Supplementary Information

Ruthenium carbonyl complexes supported by pyridine-alkoxide ligands: synthesis, structure and catalytic oxidation of secondary alcohols

Siqi Zong[a,§], Kang Liu[a,§], Xiaohui Yue[a], Zhiqiang Hao[a,*], Zhihong Ma[b,*], Zhangang Han[a], Guo-Liang Lu[c] and Jin Lin[a,*]

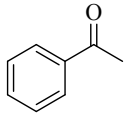
[a]National Demonstration Center for Experimental Chemistry Education, Hebei Key Laboratory of Organic Functional Molecules, College of Chemistry & Material Science, Hebei Normal University, Shijiazhuang 050024, China

[b]School of Pharmacy, Hebei Medical University, Shijiazhuang 050017, China

[c]Auckland Cancer Society Research Centre, Faculty of Medical and Health Sciences, The University of Auckland, Private Bag 92019, Auckland 1142, New Zealand

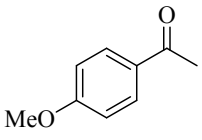
§ These authors contributed equally to this work.

NMR data for the catalytic products

1. 

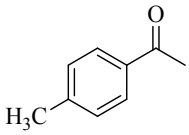
acetophenone

^{1}H NMR ($CDCl_3$, 500 MHz): δ 2.56 (s, 3H, CH_3), 7.42 (t, J = 7.5 Hz, 2H, Ph-H), 7.52 (t, J = 7.5 Hz, 1H, Ph-H), 7.92 (t, J = 7.5 Hz, 2H, Ph-H) ppm; ^{13}C NMR: ($CDCl_3$, 125 MHz) δ 26.5, 128.3, 128.5, 133.1, 137.1, 198.0 ppm.

2. 

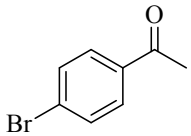
1-(4-methoxyphenyl)ethanone

^{1}H NMR ($CDCl_3$, 500 MHz): δ 2.56 (s, 3H, CH_3), 3.87 (s, 3H, OCH_3), 6.93 (d, J = 8.0 Hz, 2H, Ph-H), 7.94 (d, J = 8.0 Hz, 2H, Ph-H) ppm; ^{13}C NMR: ($CDCl_3$, 125 MHz): δ 26.3, 55.4, 113.7, 130.4, 130.6, 163.5, 196.7 ppm.

3. 

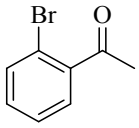
1-(4-methylphenyl)ethanone

^{1}H NMR ($CDCl_3$, 500 MHz): δ 2.34 (s, 3H, CH_3), 2.50 (s, 3H, CH_3), 7.27 (d, J = 8.0 Hz, 2H, Ph-H), 7.86 (d, J = 8.0 Hz, 2H, Ph-H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 21.3, 26.2, 128.7, 128.9, 133.7, 142.8, 197.0 ppm.

4. 

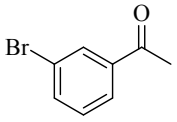
1-(4-bromophenyl)ethanone

^{1}H NMR ($CDCl_3$, 500 MHz): δ 2.58 (s, 3H, CH_3), 7.59 (d, J = 8.5 Hz, 2H, Ar-H), 7.81 (d, J = 8.5 Hz, 2H, Ar-H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 26.6, 128.4, 130.0, 132.0, 136.0, 197.1 ppm.

5. 

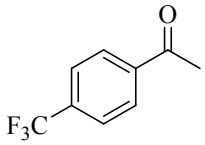
1-(2-bromophenyl)ethanone

^{1}H NMR ($CDCl_3$, 500 MHz): δ 2.54 (s, 3H, CH_3), 7.21 (t, *J* = 8.0 Hz, 1H, Ph-H), 7.28 (t, *J* = 6.0 Hz, 1H, Ph-H), 7.39-7.37 (m, 1H, Ph-H), 7.84 (d, *J* = 8.5 Hz, 1H, Ph-H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 30.3, 118.9, 127.5, 128.9, 131.8, 133.8, 141.5, 201.2 ppm.

6. 

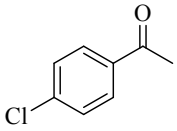
1-(3-bromophenyl)ethanone

^{1}H NMR ($CDCl_3$, 500 MHz): δ 2.57 (s, 3H, CH_3), 7.32 (t, *J* = 8.0 Hz, 1H, Ph-H), 7.66 (d, *J* = 8.0 Hz, 1H, Ph-H)，7.85 (d, *J* = 8.0 Hz, 1H, Ph-H), 8.05 (t, *J* = 8.0 Hz, 1H, Ph-H); ^{13}C NMR ($CDCl_3$, 125 MHz): δ 26.6, 122.9, 126.9, 130.2, 131.3, 135.9, 138.8, 196.5 ppm.

7. 

1-(4-(trifluoromethyl)phenyl)ethanone

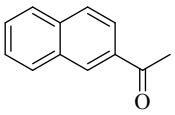
^{1}H NMR ($CDCl_3$, 500 MHz): δ 2.67 (s, 3H, CH_3), 7.75 (d, *J* = 8.0 Hz, 2H, Ph-H), 8.08 (d, *J* = 8.0 Hz, 2H, Ph-H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 26.7, 125.6, 125.7, 128.6, 134.3, 139.7, 196.9 ppm.

8. 

1-(4-chlorophenyl)ethanone

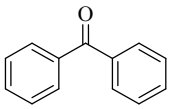
^{1}H NMR ($CDCl_3$, 500 MHz): δ 2.55 (s, 3H, CH_3), 7.38 (d, *J* = 9.0 Hz, 2H, Ph-H), 7.85 (d, *J* = 8.5 Hz, 2H, Ph-H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 26.5, 128.8,

129.7, 135.4, 139.5, 196.7 ppm.

9. 

1-(2-naphthyl)ethanone

^{1}H NMR ($CDCl_3$, 500 MHz): δ 2.70 (s, 3H, CH_3), 7.52-7.60 (m, 2H, Ph-H)，7.85 (t, *J* = 8.5 Hz, 2H, Ph-H)，7.94 (d, *J* = 8.0 Hz, 1H, Ph-H), 8.01 (dd, *J* = 8.5 Hz, *J* = 7.0 Hz, 1H, Ph-H), 8.44 (s, 1H, Ph-H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 26.7, 123.9, 127.8, 128.4, 129.6, 130.2, 132.5, 134.5, 135.6, 198.1 ppm.

10. 

benzophenone

^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.50 (d, *J* = 7.5 Hz, 4H, Ph-H), 7.60-7.63 (m, 2H, Ph-H), 7.84 (t, *J* = 9.5 Hz, 4H, Ph-H) ppm; ^{13}C NMR ($CDCl_3$, 125 MHz): δ 128.3, 130.1, 132.4, 137.6, 196.7 ppm.

References

[S1] G. Zhang, X. Han, Y. Luan, Y. Wang, X. Wen and C. Ding, *Chem. Commun.*, 2013, **49**, 7908-7910.

[S2] D.-W. Tan, H.-X. Li, M.-J. Zhang, J.-L. Yao and J.-P. Lang, *ChemCatChem*, 2017, **9**, 1113-1118.