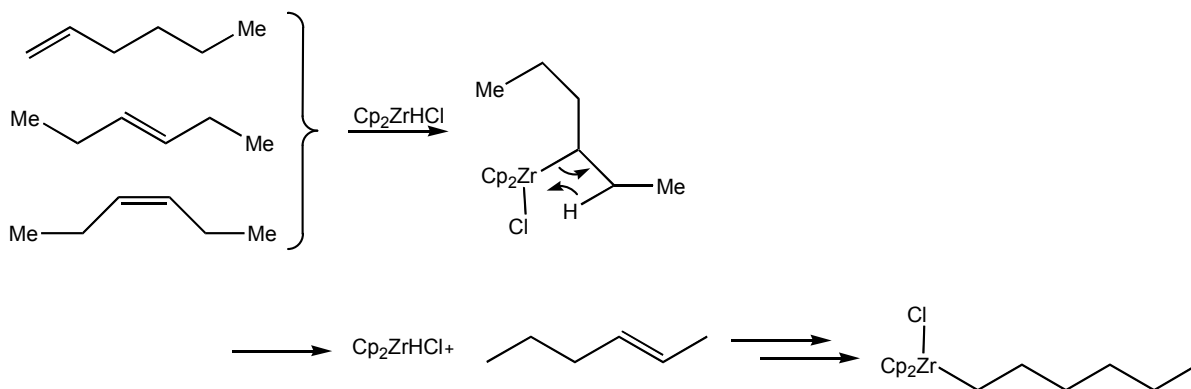
Hydrozirconation of Alkyne



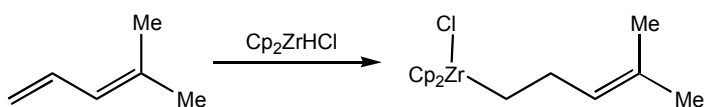
Mechanism



Hydrozirconation of Alkene



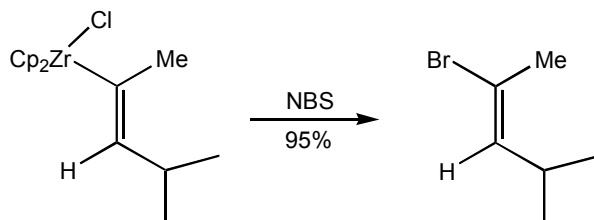
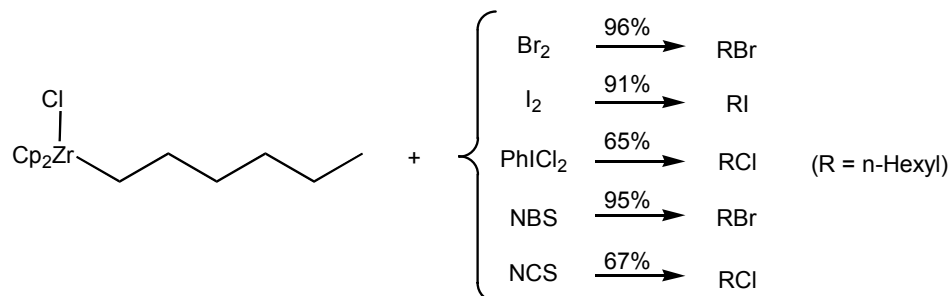
Hydrozirconation of Diene



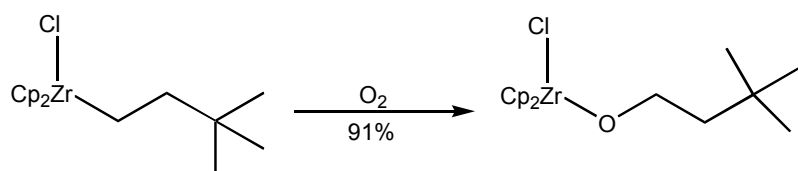
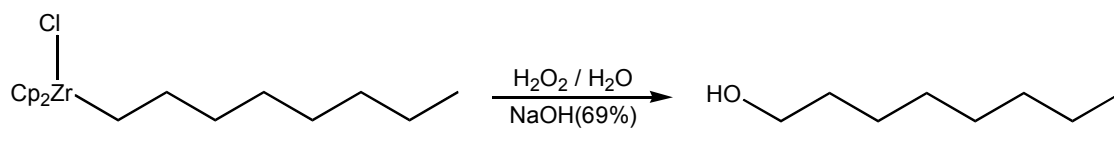
Jikkenkagaku 5th ed., 18, 254 (2004)

Reaction of Alkyl- and Alkenylzirconium Compound

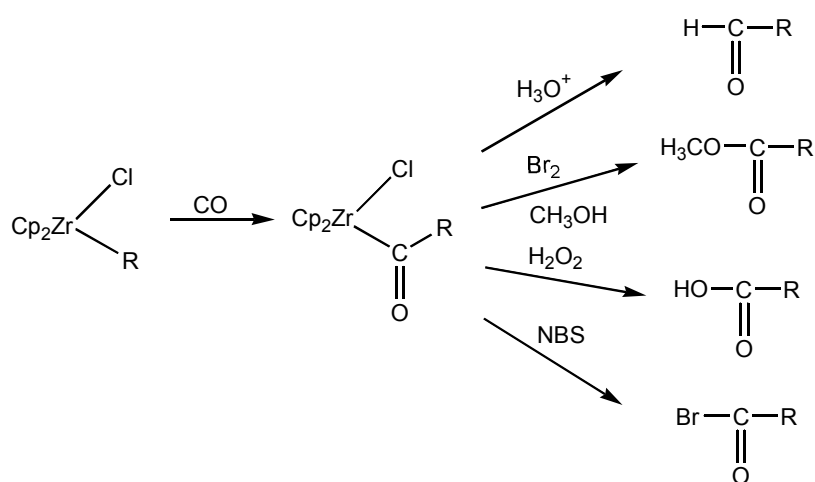
○ Synthesis of Alkyl and Alkenyl Halides



○ Synthesis of Alcohols

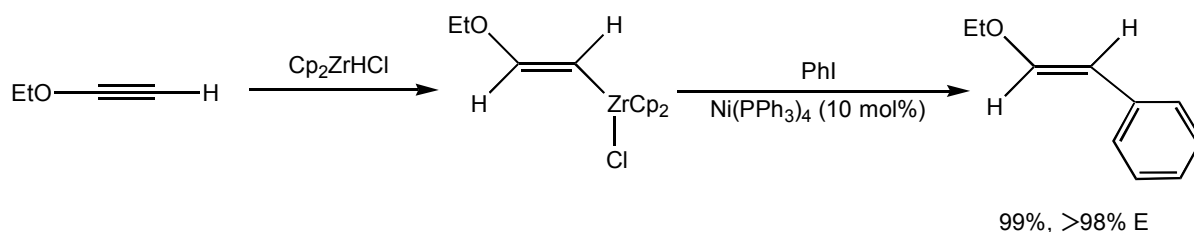
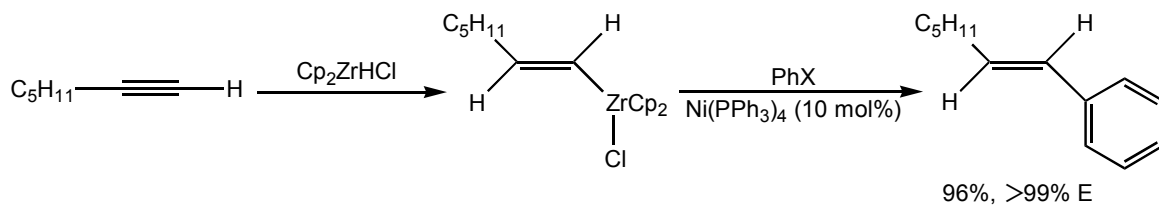


○ Insertion Reactions

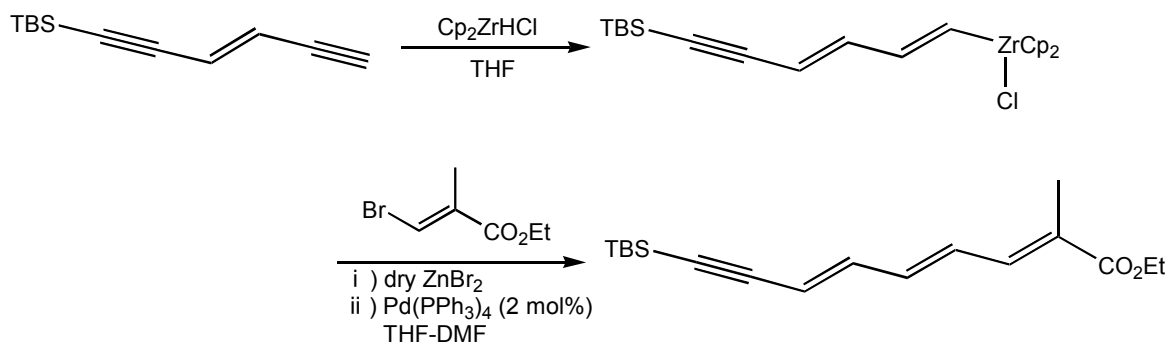


Angew. Chem. Int. Ed. Eng., 15, 333 (1976)

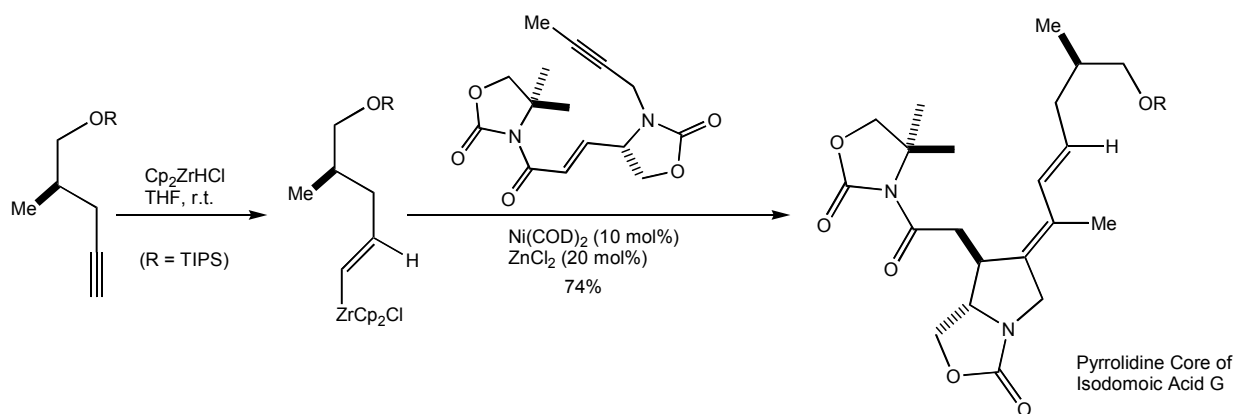
Pd- or Ni-Catalyzed Cross Coupling via Hydrozircononation



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

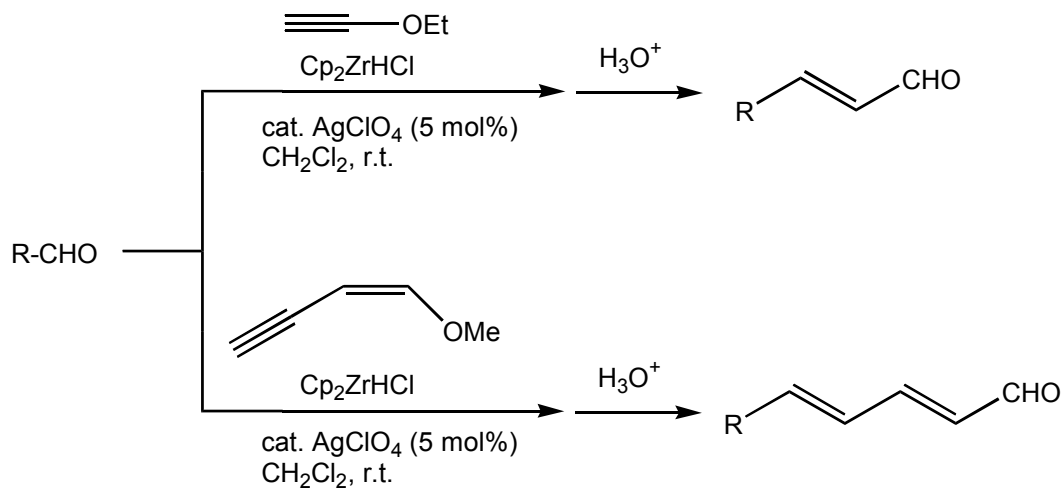


Org. Lett., **8**, (17), 3675 (2006)



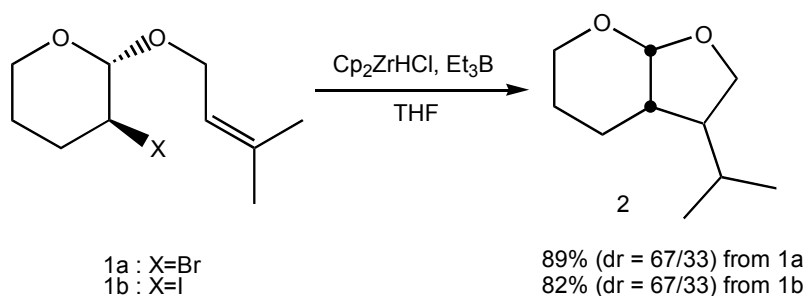
Org. Lett., **5**, (20), 3771 (2003)

Two- and Four-Carbon Homologation of Aldehyde by AgClO_4 -Catalyzed Addition of Alkoxyalkenylzirconocene Chloride

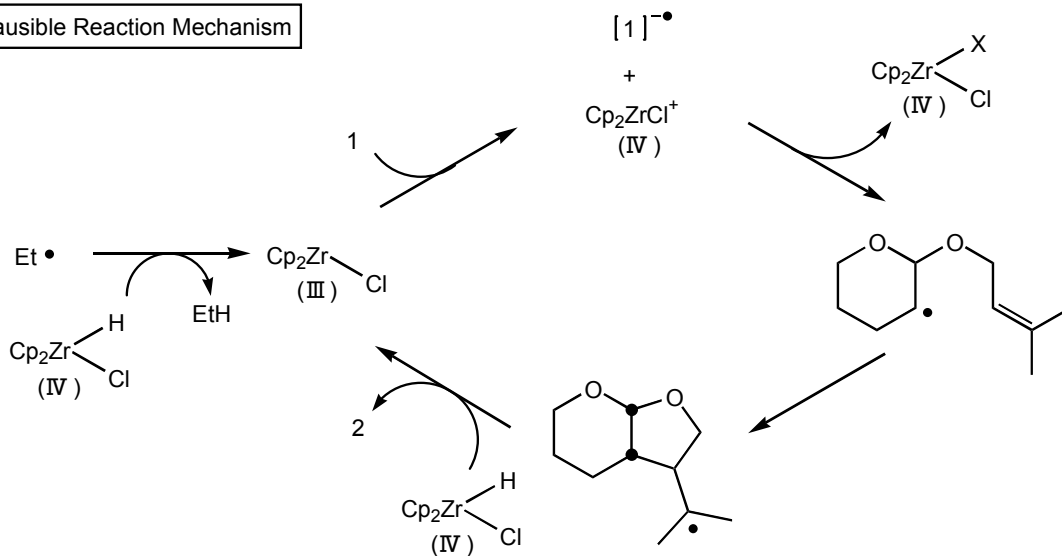


Tetrahedron, Lett., **34**, (2), 341 (1993)

Triethylborane-Induced Radical Reaction with Schwartz Reagent



Plausible Reaction Mechanism



J. Am. Chem. Soc., **123**, (13), 3137 (2001)

■ The contents of this brochure are updated as of March, 2010.

■ Reference

(The manufacturer & engineering department)

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