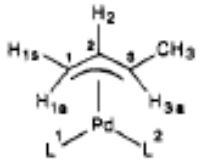
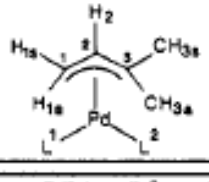
Organometallics **1987**, *6*, 620.

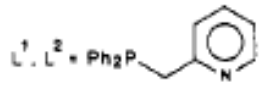
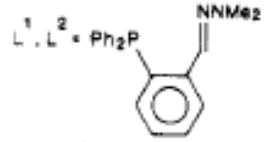
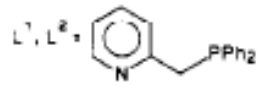
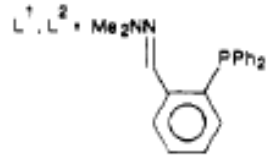
Table II. ^{13}C NMR Shifts for the η^3-Allyl Unit of (η^3-Butenyl)palladium(II) Complexes



		shifts, ppm			shift diff,
		C_1	C_2	C_3	$C_3 - C_1$
13	$L^1 = L^2 = CH_3NH_2$	56.1	116.45	74.9	19
14	L^1, L^2 = TMEDA	59.3	118.4	75.4	16
15	$L^1 = L^2$ = pyr	58.3	118.9	79.4	21
16	$L^1 = L^2 = (CH_3)_2CO$	57.05	114.2	79.5	22
17	$L^1 = L^2 = Cl^-$ (bridged)	58.3	111.4	81.5	23
18	$L^1 = L^2 = CH_3CN$	59.8	117.2	83.6	24
19	L^1, L^2 = diphos	65.6	122.8	92.0	26
20	$L^1 = L^2 = AsPh_3$	71.9	120.6	98.1	26
21	L^1, L^2 = COD	71.4	124.5	98.3	27
22	$L^1 = L^2 = PPh_3$	73.6	122.1	101.5	28
23	$L^1 = L^2 = P(OPh)_3$	68.05	123.2	102.0	34
24	$L^1 = PPh_3, L^2 = CN^-$	61.25	120.3	90.95	30
25	$L^1 = PBu_3, L^2 = Cl^-$	46.1	115.4	98.75	53
26	$L^1, L^2 = Ph_2PCH_2CH_2NMe_2$	48.1	119.9	99.4	51
27	$L^1 = PPh_3, L^2 = Cl^-$	56.3	116.95	99.6	43
28	$L^1 = P(OEt)_3, L^2 = Cl^-$	50.55	117.6	101.15	51
29	$L^1 = P(OPh)_3, L^2 = Cl^-$	51.8	117.25	101.5	50
30	$L^1 = PPh_3, L^2$ = py	54.2	120.35	101.5	47
31	$L^1 = P(OPh)_3, L^2$ = py	52.4	121.4	104.1	52
32	$L^1 = PPh_3, L^2 = CH_3CN$	55.0	119.55	105.4	50
33	$L^1, L^2 = Me_2NCH_2CH_2PPh_2$	77.6	124.0	71.2	−6

Table IV. ^{13}C NMR Shifts for the η^3-Allyl unit of Unsymmetrically Substituted (η^3-3-Methylbutenyl)Palladium(II) Complexes



		shifts, ppm			shift diff,
		C_1	C_2	C_3	$C_3 - C_1$
54	$L^1 = PPh_3$, $L^2 = CN^-$	56.9	113.6	107.4	51
55	$L^1 = CH_3NC$, $L^2 = Cl^-$	50.4	109.8	108.8	58
56	$L^1, L^2 =$ $Ph_2PCH_2CH_2NH_2$	46.5	111.6	112.65	66
57	$L^1 = PBu_3$, $L^2 = Cl^-$	42.3	108.4	114.5	72
58	$L^1 = PPh_3$, $L^2 = I^-$	57.9	111.4	115.0	57
59	$L^1 = PPh_3$, $L^2 = SCN^-$	≈56 (br)	110.9	115.2	59
60	$L^1, L^2 =$ $Ph_2PCH_2CH_2NMe_2$	43.6	111.2	115.2	72
61		45.3	111.7	115.3	70
62	$L^1 = PCy_3$, $L^1 = Cl^-$	41.9	107.7	115.5	74
63	$L^1 = PPh_3$, $L^2 = py$	50.0	112.6	116.2	66
64	$L^1 = PPh_3$, $L^2 = Cl^-$	52.2	110.2	116.5	64
65	$L^1 = PPh_3$, $L^2 =$ CH_3NC	59.1	114.0	117.5	58
66	$L^1 = P(OEt)_3$, $L^2 = Cl^-$	46.3	110.3	118.1	72
67	$L^1 = P(OMe)_3$, $L^2 = Cl^-$	46.3	110.4	119.0	73
68	$L^1 = P(OPh)_3$, $L^2 = Cl^-$	47.5	110.05	120.05	73
69	$L^1 = P(OPh)_3$, $L^2 = py$	47.55	113.0	120.35	73
70	$L^1 = PPh_3$, $L^2 =$ CH_3CN	50.8	112.2	122.7	72
71		44.7	111.6	123.0	78
72	$L^1, L^2 =$ $Me_2NCH_2CH_2PPh_2$	73.5	118.6	85.6	
73		73.3	118.8	86.2	
74		78.2	118.6	86.5	
75	$L^1, L^2 =$ $H_2NCH_2CH_2PPh_2$	67.8	116.5	88.3	

Scheme 1[a]

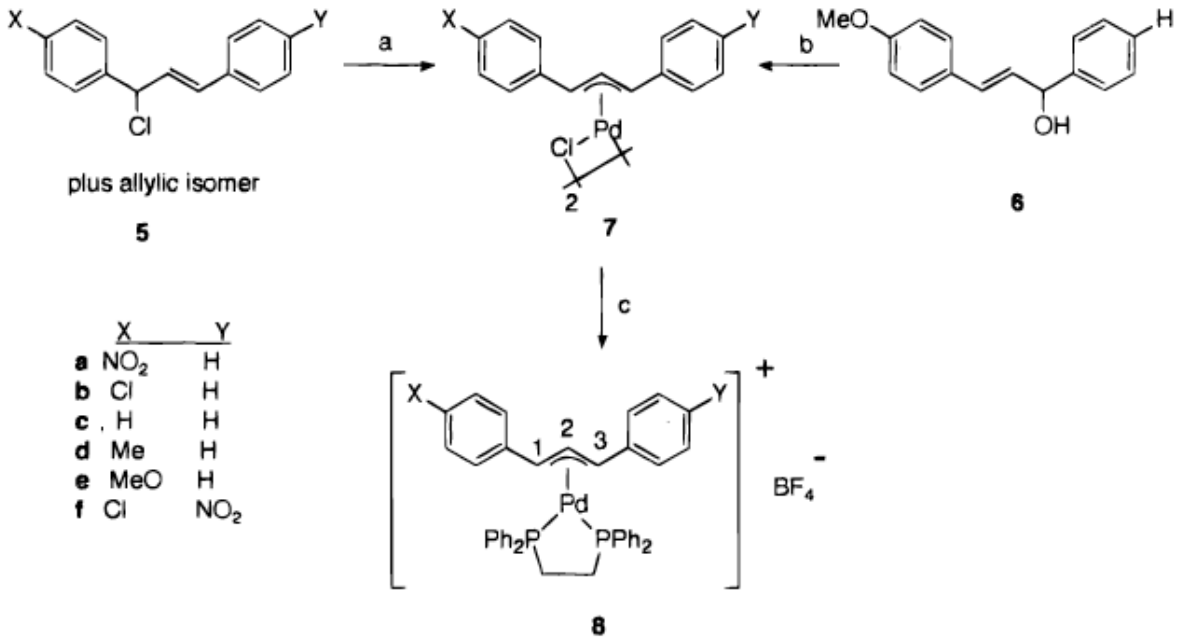
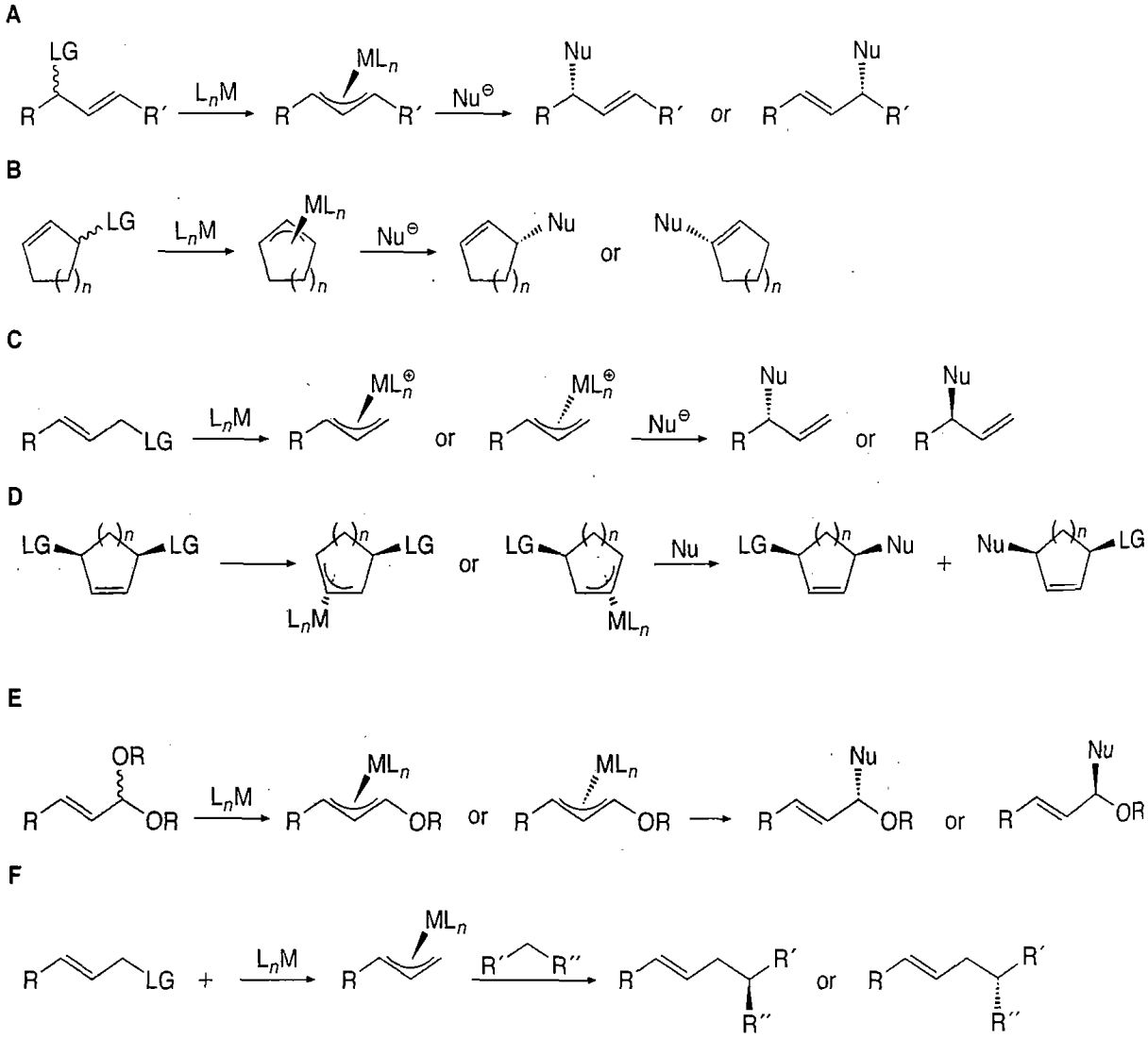


Table 1. ^{13}C NMR Chemical Shifts in δ Units ($CDCl_3$) of Allyl Carbon Atoms in Compounds 8a–f

8	X	Y	δ(C-1)	δ(C-2)	δ(C-3)
8a	NO_2	H	84.70	113.11	93.95
8b	Cl	H	88.17	111.78	91.14
8c	H	H	90.10	111.60	90.10
8d	Me	H	90.72	111.04	89.54
8e	MeO	H	91.45	110.32	88.90
8f	Cl	NO_2	91.84	113.75	85.41

Forms of Asymmetric Allylic Substitution Reactions



Scheme 20.10

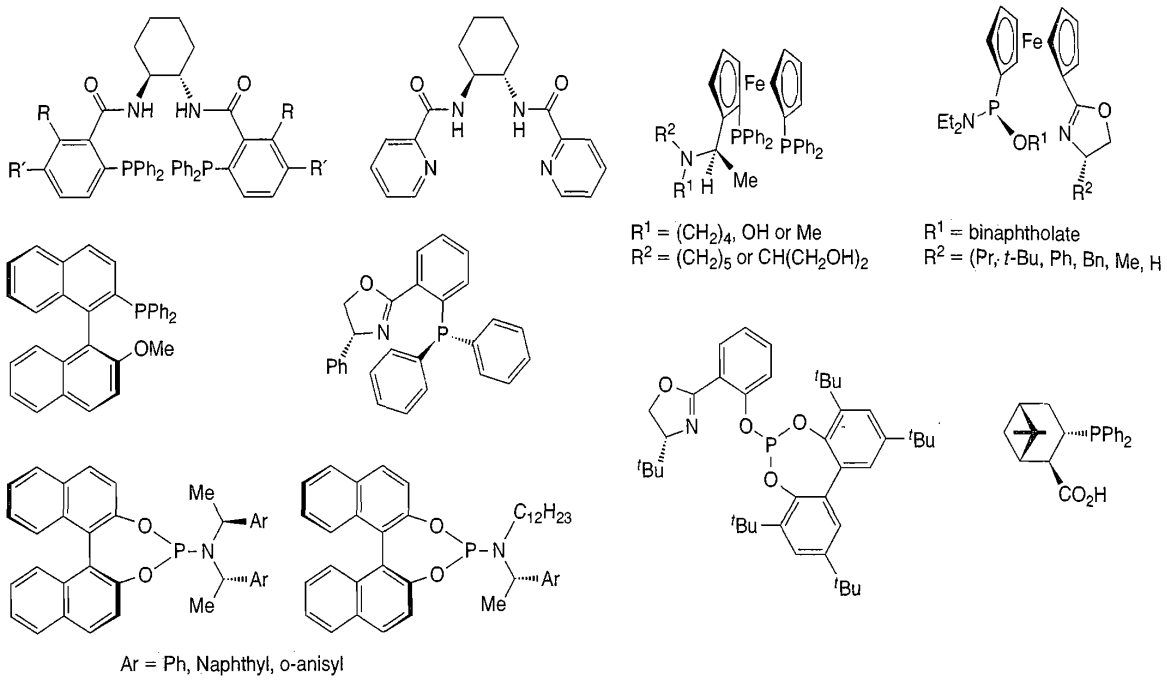


Figure 20.2.
Some of the ligands that generate highly enantioselective catalysts for allylic substitution with palladium, molybdenum, and iridium.