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Hornillos, Valentin; Perez, Manuel; Fananas-Mastral, Martin; Feringa, Ben L.

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Cu-Catalyzed Asymmetric Allylic Alkylation of Phosphonates and Phosphine Oxides with Grignard Reagents

Valentín Hornillos, Manuel Pérez, Martín Fañanás-Mastral, and Ben L. Feringa^{*[a]}

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NMR spectra of mechanistic studies:

Figure 1S. ³¹P-NMR spectra of the treatment of phosphine oxide **2f** with MeMgBr at -80°C in CD₂Cl₂

Figure 2S. ^{31}P -NMR spectra of the treatment of allyldiphenylphosphine oxide **11** with MeMgBr at r.t. in CD_2Cl_2

Figure 3S. ^{31}P -NMR spectra of the treatment of 2-methylbut-3-en-2-yl-diphenylphosphine oxide **12** with MeMgBr at r.t. in CD_2Cl_2

NMR spectra of new compounds

Small ¹H- and ³¹P NMR peaks are due to the presence of (Z)-isomer.

Small ^1H - and ^{31}P NMR peaks are due to the presence of (Z)-isomer.

Small ^1H - and ^{31}P NMR peaks are due to the presence of (*Z*)-isomer.

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Representative HPLC traces

PDA Ch1 217nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Area%
1	37.429	7962	224	0.000		M	0.453
2	40.957	1750773	34012	0.000		M	99.547
Total		1758735	34236				100.000

Pk #	Name	Retention Time	Area	Area Percent
1	Peak @ 29,740 Minutes	29,740	38784	1,984
2	Peak @ 31,300 Minutes	31,300	1916303	98,016
Totals			1955087	100,000

PDA Ch1 220nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Area%
1	19.041	4744518	134365	0.000		M	94.900
2	21.575	254969	7133	0.000		M	5.100
Total		4999488	141498				100.000

PK #		Name	Retention Time	Area	Area Percent
1	1		30,884	4876357	96,336
2	2		34,556	185459	3,664
Totals				5061816	100,000

Retention Time	Area	Area Percent
33,660	1023082	95,498
37,764	48231	4,502

1: 220 nm,
2 nm Results

Pk #	Name	Retention Time	Area	Area Percent
1	1	33,800	60126	4,871
2	2	37,828	1174121	95,129

PDA Ch1 236nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Area%
1	16.670	145655	5476	0.000		M	21.330
2	17.545	537212	15759	0.000		M	78.670
Total		682867	21235				100.000