Supporting Information for

Transfer hydrogenation with a ferrocene diamide ruthenium complex

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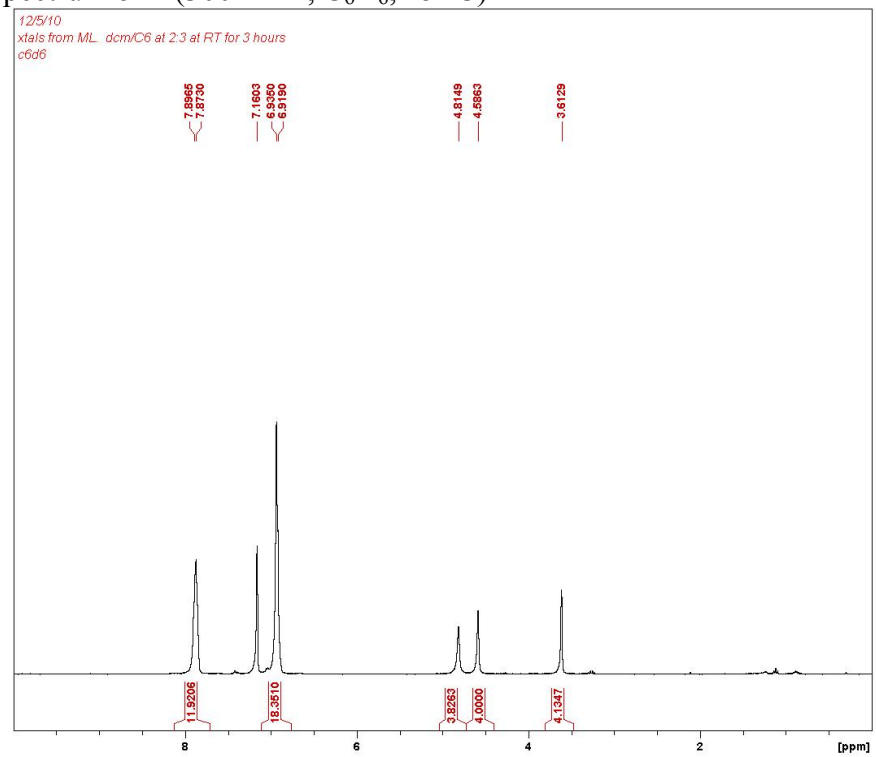
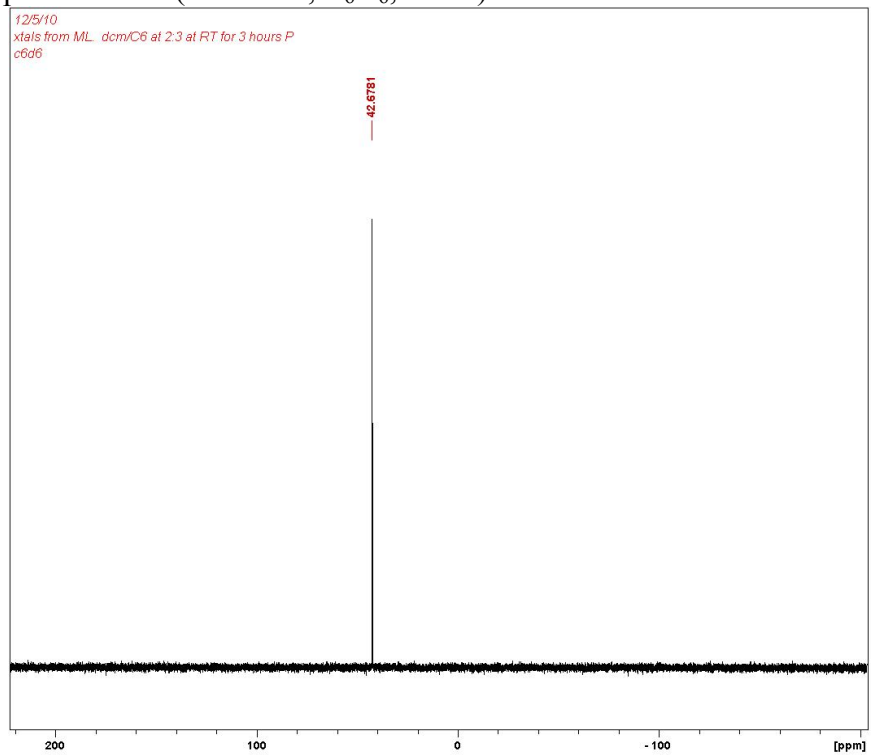
General procedures: All experiments were performed under a dry nitrogen atmosphere using standard Schlenk techniques or an MBraun inert-gas glovebox. Solvents were purified using a two-column solid-state purification system by the method of Grubbs[1] and transferred to the glove box without exposure to air. Acetophenone, 2-heptanone and pinacolone were purchased from Sigma and purified by vacuum distillation then stored over sieves in a nitrogen atmosphere. Benzophenone was purchased from Sigma and purified by crystallization from hexanes. $RuCl_3 \cdot nH_2O$ and PPh_3 were purchased from Acros. $RuCl_2(PPh_3)_3$[2], $fc(NH_2)_2$[3] and 1,1'-bis(diphenylphosphino)ferrocene[4] (dppf) were synthesized according to previously published procedures. NMR solvents were obtained from Cambridge Isotope Laboratories, degassed, and stored over activated molecular sieves prior to use. ^1H NMR spectra were recorded on Bruker300 or Bruker500 spectrometers at room temperature in C_6D_6 (the UCLA NMR spectrometers are supported by the NSF grant CHE-9974928). Chemical shifts are reported with respect to internal solvent, 7.16 ppm (C_6D_6) for ^1H NMR spectra. For ^{31}P NMR spectra, chemical shifts are reported with respect to an external standard, 0 ppm (neat H_3PO_4). GS-MS data were obtained on an Agilent 6890-5975 GC-MS equipped with an Agilent HP-5MS column and autosampler. Helium was used as the mobile phase at a column pressure of 14.25 psi. The injector temperature was 280 °C. Quadrupole MS was used for detection, with the MS source at 230 °C and the quadrupole at 150 °C.

NMR Spectra

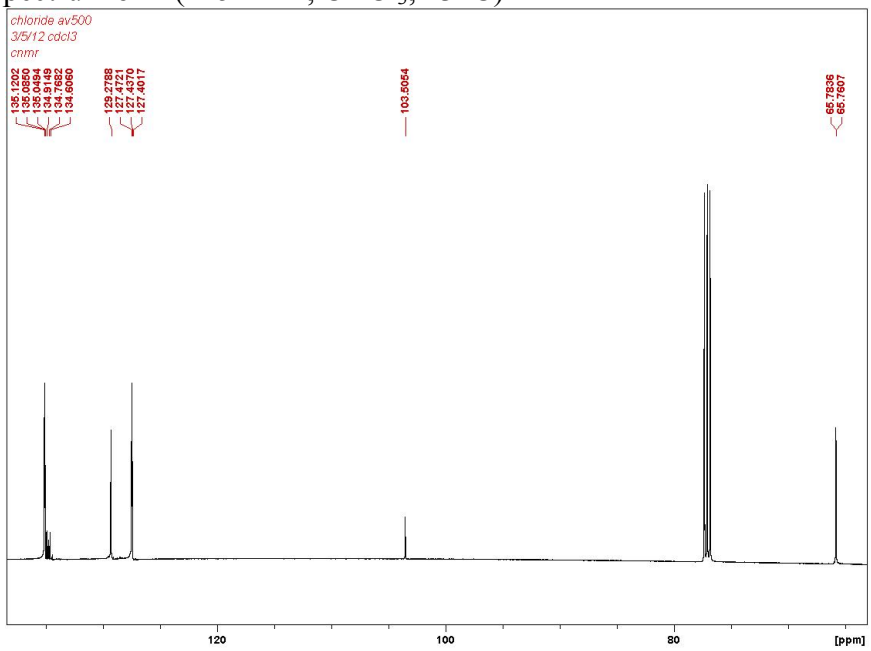
^{1}H NMR spectrum of **1** (300 MHz, C_6D_6, 25 ^{o}C)



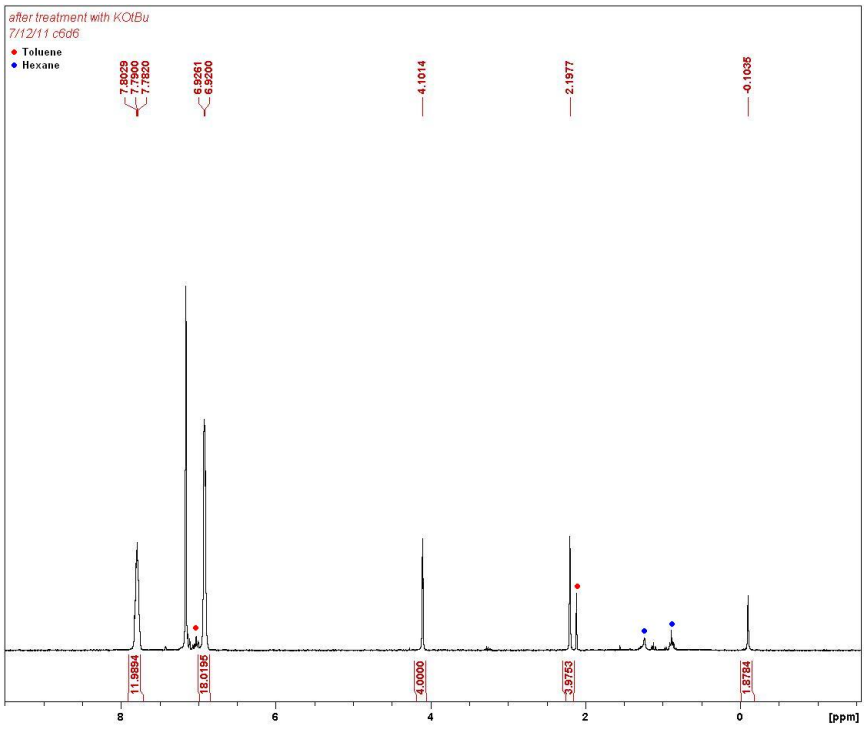
^{31}P NMR spectrum of **1** (121 MHz, C_6D_6, 25 ^{o}C)



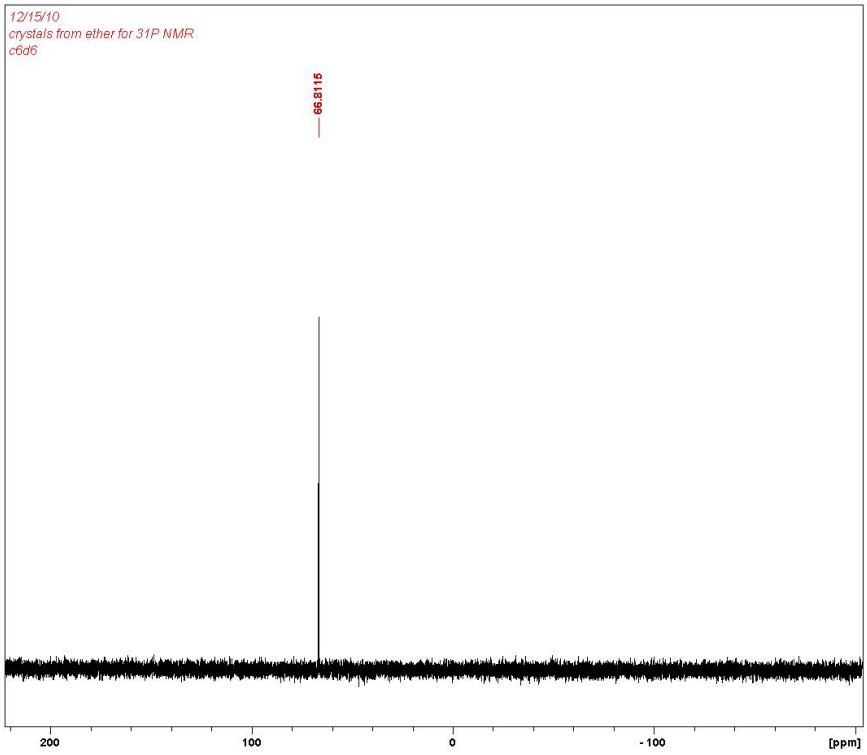
^{13}C NMR spectrum of **1** (125 MHz, $CDCl_3$, 23 ^{o}C)



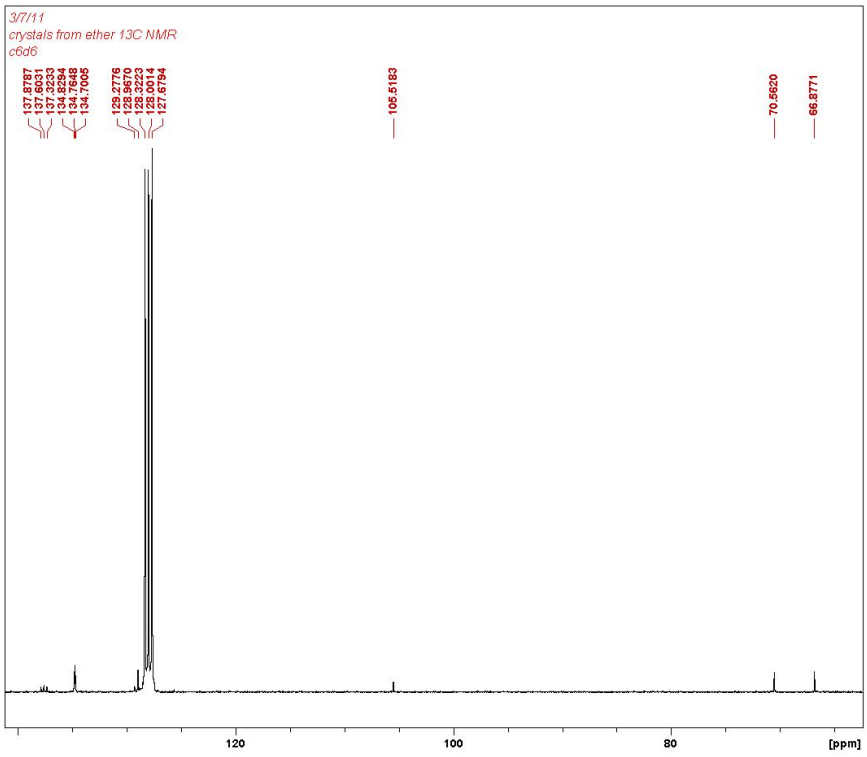
^{1}H NMR spectrum of **2** (300 MHz, C_6D_6, 25 ^{o}C)



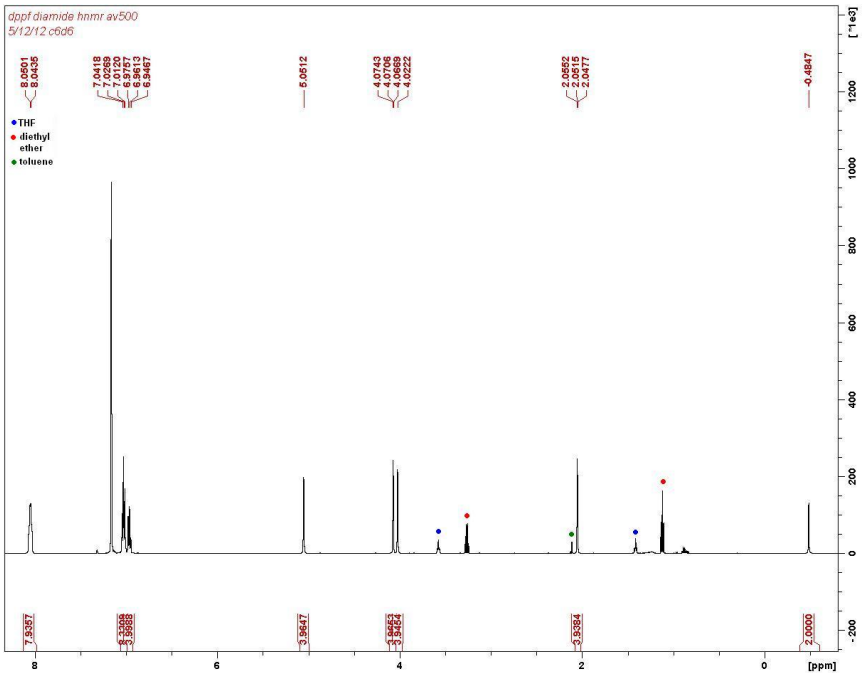
^{31}P NMR spectrum of **2** (121 MHz, C_6D_6, 25 ^{o}C)



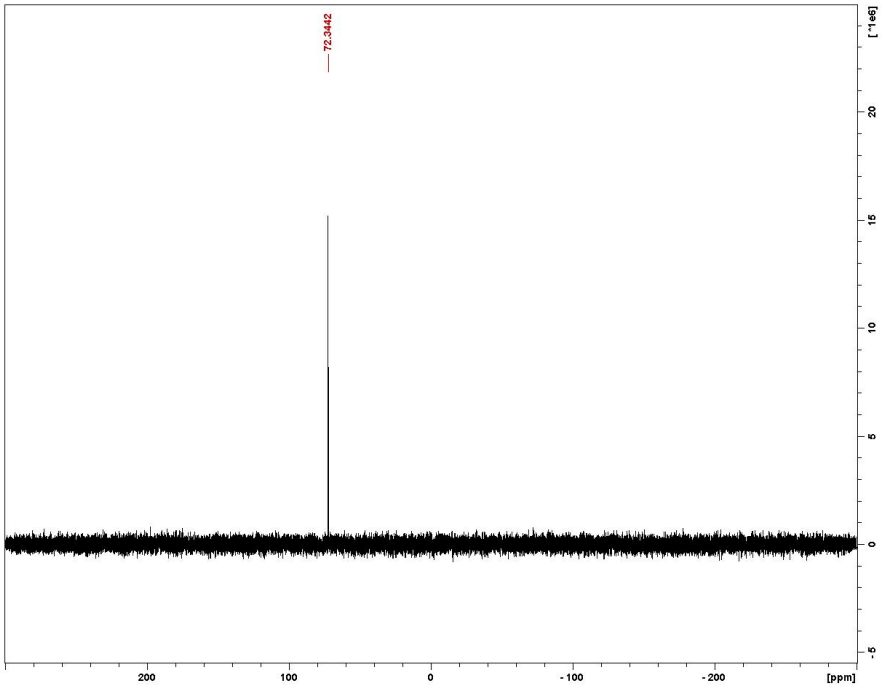
^{13}C NMR spectrum of **2** (75 MHz, C_6D_6, 25 ^{o}C)



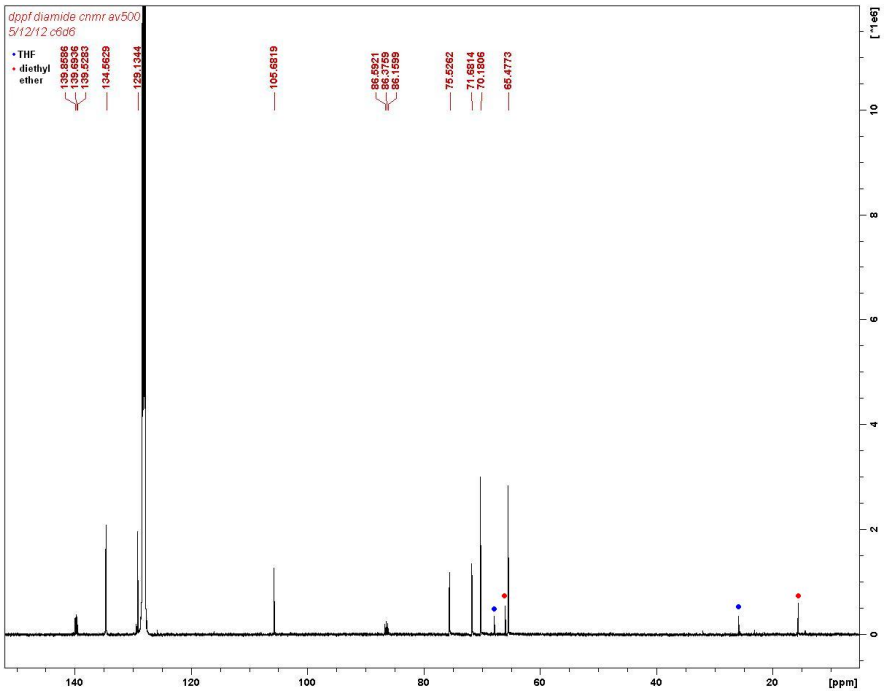
^{1}H NMR spectrum of **3** (300 MHz, C_6D_6, 23 ^{o}C)



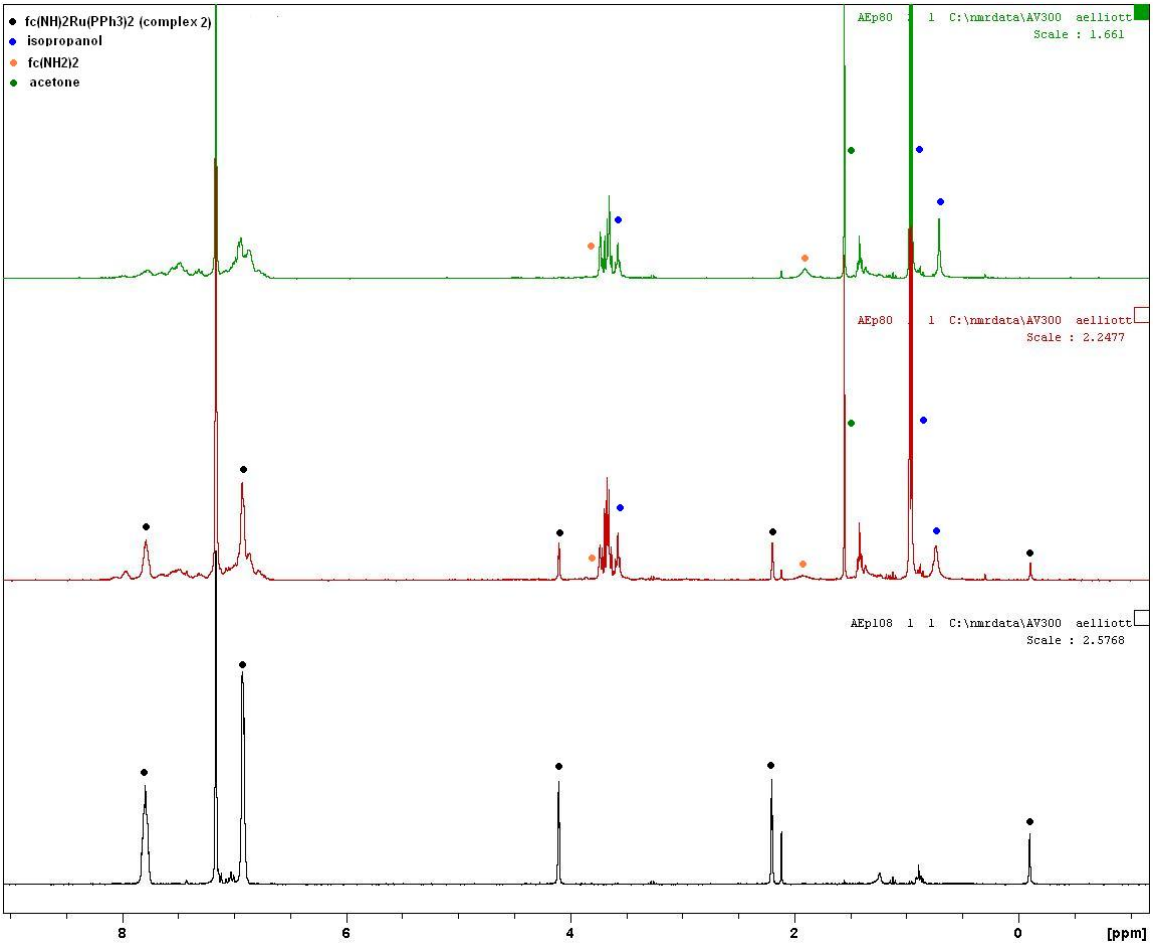
^{31}P NMR spectrum of **3** (121 MHz, C_6D_6, 25 ^{o}C)



^{13}C NMR spectrum of **3** (125 MHz, C_6D_6, 23 ^{o}C)

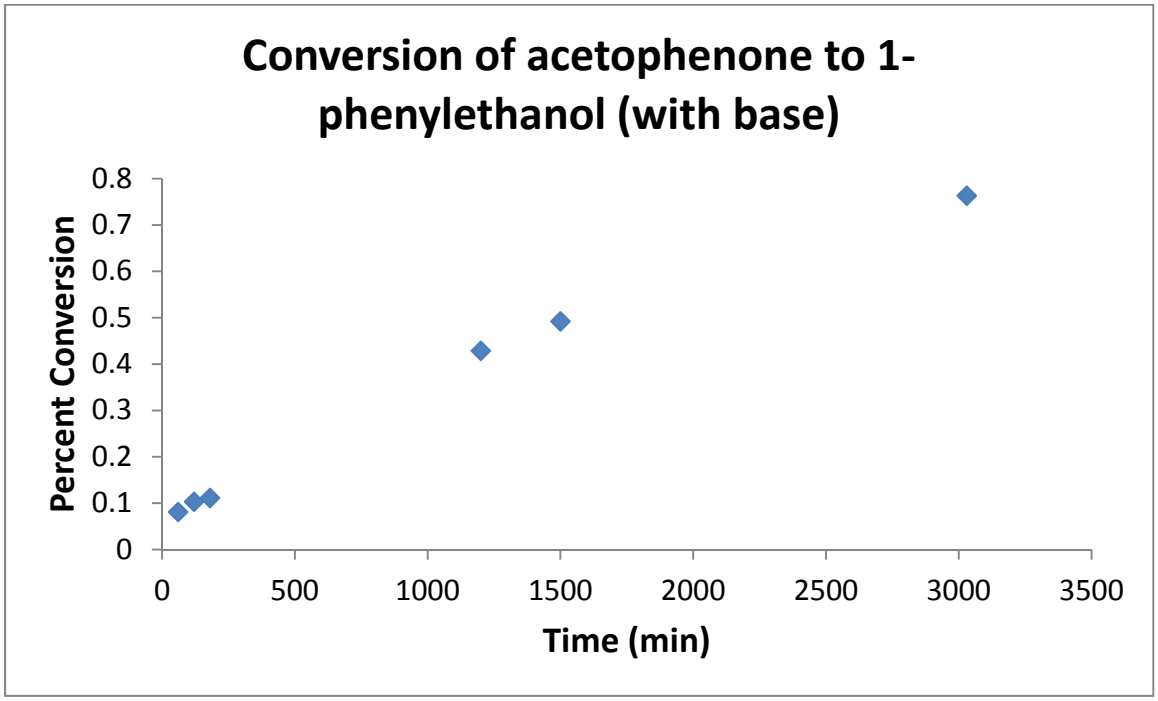


Reaction of **2** with isopropanol

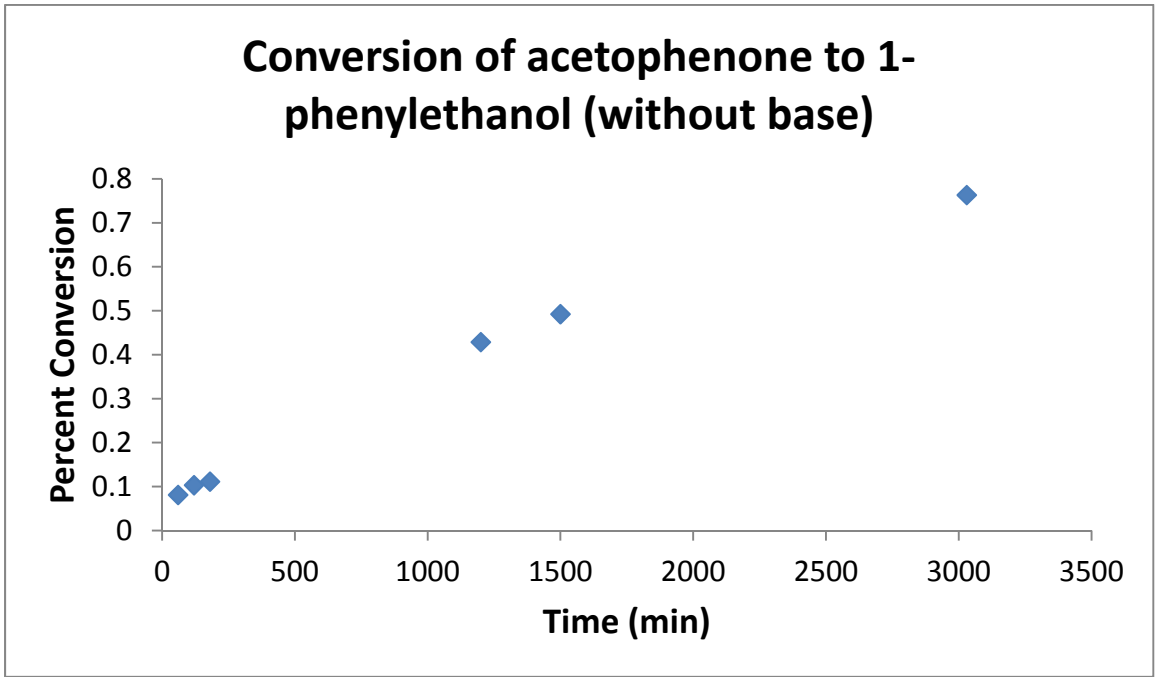


Upon treatment of **2** with excess isopropanol, the complex decomposes to form free $fc(NH_2)_2$.

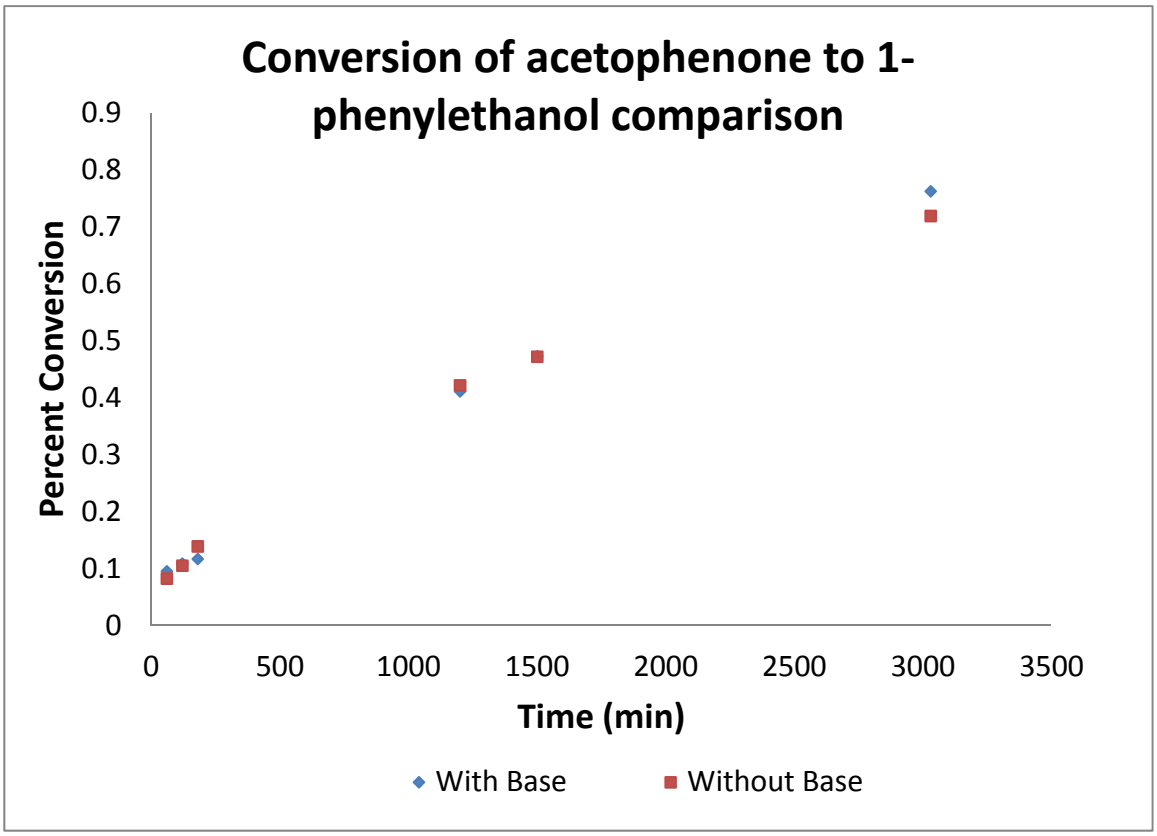
Transfer hydrogenation of acetophenone by 2



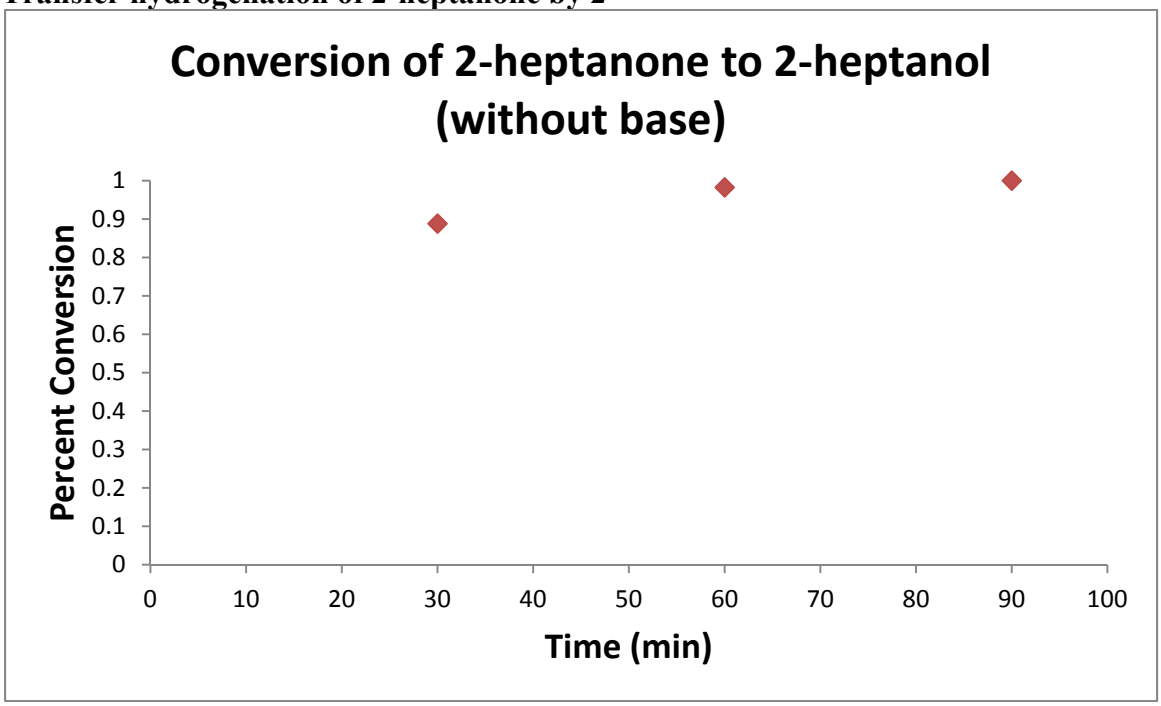
TON: 153
TOF: 19 h^{-1}
76% conversion in 50 h



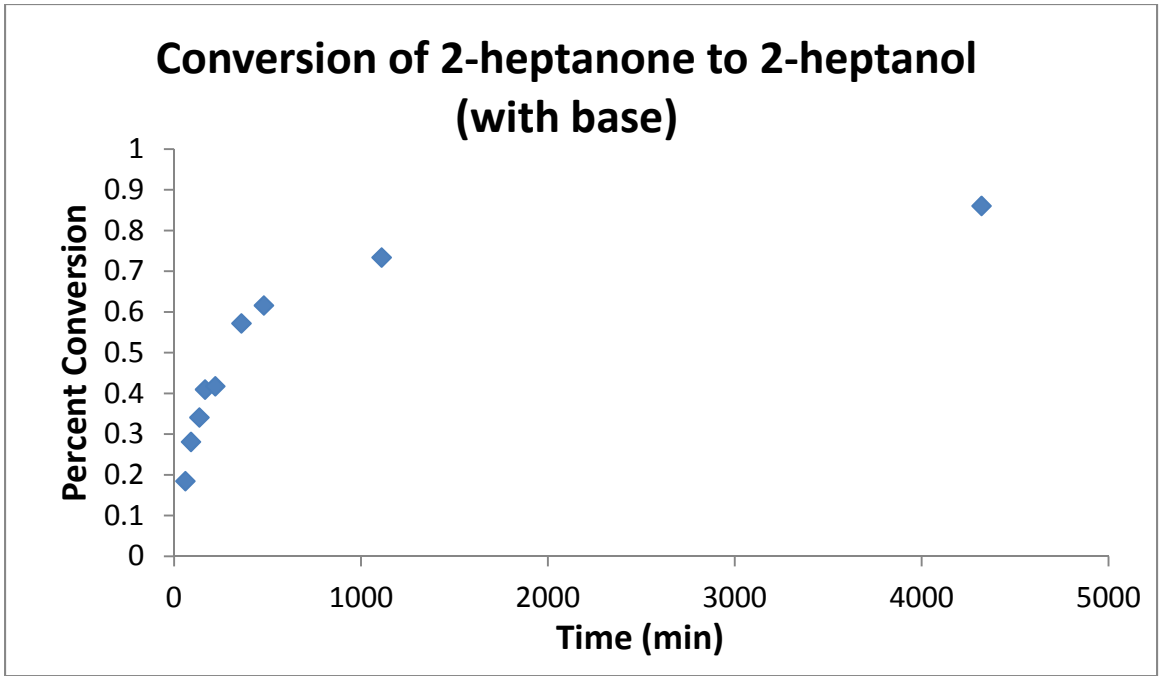
TON: 144
TOF: 16.5 h^{-1}
72% conversion in 50 h



Transfer hydrogenation of 2-heptanone by 2

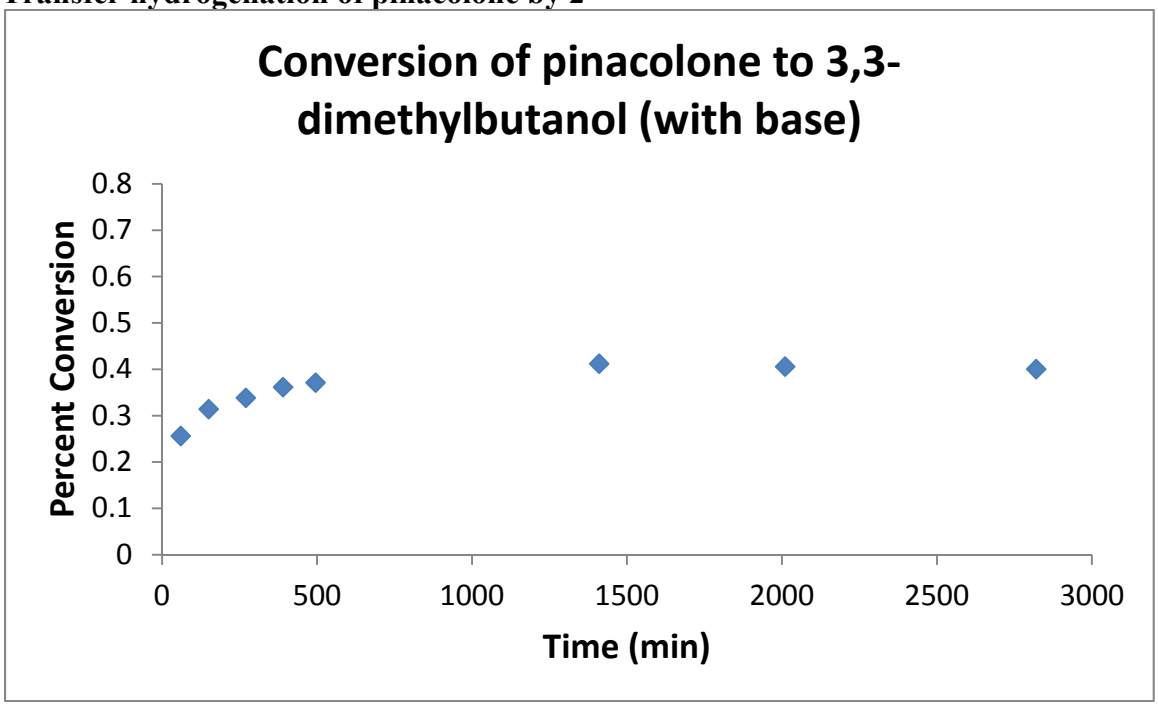


TON: 200
TOF: 339 h^{-1}
100% conversion in 1.5 h

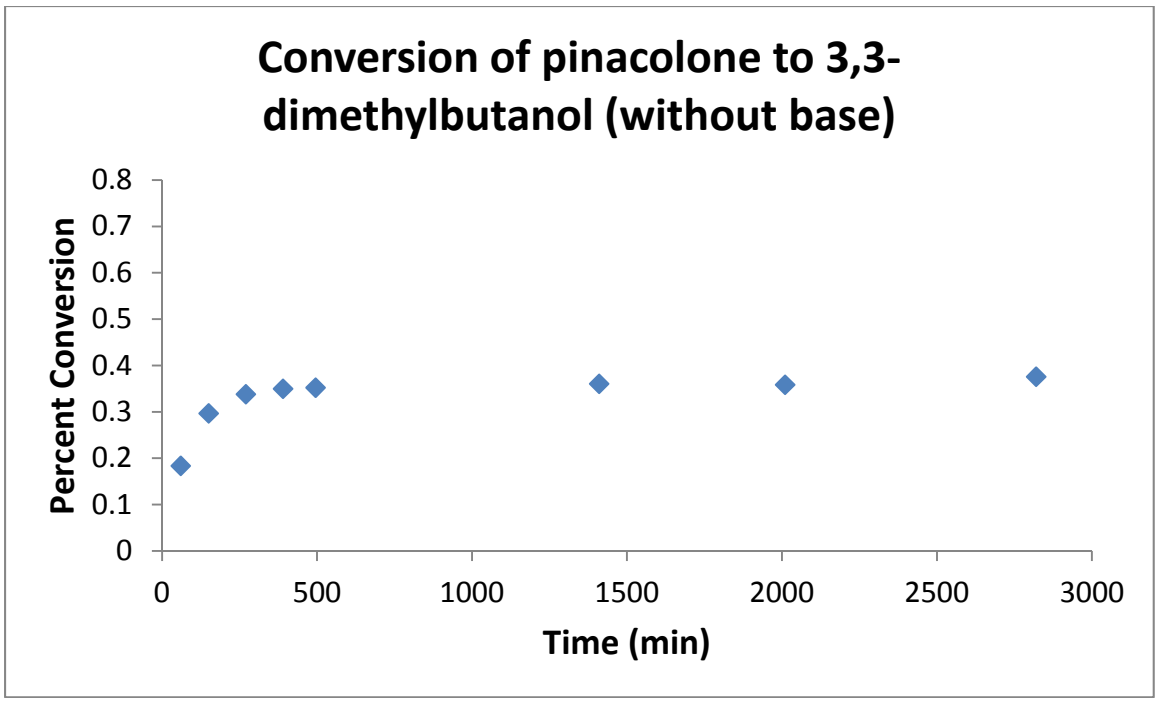


TON: 172
TOF: 36 h^{-1}
84% conversion in 72 h

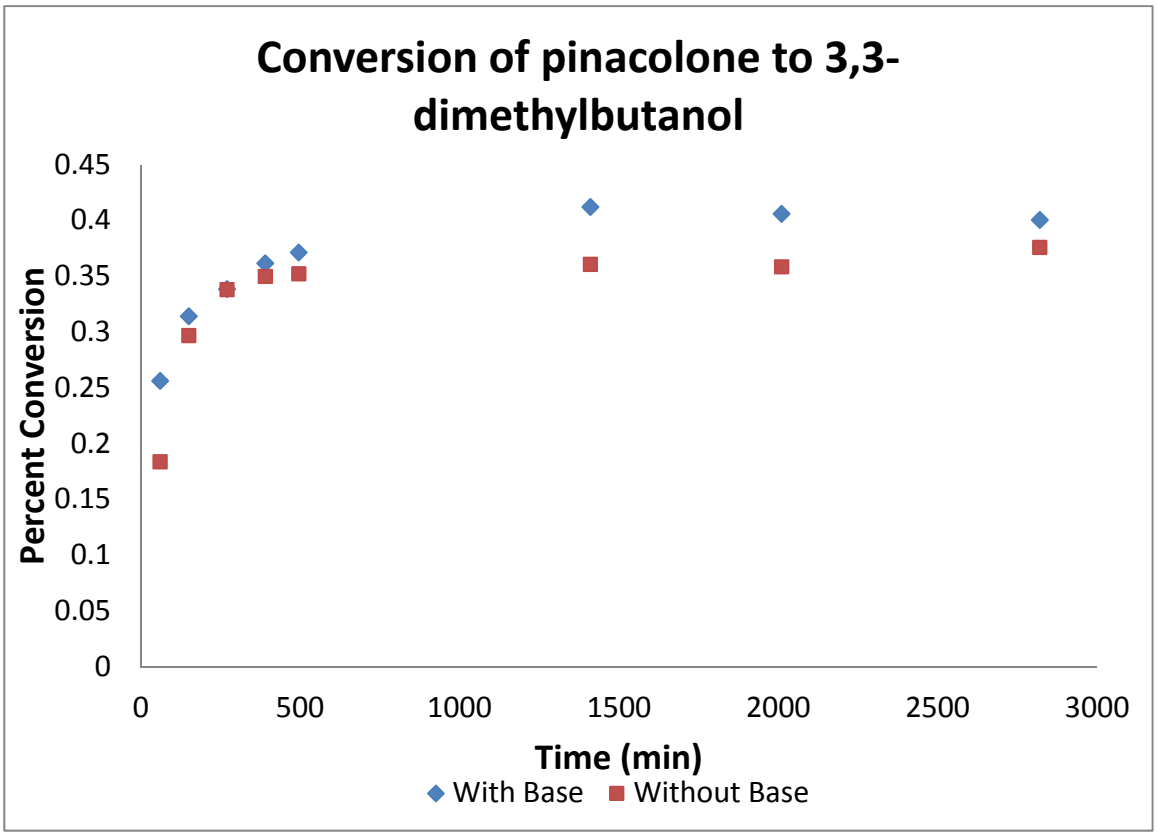
Transfer hydrogenation of pinacolone by 2



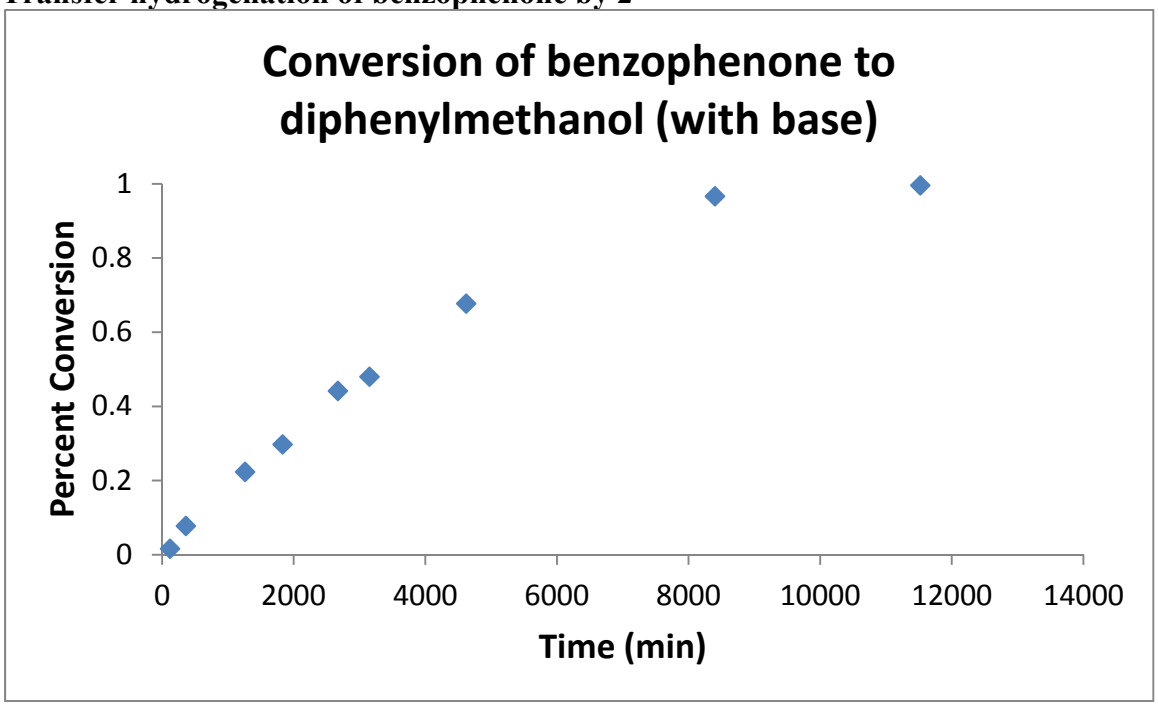
TON: 82
TOF: 51 h^{-1}
41% conversion in 24 h



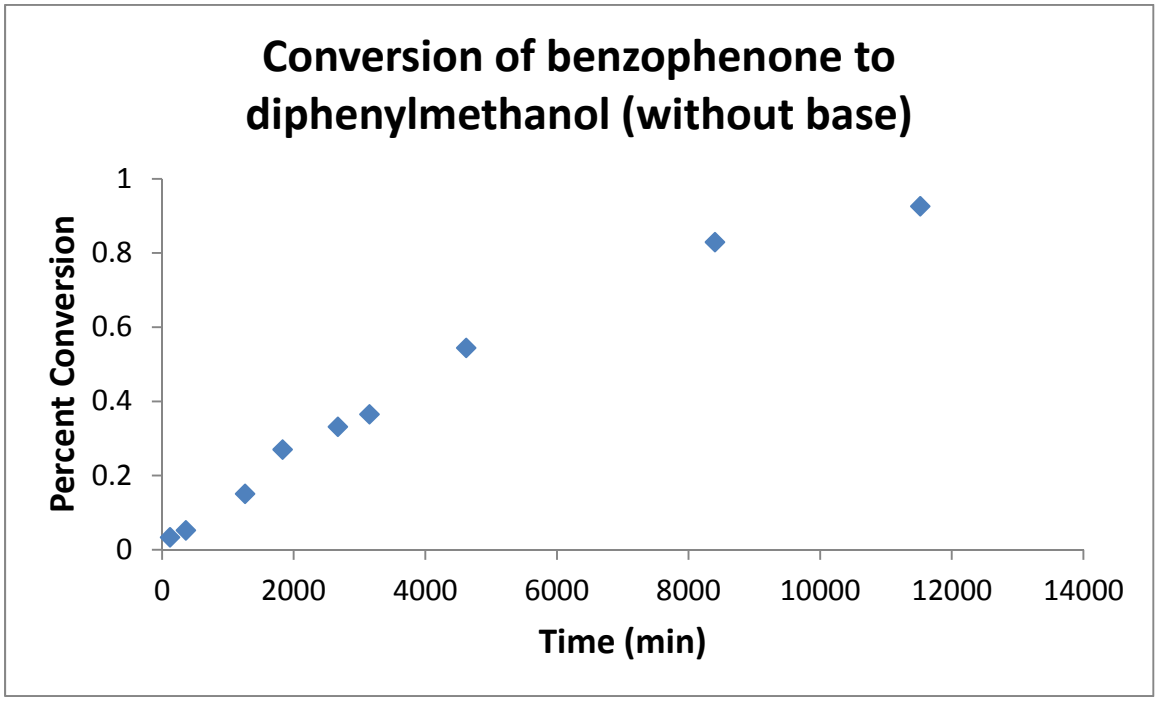
TON: 75
TOF: 37 h^{-1}
36% conversion in 24 h



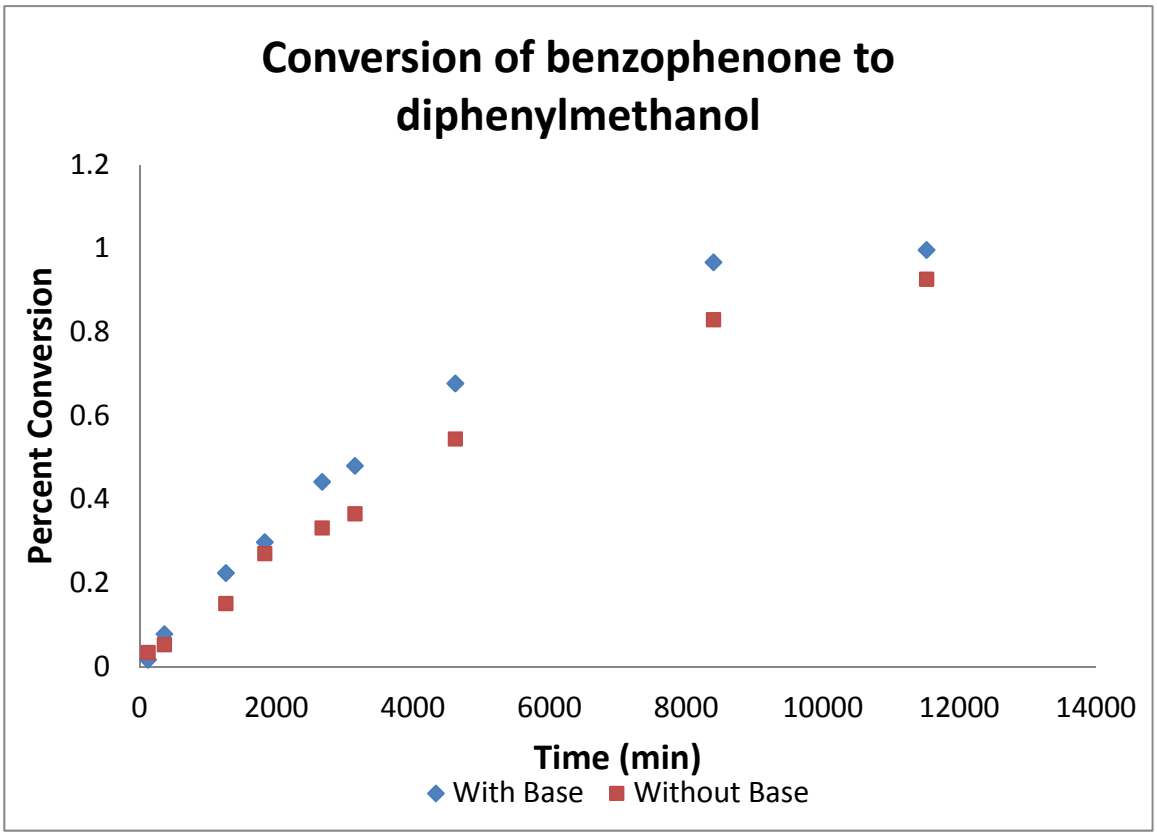
Transfer hydrogenation of benzophenone by 2



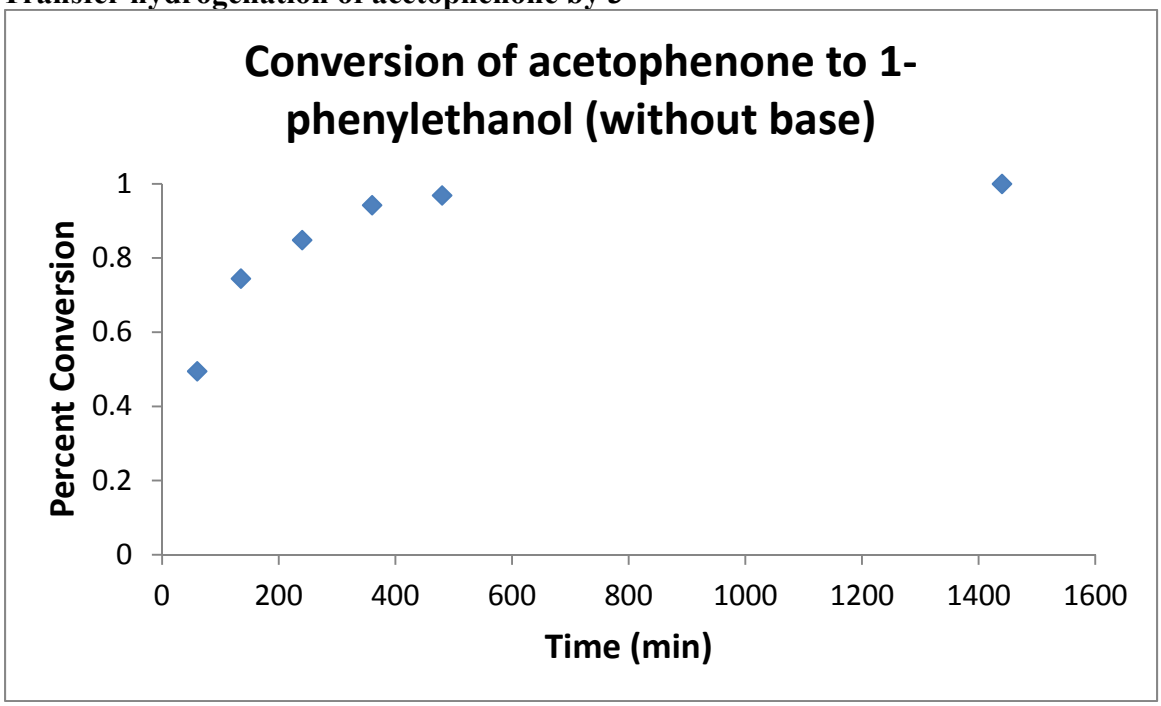
TON: 199
TOF: 3 h^{-1}
99% conversion in 1 week



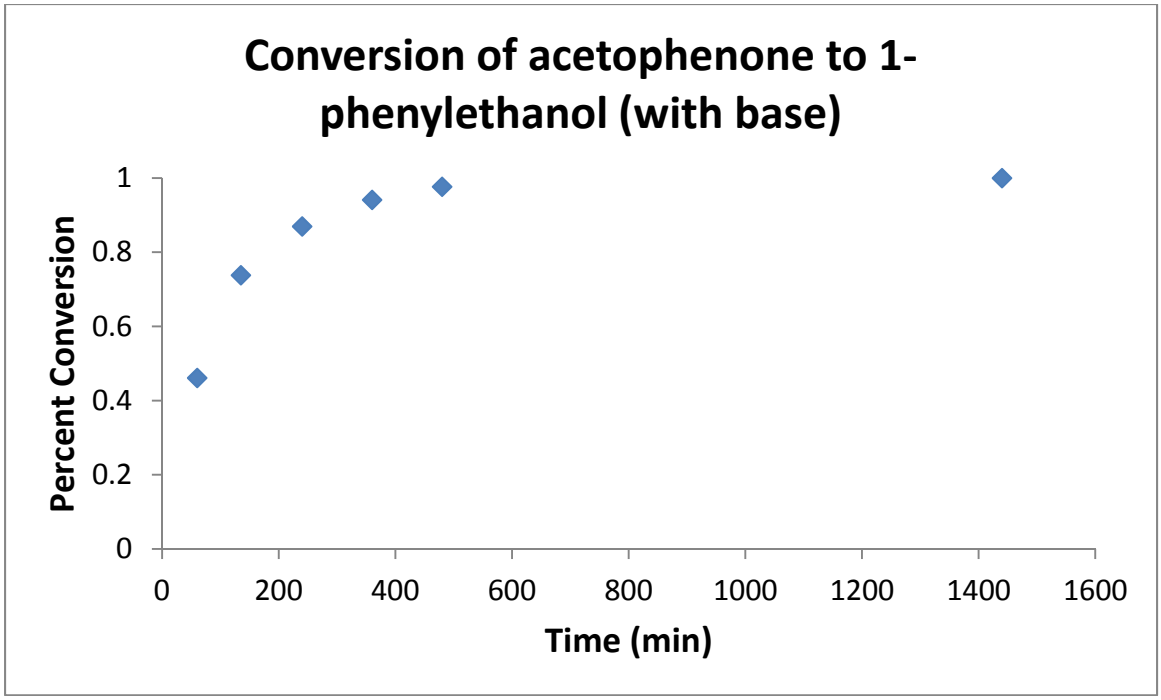
TON: 185
TOF: 7 h^{-1}
93% conversion in 1 week



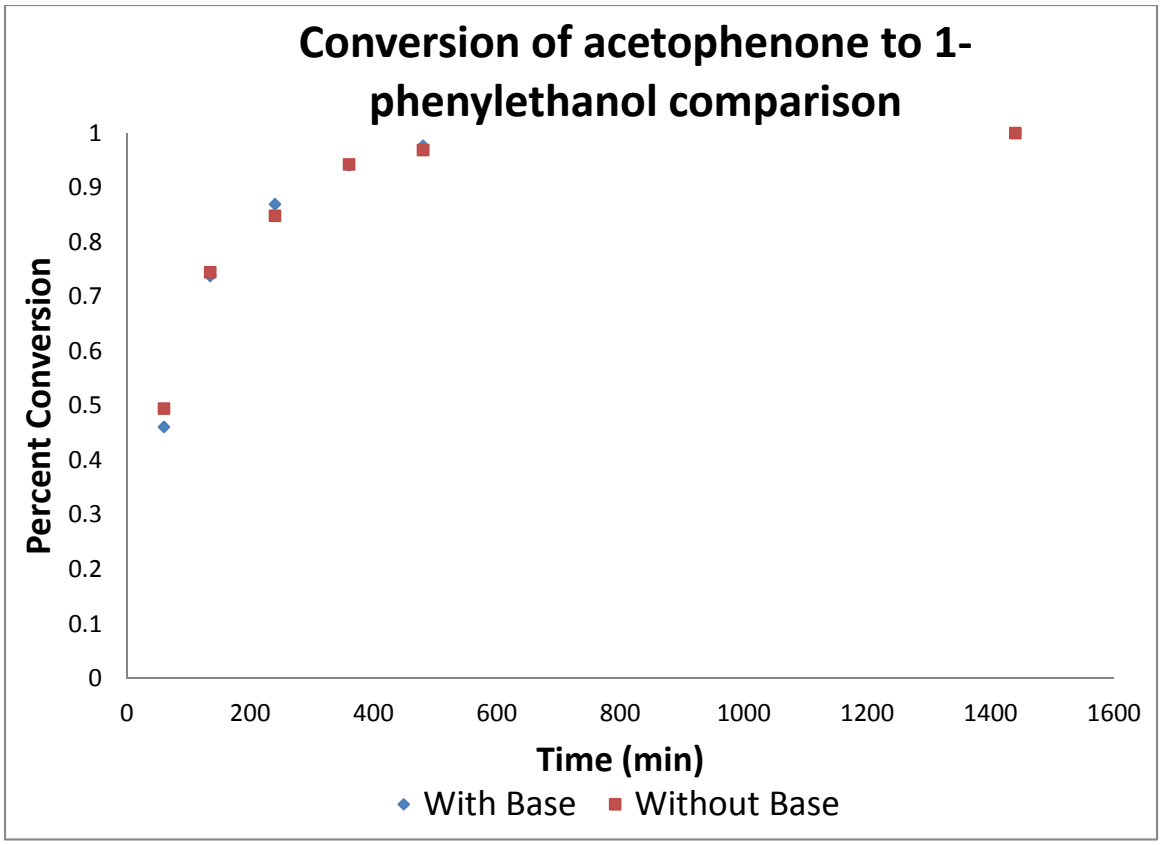
Transfer hydrogenation of acetophenone by 3



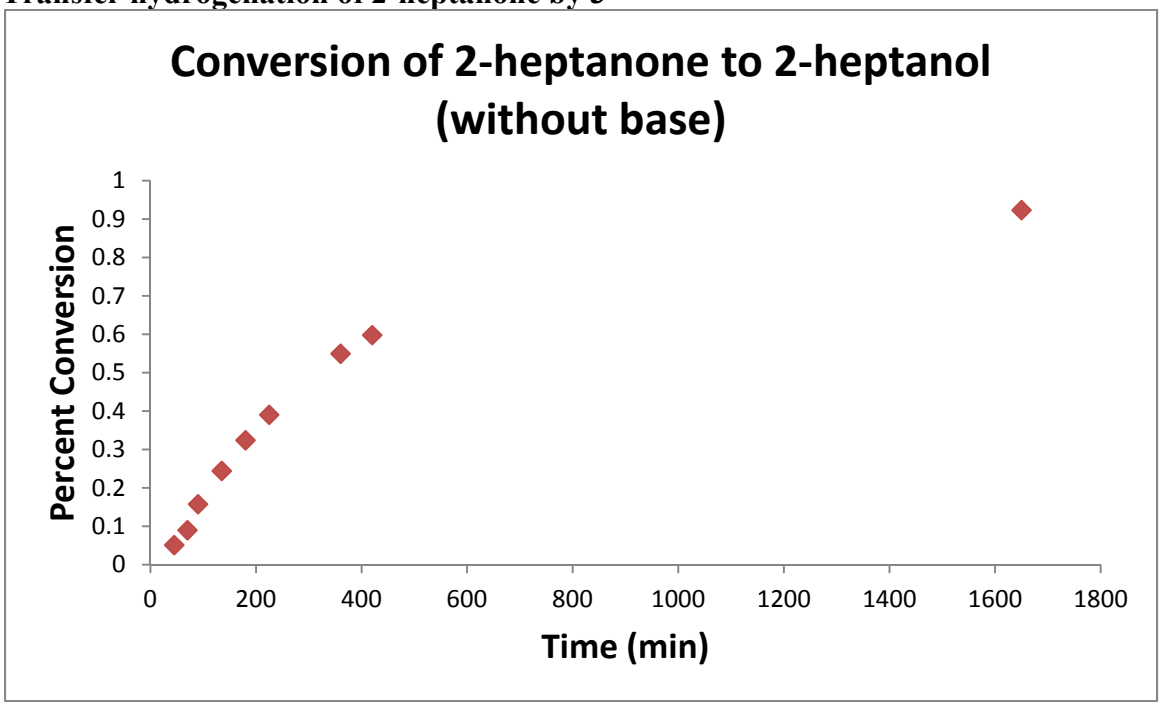
TON: 200
TOF: 99 h^{-1}
100% conversion in 1 day



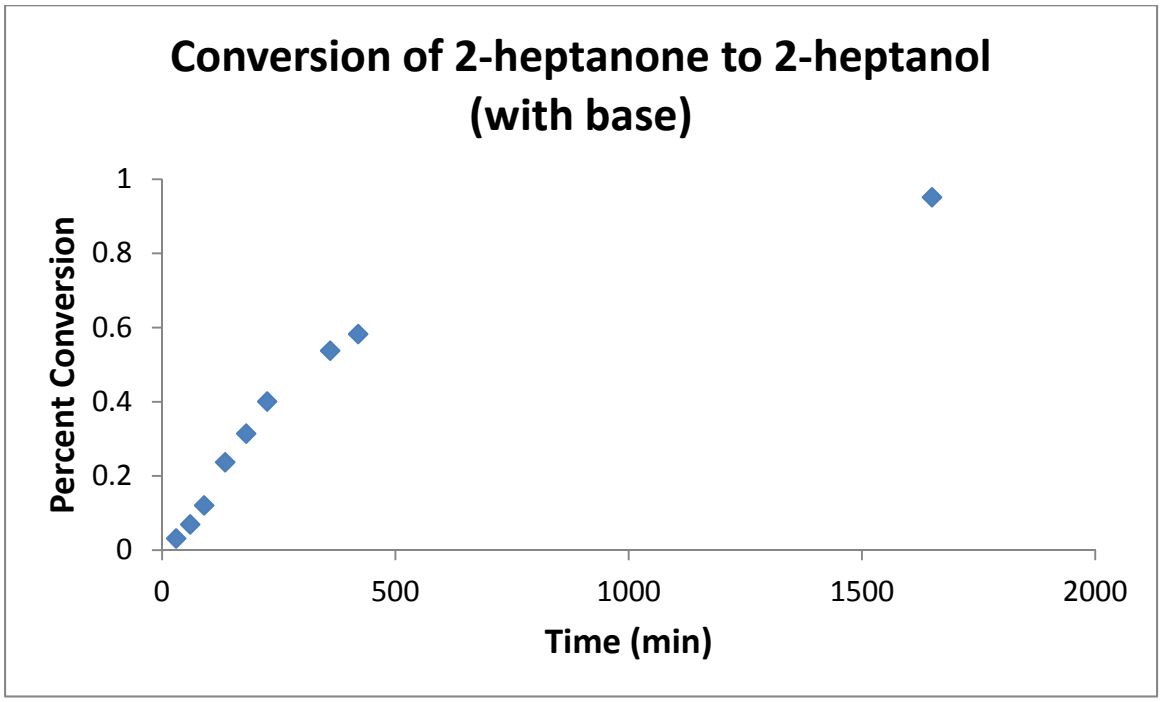
TON: 200
TOF: 92 h^{-1}
100% conversion in 1 day



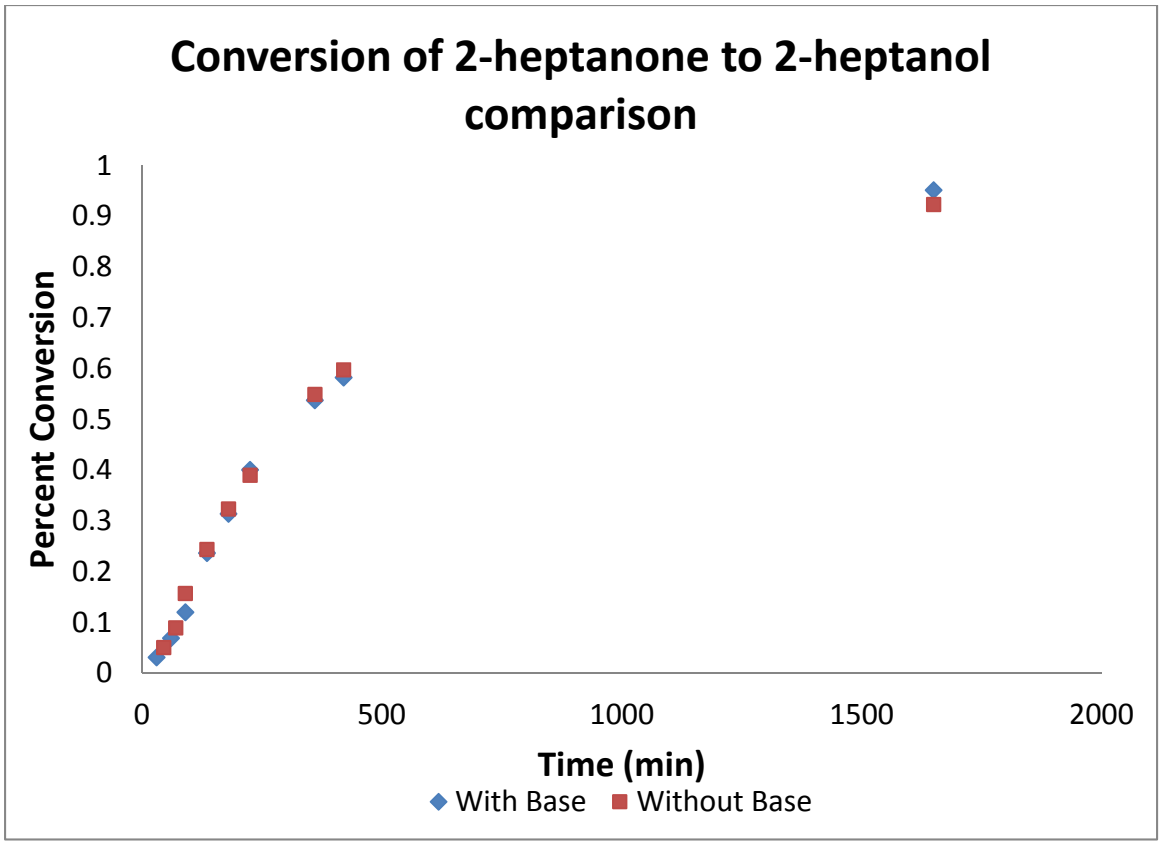
Transfer hydrogenation of 2-heptanone by 3



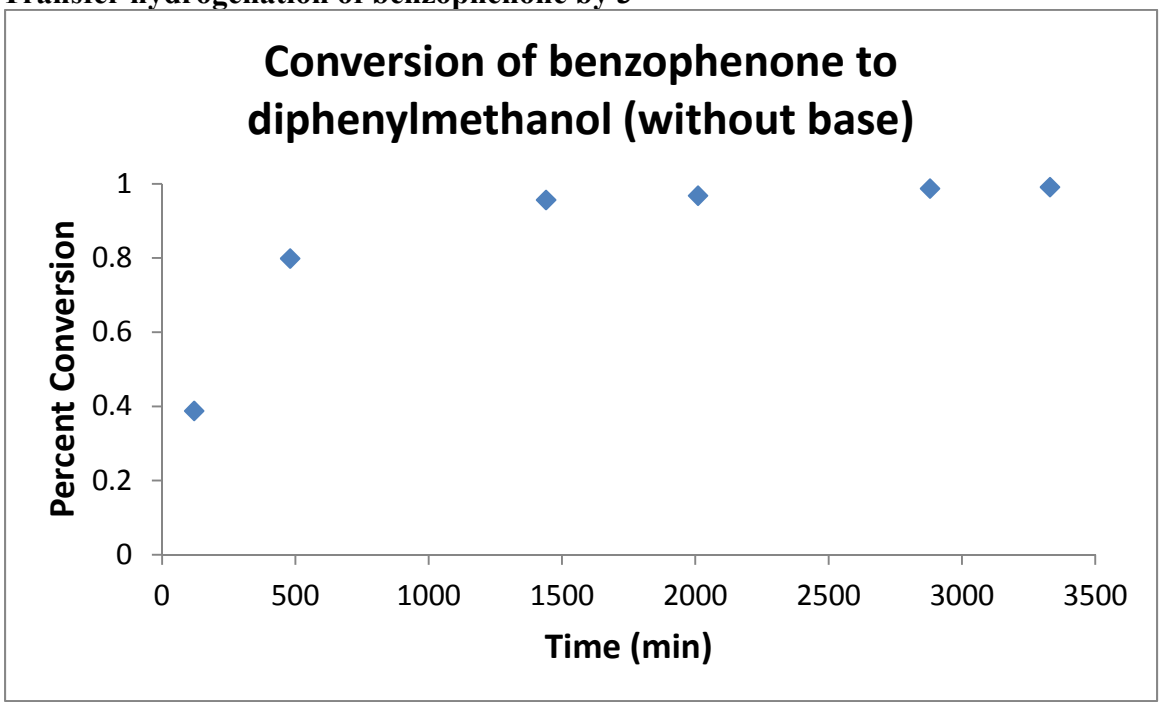
TON: 185
TOF: 41 h^{-1}
92% conversion in 27.5 hours



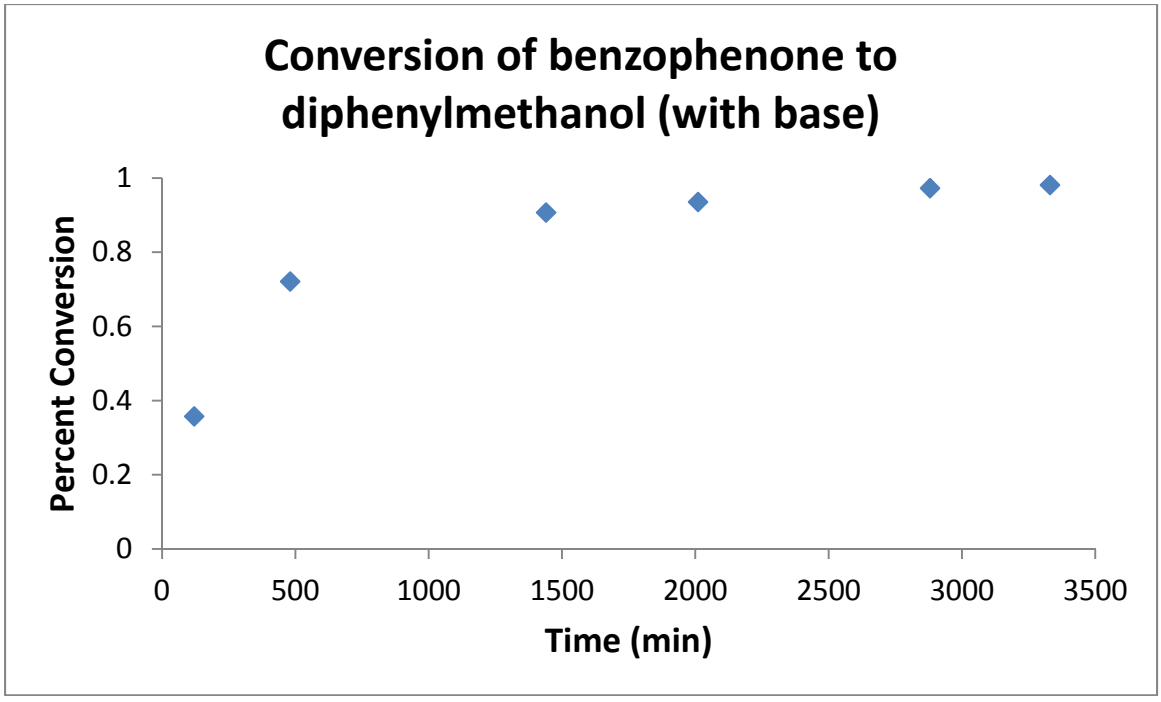
TON: 190
TOF: 36 h^{-1}
95% conversion in 27.5 hours



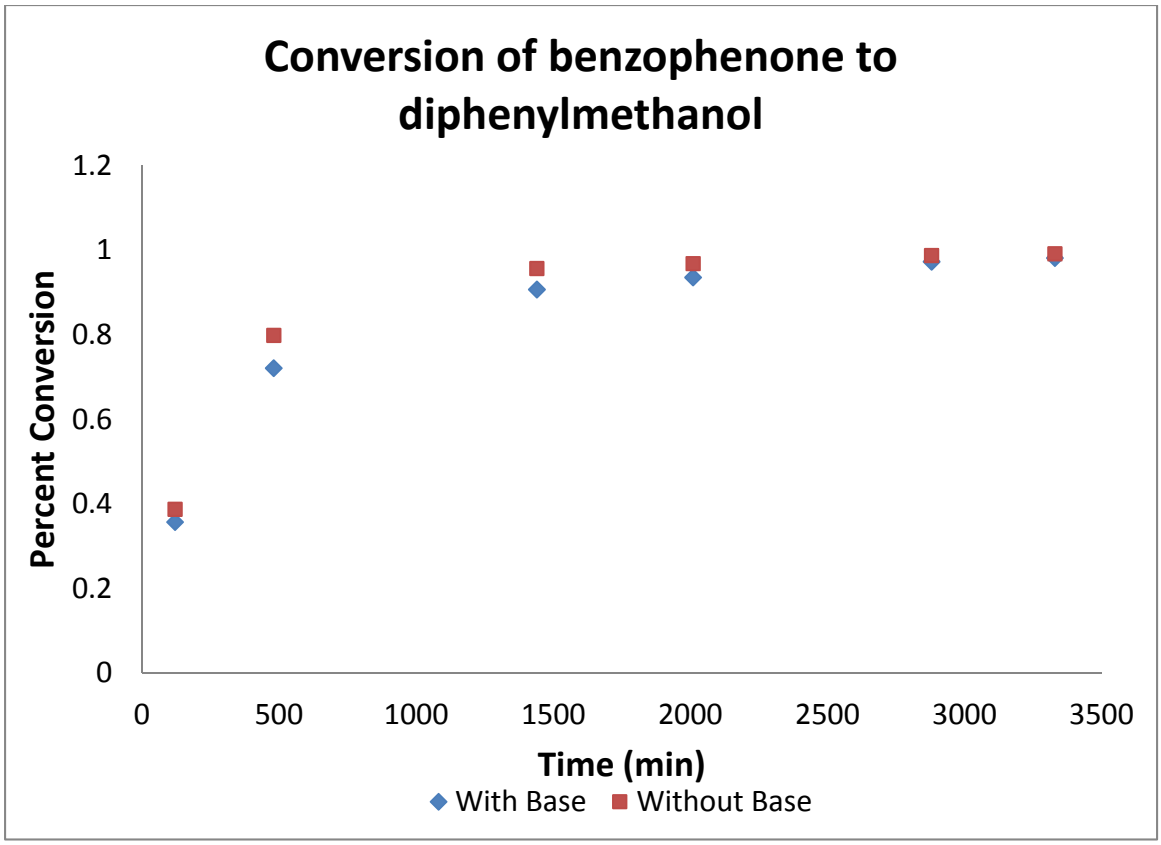
Transfer hydrogenation of benzophenone by 3



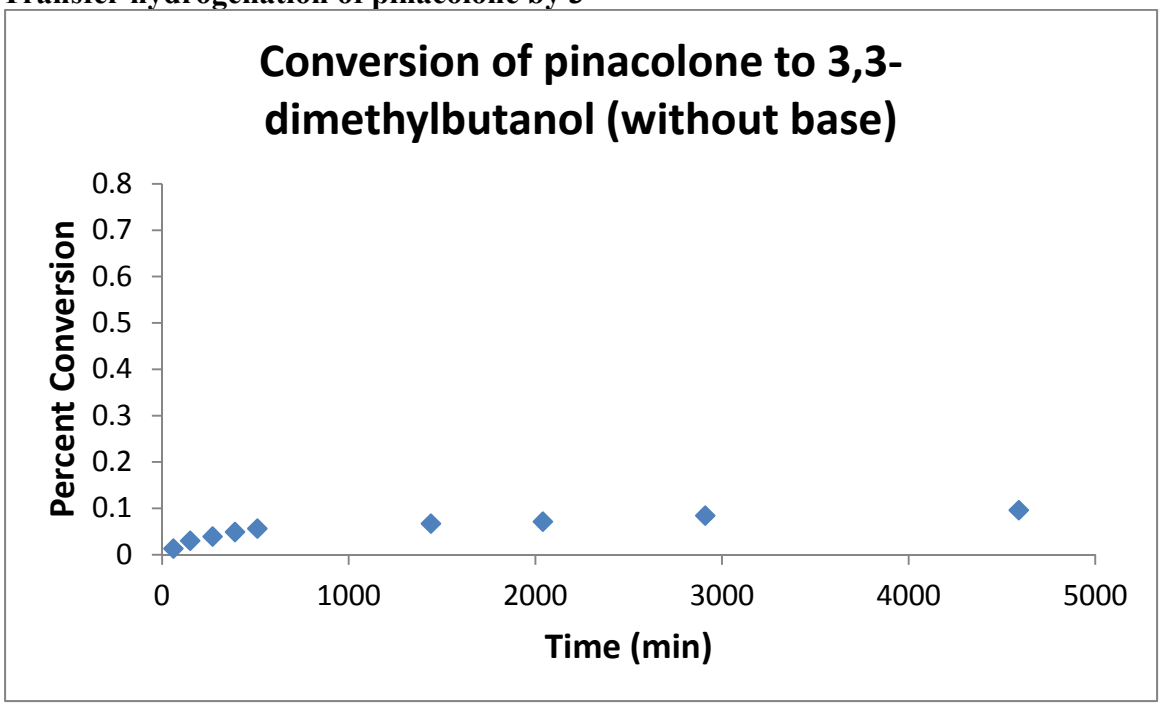
TON: 198
TOF: 38 h^{-1}
99% conversion in 55.5 hours



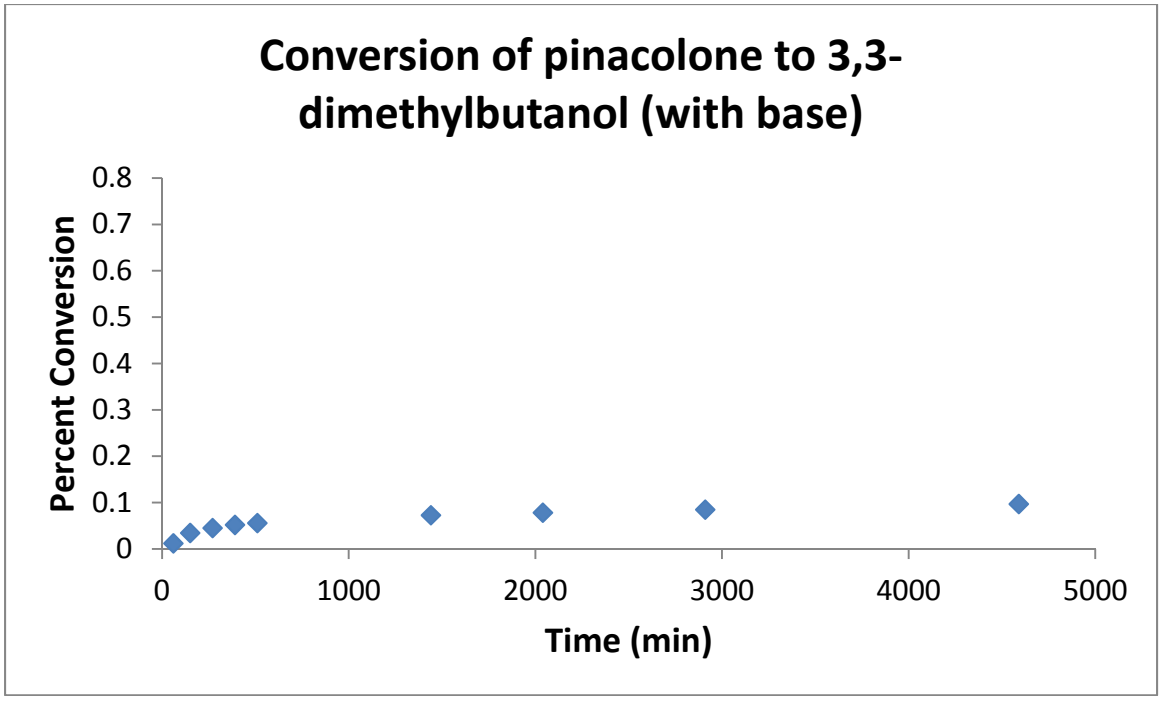
TON: 196
TOF: 36 h^{-1}
98% conversion in 55.5 hours



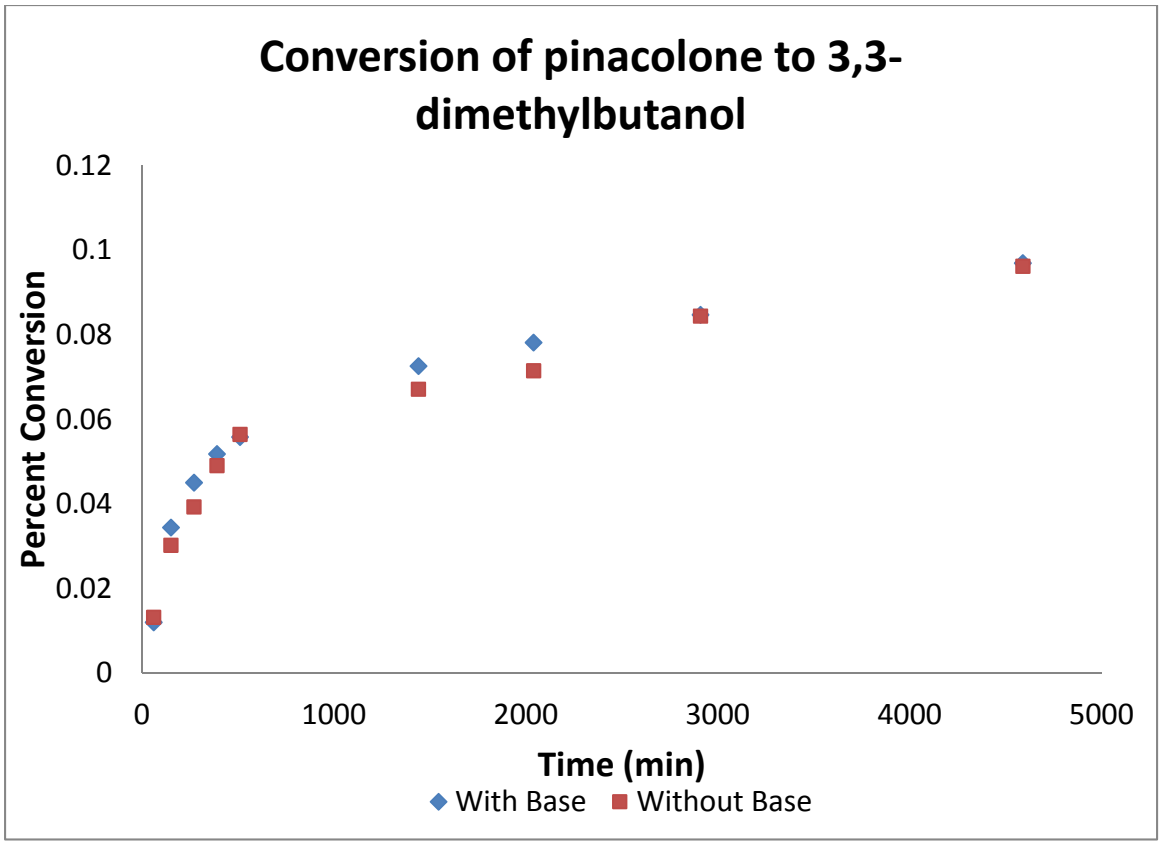
Transfer hydrogenation of pinacolone by 3



TON: 19
TOF: 3 h^{-1}
10% conversion in 76.5 hours



TON: 19
TOF: 3 h^{-1}
10% conversion in 76.5 hours



References

1. A. B. G. Pangborn, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J., *Organometallics*, 1996, **15**, 1518.
2. M. A. H. Fox, J. E.; Heider, S.; Pérez-Gregorio, V.; Zakrzewska, M. E.; Farmer, J. D.; Yufit, D. S.; Howard, J. A.K.; Low, P. J., *J. Organomet. Chem.*, 2009, **694**, 2350.
3. M. J. Monreal, C. T. Carver and P. L. Diaconescu, *Inorg. Chem.*, 2007, **46**, 7226-7228.
4. J. J. Bishop, A. Davison, M. L. Katcher, D. W. Lichtenberg, R. E. Merrill and J. C. Smart, *J. Organomet. Chem.*, 1971, **27**, 241-249.