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Stereo- and Regio-Selective Synthesis of Silicon-Containing Diborylalkenes via Platinum-Catalyzed Mono-Lateral Diboration of Dialkynylsilanes

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A highly chemoselective platinum-catalyzed mono-lateral diboration of dialkynylsilanes for the construction of silicontethered alkynyl diborylalkenes is described, in which the tris(4methoxyphenyl)phosphine was found to be an effective ligand for *cis*-addition of diboron agent to the silicon-tethered alkynes, and the chiral ligand (AFSi-Phos) -mediated diboration of dialkynylsilanes resulted into desymmetric construction of siliconstereogenic center in promising enantioselectivity.

The organoboron compounds have been widely applied in organic and medicinal chemistry as building $block^1$ due to their versatile reactivity.² Especially, the alkenylboron compounds are valuable synthon for varied natural product³ and electronic materials.⁴ In this context, the transition-metal-catalyzed boration of alkynes is one of facile approaches to access alkenylboron compounds, including diborylalkenes, that are essential elements in functional materials and crucial intermediate for multisubstituted alkenes, bioactive compounds, and π -conjugated materials.⁵ Over the past years, transition-metal-catalyzed boration and diboration reactions of alkynes have been extensively studied, in which the borylation of internal and terminal alkynes with B₂pin₂ could be achieved with defined regio- and stereochemistry (Figure 1a).⁶

Although catalytic diboration of alkynes with *cis*-selectivity is well established, the discovery of a new catalyst can enhance the synthetic efficiency of the boration and provide alternative approach to the construction of structurally diverse organoboron compounds. Based on our previous studies on silicon-mediated organic synthesis (SiMOS),⁷ we are interested in the catalytic synthesis of silicon-containing diborylalkenes and alkynes that have potential capability of transformation into various organosilicon

compounds and as highly versatile substrate sources for the transformation of another alkynes to the construction of cyclic ring structures.^{8,9} To the best of our knowledge, there are no reports about mono-lateral diboration of dialkynlsilanes. Herein we document a highly stereo- and chemoselective synthesis of silicon-containing diborylalkenes via platinum-catalyzed mono-lateral diboration of dialkynlsilanes. The pronunced ligand effect and DFT calculations suggest that diboration reactions initiated by oxidation of the B-B bond to Pt and the rate-determining step is found to be phosphine dissocaitaion step.



Figure 1 The synthesis of silicon-tethered alkynyl diborylalkenes through mono-lateral diboration of dialkynylsilanes

We started our investigations with the reaction of di(hex-1-yn-1-yl)(methyl)(phenyl)silane (1a) and B_2pin_2 (2a) with Pt(dba)₃ as catalyst. After screening of various phosphine ligands, the desired mono-lateral diboration product **3a** was accessed at 78% yield in the presence of triphenylphosphine (Table 1, entry 9). And then the best ligand was identified as tris(4-methoxyphenyl)phosphine, which gave the desired *cis*-addition diborylalkene **3a** in 83% yield with >99:1 c.r. and 99:1 Z/E (Table 1, entry 14). Other phosphine ligands, such as XantPhos, SPhos, DPEPhos, XPhos, JohnPhos and phosphine ligands **L1-L3** evaluated in this work, were found to be no activities that totally suppress the reaction. Therefore, only the triphenylphosphine and its derivatives that have a donor group at

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para-position of phenyl ring were suitable P-ligand in this transformation (Table 1, entries 9 and 13-14). Notably, we did not determine formation of **4a** that theoretically generated by double diboration of **1a** with 2 eq. of B_2pin_2 , which revealed the good chemoselectivity of Pt/P(4-MeOPh)₃ in this reaction. In addition, the structure of **3a** was determined by COSY and NOE spectra, which signified the process of *cis*-addition across the reaction.

Table 1 Screen of ligands in the Pt-catalysed diboration of Si-linked bisalkyne ${f 1a}^a$								
n-Bu Si	B ₂ pin ₂ (1.2 eq) Pt(dba) ₃ (3 mol %) Ligand (3 mol %) Tol, 50 °C, 20 h	n-Bu 3	nBu Bpin + Bpin a	Bu n-Bu Si Bpin Bpin Bpin 4a				
Entry	ligand	3a/4a ^c	Yield (%) ^b	Z/E ^c				
1	XantPhos	-	n.r.	-				
2	RuPhos	-	n.r.	-				
3	t-Bu₃P·HBF₄	-	n.r.	-				
4	JohnPhos	-	n.r.	-				
5	XPhos	-	n.r.	-				
6	DPENPhos	-	n.r.	-				
7	Cy ₃ P·HBF ₄	-	n.r.	-				
8	SPhos	-	n.r.	-				
9	PPh ₃	>99:1	78	97/3				
10	L1	-	n.r.	-				
11	L2	-	n.r.	-				
12	L3	-	n.r.	-				
13	P(p-toyl) ₃	>99:1	72	98/2				
14	P(4-MeOPh)₃	>99:1	83	99/1				

^o**1a** (0.1 mmol), B₂pin₂ (0.12 mmol), catalyst and ligand (3 mol %) and solvent (1 mL) at 50 °C for 20 h. ^b Yields are determined by GC. ^cThe c.r. (**3a/4a**) and the ratio of Z/E were determined by GC-MS and confirmed by ¹H-NMR.



We next explored the catalytic activity of other transition-metal complexes in the presence of tris(4-methoxyphenyl)phosphine. Interestingly, the corresponding Pt(dba)₃ complexes with P(4-MeOPh)₃ was the only effective catalyst for the highly chemoselective mono-lateral diboration of Si-linked bisalkyne **1a**, and other metal complexes, e.g., [Rh(COD)Cl]₂, Pd₂(dba)₃, [Pd(η^3 -C₃H₅)Cl]₂, [Ir(COD)Cl]₂ and [Ru(*p*-cymene)Cl]₂ were ineffective in this reaction (Table 2, entries 1-5). These results suggested that the oxidative addition of B-B bond to Pt is expected to be favored over other metal catalysts. Based on these preliminary findings that the Pt/P(4-MeOPh)₃ was a suitable catalyst, the effect of solvents on diboration revealed that toluene was superior to other solvents, whereas other solvents involved polar and non-polar solvents lowered yield or totally inhibited the reaction (Table 1, entries 6-11).

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In addition, running the reaction at 100 °C or 80_{Vi} c, $ked_{le}t_{9ni}$ p increased yield with 90% or 95% respectively (7ab 2, 6nt 13 and 14).

 Table 2 Optimization studies on the optimization of reaction parameters

n-Bu	B2pin2 (1.2 eq Catalyst (3 mol r-Bu P(4-MeOPh) ₃ (3 r Solvent, T, 20	l) %) <u>nol %)</u> I h <i>n</i> -Bu∕	Si Bpi 3a	Bpin Bpin	n-Bu Si Bpin Bpin 4a	pir
Entry	Catalyst	Solvent	Т	Yield	Z/E ^c	
			(°C)	(%)		I.
1	[Rh(COD)Cl] ₂	Toluene	50	n.r	-	
2	Pd ₂ (dba) ₃	Toluene	50	n.r	-	
3	$[Pd(\eta^{3}-C_{3}H_{5})Cl]_{2}$	Toluene	50	n.r	-	
4	[Ir(COD)CI] ₂	Toluene	50	n.r	-	
5	[Ru(p-cymene)Cl] ₂	Toluene	50	n.r	-	
6	Pt(dba)₃	EA	50	63	99/1	
7	Pt(dba)₃	DCM	50	n.r	-	
8	Pt(dba)₃	THF	50	32	99/1	
9	Pt(dba)₃	CH₃CN	50	trace	-	
10	Pt(dba)₃	Hexane	50	n.r	-	
11	Pt(dba)₃	Toluene	60	73	99/1	
12	Pt(dba)₃	Toluene	80	91	98/2	
13	Pt(dba)₃	Toluene	100	90	97/3	
14	Pt(dba)₃	Toluene	80	95(88) ^d	99/1	

^{*a*} **1a** (0.1 mmol), B₂pin₂ (0.12 mmol), catalyst and ligand (3 mol %) and solvent (1 mL) at 50 °C for 20h. ^{*b*} Yields are determined by GC. ^{*c*} Determined by GC-MS and confirmed by ¹H-NMR. ^{*d*} Both the catalyst and ligand are 2 mol % in solvent (0.5 mL), isolated yield is in parentheses.

With the established optimal conditions in hand, we investigated the substrates scope of mono-lateral diboration using a variety of Si-linked bisalkynes 1a-1s bearing various substituted groups at the aromatic ring or silicon center. As shown in Scheme 1, the substrates 1a-1I that with varied substituents on the phenyl ring reacted with B₂pin₂ efficiently to afford desired products in high yields (76-90%) with >99:1 c.r. and high Z/E ratio (>99:1). When electron-donating group (1c) on the para-position of phenyl rings attached on silicon center, an improved yield was obtained (90% yield for 3c). And the electron-withdrawing substituents would slightly inhibit the reaction (76% yield for 3I). In fact, the variation of alkyl substituents on phenyl group and alknyl group linked to the silicon center did not play crucial role in this reaction. However, when the introduction of phenylethyny and tert-butyl group at the terminal alkyne and Si-center respectively, corresponding products were obtained with decreased yields (43% yield for 3q and 55% yield for 3r), which suggested the important role of steric repulsion and electronic effect during the coordination of alkyne with Pt catalyst for the formation of a π -complex.

Based on our previous work on the enantioselective construction of silicon-stereogenic organosilicon compounds,¹⁰ we envisaged that chiral P-ligand can make a promising enantioselective induction in the desymmetrization of Si-linked alkynes to give alkynyl Sistereogenic organoboron compounds. Then we screened various chiral P-ligands under the optimized reaction conditions (Scheme 2 and see Table S5 and Table S6 in Supporting Information). It was proved that the desymmetrization of prochiral Si-centered

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dialkynlsilanes was not an easy task at present. After extensive screening of chiral P-ligands, we found that only our Ar-NNPs¹¹ and its derivatives¹² could be worked as an effective P-ligand to give promising enantiomeric excess for the desired product *Z*-**3a** or *E*-**3a'** (up to 73.5:26.5 *er*). And more importantly, the bulkyl and chiral P-ligand could cause *trans*-addition of diboration to give unusal *E*-**3a'** in moderate yield (Scheme 2). The DFT calculations for the Pt-catalyzed diboration could provide useful information for the unexpected diboration of Si-linked bisalkyne with *E*-selective conversion.



Scheme 1 Substrates of scope. Reaction conditions: 1 (0.1 mmol), 2a (1.2 equiv), Pt(dba)₃ (2 mol %), P(4-MeOPh)₃ (2 mol%), 20 h, 80 °C. Isolated yields were achieved from flash column chromatograph.

On the basis of the experimental results and DFT calculations (See ESI, Figure S1-S5) 1-for the platinum-catalyzed diboration of alkynes,^{6,13} we proposed a plausible catalytic cycle for the reaction (Figure 2, path A is expected to be favored over path B). The adduct **C1** derived from the reaction of **2a** and species **O1** generated from association of Pt(dba)₃ with phosphine ligand was expected to react with alkynyl moiety of **1a** selectively, which led to intermediate **D1** or **E1** that possibly diverge into *Z*- or *E*-configuration intermediate impacted by the bulkyl P-ligand. Finally, the reductive elimination of intermediate **F1** gave the desired product and Pt species **O1**. In this regard, the mechanistic process gave important information that the desymmetrization of prochiral dialkynylsilanes is not an easy



Scheme 2 Preliminary results for the enantioselective construction of siliconstereogenic center via desymmetric platinum-catalyzed mono-lateral diboration of prochiral **1a** with B₂pin₂.



Figure 2 Proposed catalytic cycle for Pt-catalyzed diboration of Si-linked bisalkynes.



Figure 3 The energy profile [kcal/mol] for P-ligated Pt Catalyst [PtL1] of reaction. The energy of A, B and P-ligated Pt complex [PtL1] is set to be relative zero reference (Also see Figure S1-S5 and Table S9-S12 of Supporting information).

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task because the energy profile for the formation of (S)-isomer and (*R*)-isomer is very close (see Figure 3, 9.0 kcal/mol versus 8.7 kcal/mol). In addition, the steric repulsion of chiral phosphine ligand **L6** plays an essential role. The *trans*-adducts **3a'** shown in Scheme 2 could be produced through isomerization of η^2 -vinyl Pt-complex (**E1** or **E2**) due to the less sterically hindrance between the Bpin-Pt-L6 and the other Bpin moiety in comparison to that of *cis*-addition process The steric effect was also supported by the experiment results that phosphine ligands (**L3**, **L5** and **L6**) bearing a bulky group produced *E*-isomer with high E/Z ratio (up to 44/56) that has never been reported in previous literatures.⁶

In summary, we have developed a novel platinum-catalyzed mono-lateral diboration of prochiral Si-linked dialkynylsilanes with B₂pin₂. It was found that the employment of a monophosphine ligand P(4-MeOPh)₃ led to facile synthesis of a series of siliconcontaining diborylalkenes in high yields with good stereo- and Preliminary studies regioselectivities. suggested that enantioselective construction of silicon-stereogenic Si-linked diborylalkenes via this platinum-catalyzed mono-lateral diboration of prochiral dialkynylsilanes is a challenging task, in which our new AFSi-Phos gave the best enantioselectivity. Further work on the exploration of conceptually new ligand for the enantioselective diboration of alkynes is currently in progress.

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Conflicts of interest

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There are no conflicts to declare.

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