

Supporting Information

Development of Silica Supported Frustrated Lewis Pairs: Highly Active Transition Metal-Free Catalysts for Z-Selective Reduction of Alkyne

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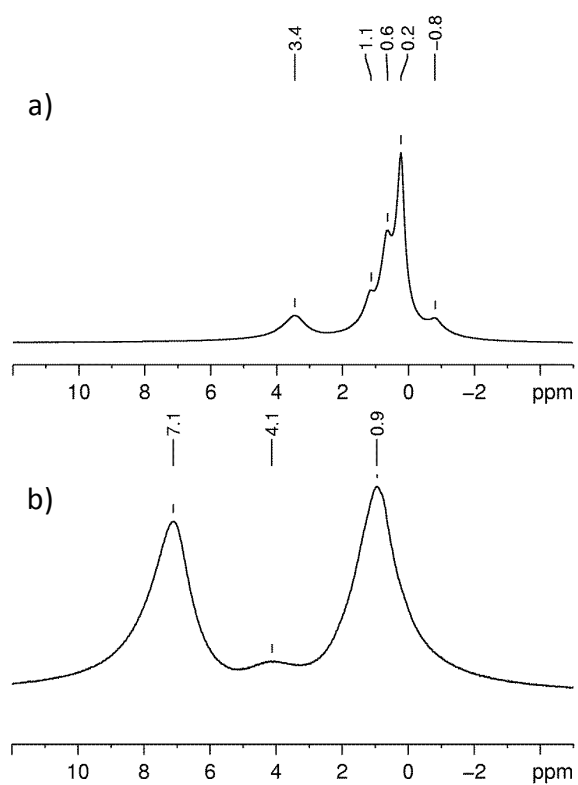


Figure S1. ^1H MAS NMR (500 MHz, 8 scans, relaxation delay of 5 s, 10 kHz spinning speed) spectra of **1** (a) and **2** (b).

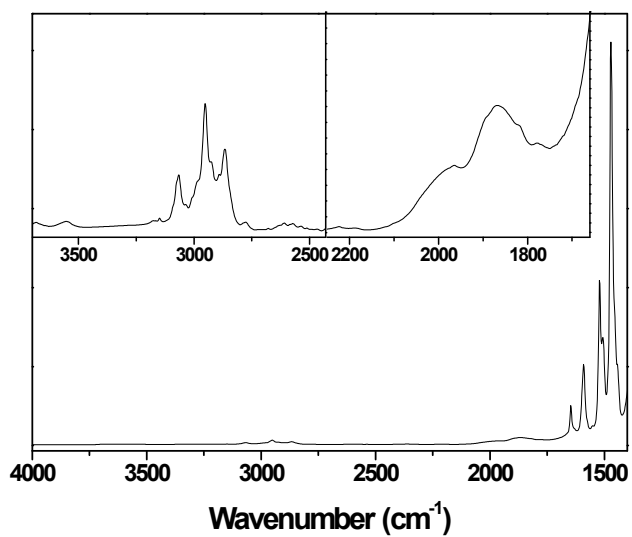


Figure S2. DRIFT spectrum of **3b**.

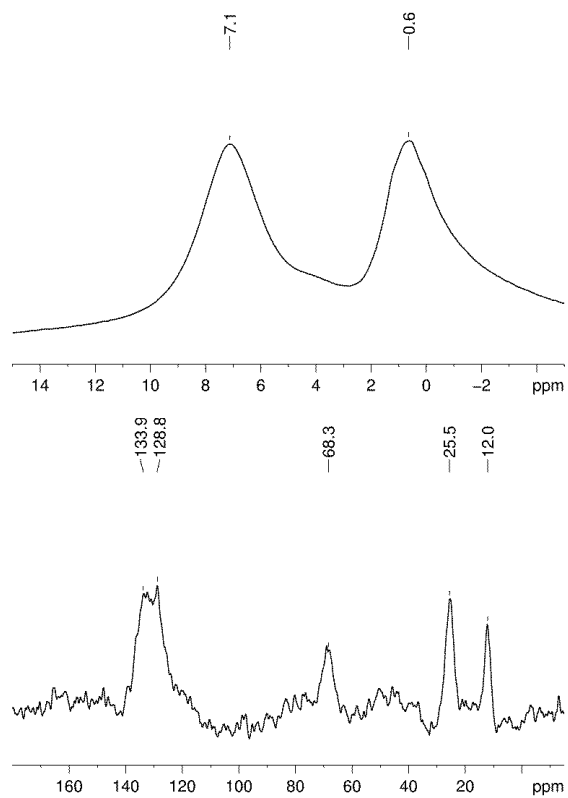


Figure S3. ^1H MAS (500 MHz, 8 scans, relaxation delay of 5 s, 10 kHz spinning speed) and ^{13}C CP/MAS (125.7 MHz, 30000 scans, relaxation delay of 5 s, 10 kHz spinning speed) NMR spectra of **3a**.

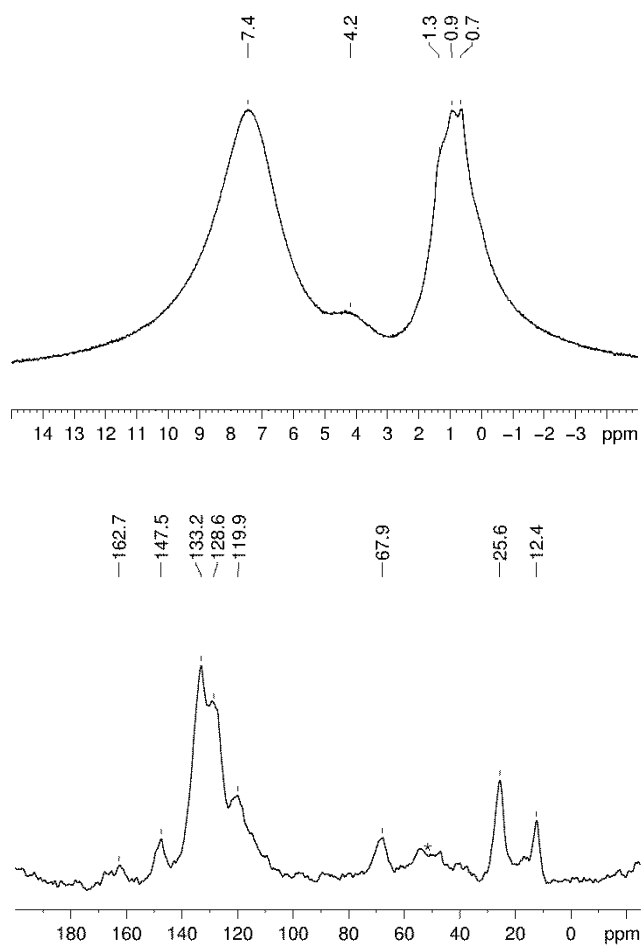


Figure S4. ^1H MAS (500 MHz, 8 scans, relaxation delay of 5 s, 10 kHz spinning speed) ^{13}C CPMAS NMR (125.7 MHz, 30000 scans, relaxation delay of 5 s, 10 kHz spinning speed) spectra of **3b**.

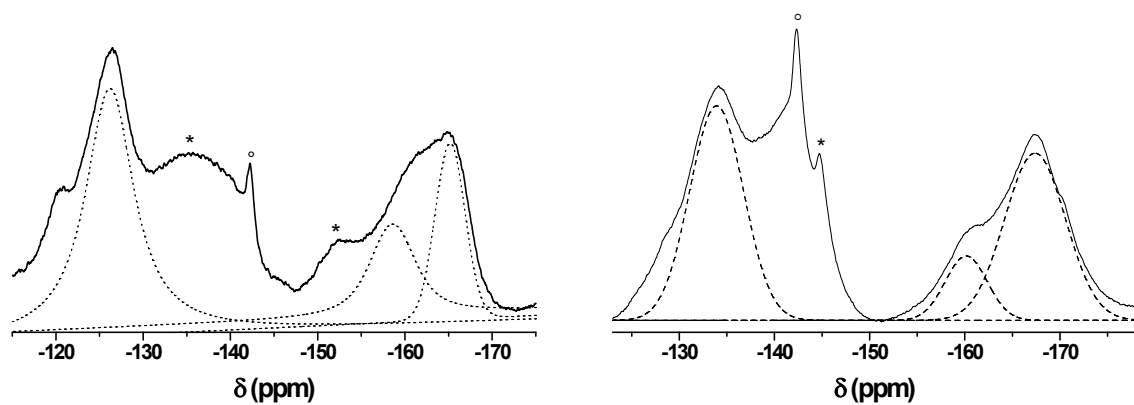


Figure S5. ^{19}F MAS NMR (476.5 MHz, 64 scans, relaxation delay of 5 s, 12 kHz spinning speed) spectra of **3a** (left, dotted curves represent deconvoluted peaks) and **3b** (right, dashed curves present deconvoluted peaks), spinning side bands (*) were determined by changing the spinning rate (7 kHz, 10 kHz), "o" corresponds to signal from Krytox[®] vacuum grease (DuPont).

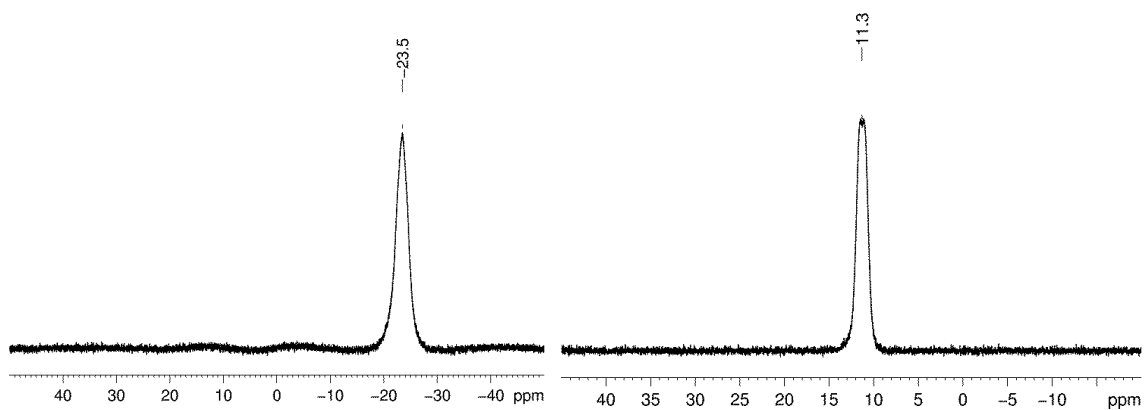


Figure S6. ^{11}B NMR spectrum (left) and ^{31}P NMR spectrum (right) of $\text{PPh}_3\cdot\text{HB}(\text{C}_6\text{F}_5)_2$ in C_6D_6 .

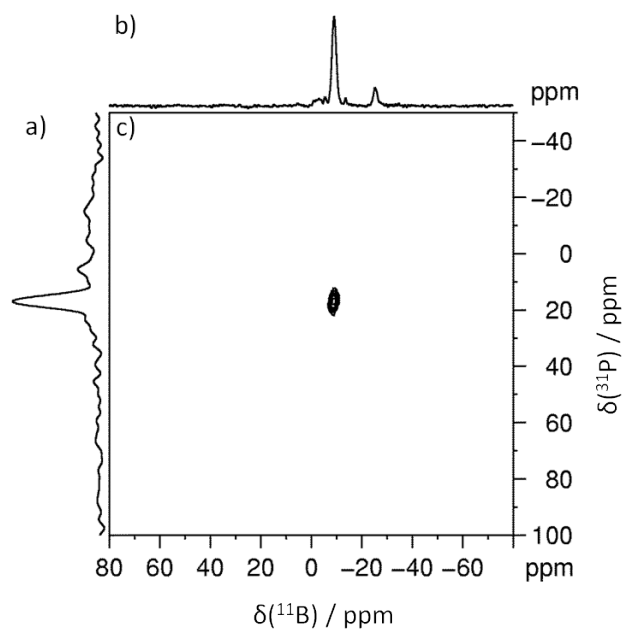
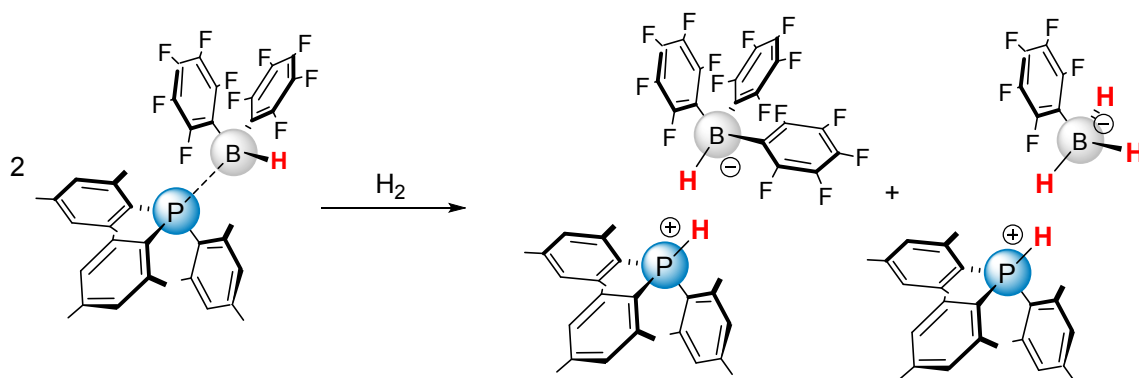


Figure S7. MAS-D-HMQC experiment of **3b** to a pair of nuclei $\{^{11}\text{B}, ^{31}\text{P}\}$



Scheme S1. Restructuration of $[\text{HB}(\text{C}_6\text{F}_5)_2]\cdot[\text{PPh}_3]$ in solution after hydrogen addition.

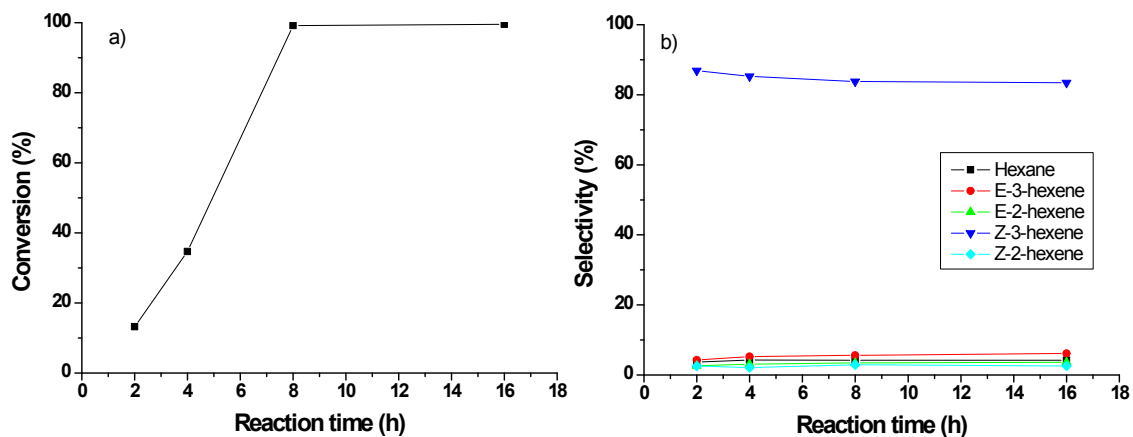


Figure S8. Kinetic study of the conversion of 3-hexyne at 10 bar hydrogen, 80 °C and 2 mol% of **3a** in pentane.

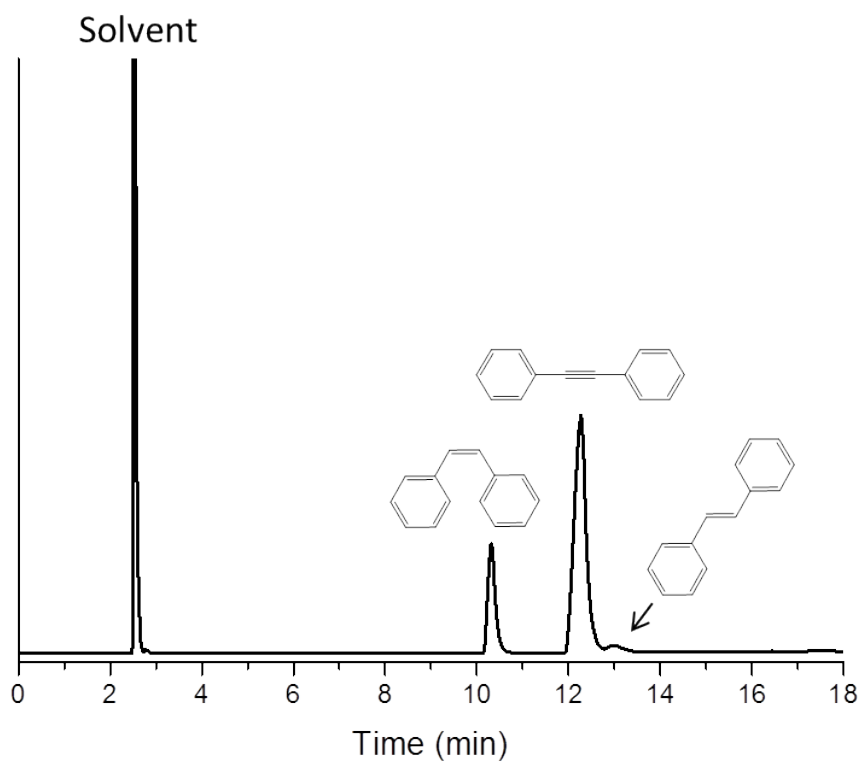


Figure S9. GC chromatogram of the hydrogenation of a) 1,2-diphenylethyne.

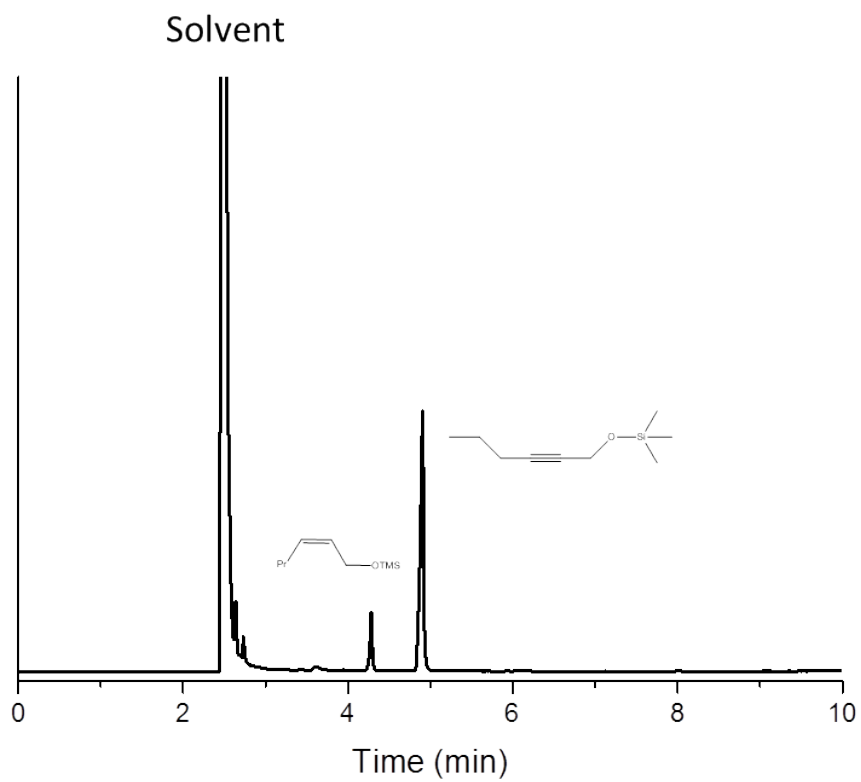


Figure S10. GC chromatogram of the hydrogenation of b) (hex-2-yn-1-yloxy)trimethylsilane.

Solvent

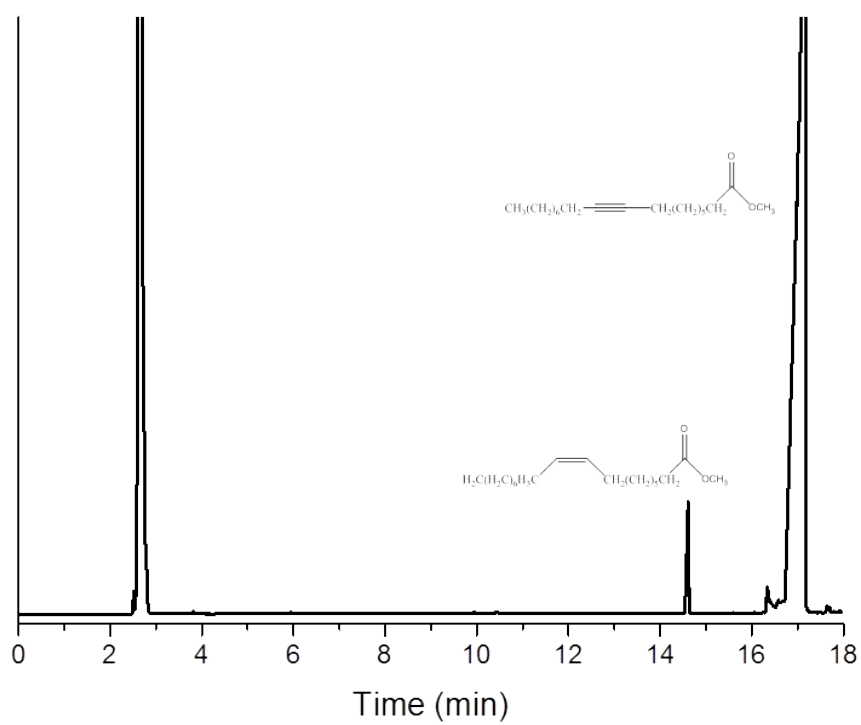


Figure S11. GC chromatogram of the hydrogenation of c) alkyne derived from oleic methyl ester: methyl octadec-9-ynoate..