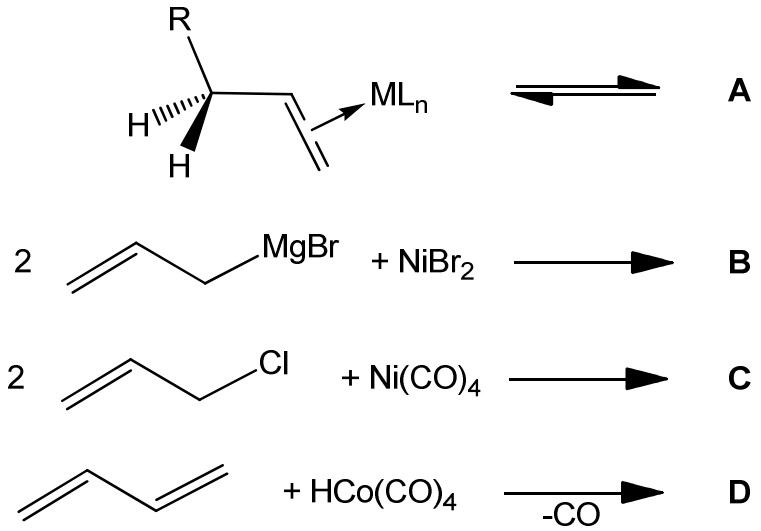
T5. OMCh Problems

1 Predict the products of the following reactions:



A: hydride allyl complex; B: homoleptic allyl complex, C: binuclear allyl complex, D: allyl complex, *syn* isomer.

a. Indicate the reaction type.

b. Compound B undergoes CO_2 insertion, describe the reaction product.

c. Indicate the differences in ^{1}H-NMR spectra for compound B and allylmagnesium bromide precursor.

VOE & OP, 2010

2 For the anionic allyl group

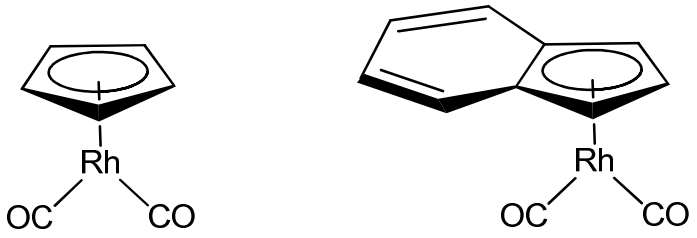
a. Draw the frontier orbitals.

b. Describe the coordination modes to metals.

c. Propose a mechanism for the fluxional behaviour of the palladium complexes.

3 Describe the synthesis, molecular structure and crystal packing of $[\eta^3\text{-}C_3H_5PdCl]_2$.

4 The following complexes undergo simple ligand substitution via an associative mechanism. Expalin why the rate for the indenyl complex is 10^8 greater than for the cyclopentadienyl analogue.



http://www.ilpi.com/organomet/cp.html

Rerek; Ji; Basolo, *JCS, Chem. Comm.* **1983**, 1208-9

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a. Describe the bonding modes for the pentadienyl ligand ($C_5H_7^-$).

b. Comment the structural data for the following bis(dimethylpentadienyl) metal complexes

Complex	refcode	M-C (pm)	M-centroid (pm)	M-plane (pm)	C-C (pm)	θ (º)
[**V**($Me_2C_5H_5$)$_2$]	COGXOL	216-224	163	152	138 - 142	86.8
[**Cr**($Me_2C_5H_5$)$_2$]	COGXUR01	214-218	160.0	151.9	137 - 140	80.6
[**Fe**($Me_2C_5H_5$)$_2$]	MEPEFE10	206-212	150 - 151	145 - 147	140 - 142	59.2
[**Ru**($Me_2C_5H_5$)$_2$]	HANYIE	216-221	164	158	133 - 144	50.3
[**Os**($Me_2C_5H_5$)$_2$]	GEPJEP	215-225	164 - 165	157 - 158	127 -148	48.5

c. Pentadienyl is a more strongly bound and more reactive ligand than cyclopentadienyl. Explain.

Additional problems

Crabtree, *The Organometallic Chemistry of Transition Metals, 4 ed,* Wiley, Hoboken, 2005. Chap. 5: 7, 9.

Douglas, McDaniel, Alexander *Concepts and Models of Inorganic Chemistry,* Wiley, New York, 1994. 13.4; 12.5.