Electrical Supplementary Information (ESI)

First example of a heterobimetallic ‘Pd–Sn’ catalyst for direct activation of alcohol: Efficient allylation, benzylolation and propargylation of arenes, heteroarenes, active methylenes and allyl-Si nucleophiles

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S-1. Study for substrate catalyst interaction

(a) Experimental procedure to study and observation for the interaction of alpha-allyl benzyl alcohol with [Pd-Sn] by $^1$H NMR

To see the initial activation the spectrum of alpha-allyl benzyl alcohol 2b (1.4 mg, 0.01 mmol) was recorded in C$_6$D$_6$ solvent at room temperature in the absence as well as in the presence of catalyst 1a (4.75 mg, 0.01 mmol). In the absence of catalyst 1a the alcohol 2b shows an unresolved broad singlet at 4.86 ppm for allylic proton and a singlet at 1.21 ppm for -OH proton. Upon addition of the catalyst 1a, the initial broad singlet of the allylic -CH proton of 2b was converted to a well resolved doublet ($J=$5.6 Hz) at 5.45 ppm, while the peak for -OH proton almost vanishes.
(b) Procedure for the In situ $^{13}$C NMR study

$^{13}$C NMR of cinnamyl alcohol/benzyl alcohol was recorded at room temperature in the absence as well as in the presence of 1 eqv. of catalyst 1a with respect to alcohol in CDCl$_3$.

![NMR spectra](image1)

S-2. Reaction of Vinylsilane: Formation of reduced product (E)-1,3-di(p-tolyl)prop-2-en (5)

A mixture of allyl alcohol 2f (1 mmol), vinyltrimethylsilane (2 mmol), and [Pd(COD)Cl(SnCl$_3$)] (2 mol %) in 2 mL of nitromethane was stirred at 85 °C for 1 hr. After that the reaction mixture was concentrated and purified by column chromatography to give 40% yield of 5.

![Reaction schematic](image2)
S-3. Spectra of complexes and alkylated products

$^1$H and $^{13}$C spectra of catalyst 1a
DEPT spectra of catalyst 1a
$^1$H and $^{13}$C spectra of catalyst 1b
$^{31}$P spectra of catalyst 1b

$^{31}$P NMR

Pd($\text{PPh}_3)_2\text{ClSnCl}_3$
$^1$H and $^{13}$C spectra of compound 4b'}
DEPT spectra of compound 4b′
$^1\text{H}$ and $^{13}\text{C}$ spectra of compound 4f and 4f'

![NMR Spectra](image-url)
$^1$H and $^{13}$C spectra of compound 4h and 4h'
DEPT spectra of compound 4h and 4h'
$^1$H and $^{13}$C spectra of compound 4j
$^1$H and $^{13}$C spectra of compound 4k
DEPT spectra of compound 4k
$^1$H and $^{13}$C spectra of compound 4l
DEPT spectra of compound 4l
$^1$H and $^{13}$C spectra of compound 4o
$^1$H and $^{13}$C spectra of compound 4t
$^1$H and $^{13}$C spectra of compound 4v
DEPT of compound 4v
$^{1}\text{H}$ and $^{13}\text{C}$ spectra of compound 4z