

Electronic Supplementary Information

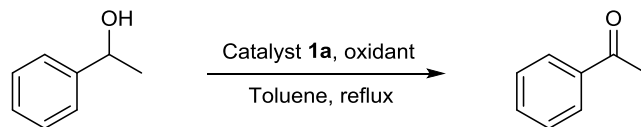
Ruthenium Carbonyl Complexes with Pyridylalkanol ligands: Synthesis, Characterization and Catalytic Properties for Aerobic Oxidation of Secondary Alcohols

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Table S1 Aerobic oxidation of 1-phenylethanol catalyzed by complex **1a** with various of oxidants^a



Entry	Catalyst (mol%)	Oxidant	Solvent	Yield (%) ^b
1	2.5	NMO	toluene	67
2	2.5	H ₂ O ₂	toluene	59
3	2.5	Bu ^t OOH	toluene	62

^aReaction conditions: 1-phenylethanol (1.0 mmol), toluene (5.0 mL), oxidant (2.5 mmol), reaction time 6 h.

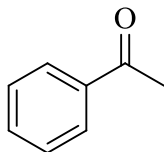
Table S2 Crystallographic data and structure refinement parameters for **1a**, **1c**, **1e**, **1g** and **1i**.

Complex	1a	1c	1e	1g	1i
Empirical formula	C ₂₈ H ₂₄ N ₂ O ₁₀ Ru ₃	C ₂₄ H ₂₀ N ₂ O ₁₀ Ru ₃	C ₃₂ H ₂₀ N ₂ O ₁₀ Ru ₃	C ₃₄ H ₂₄ N ₂ O ₁₂ Ru ₃	C ₃₂ H ₁₈ Br ₂ N ₂ O ₁₀ Ru ₃
Formula weight	851.71	799.63	895.72	955.77	1053.51

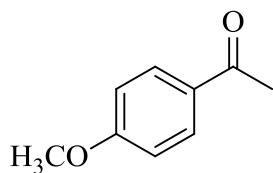
Temperature (K)	298(2)	298(2)	298(2)	298(2)	298(2)
Crystal system	Tetragonal	Orthorhombic	Tetragonal	Monoclinic	Monoclinic
Space group	$P4_32_12$	$P2_12_12_1$	$I\bar{4}2d$	$C2$	$P2_1/n$
a (Å)	12.0348(13)	11.2284(9)	14.677(4)	37.380(3)	16.4503(14)
b (Å)	12.0348(13)	15.3788(12)	14.677(4)	11.6310(11)	10.8605(9)
c (Å)	21.3648(17)	15.7738(13)	29.911(16)	14.8401(12)	20.7249(17)
α (°)	90	90	90	90	90
β (°)	90	90	90	94.3980(10)	106.928(2)
γ (°)	90	90	90	90	90
V (Å ³)	3094.4(5)	2723.8(4)	6443(4)	6433.0(10)	3542.2(5)
Z	4	4	8	6	4
$F(000)$	1672	1650	3504	2816	2024
Dcalc (g/cm ³)	1.828	1.950	1.847	1.096	1.975

Crystal dimensions (mm)	0.40 × 0.27 × 0.21	0.43 × 0.40 × 0.35	0.46 × 0.41 × 0.40	0.45 × 0.15 × 0.12	0.40 × 0.30 × 0.25
θ Range (°)	2.39-25.02	2.58-25.02	2.39-25.01	2.32-25.02	2.28-25.02
Reflections collected	15625/2735	13715/4803	15507/2846	16509/10515	17179/6233
Independent reflections	2735	4803	2846	10515	6233
R_{int}	0.0395	0.0235	0.0739	0.0755	0.0464
Parameters	195	357	213	693	443
Goodness of fit on F^2	1.087	1.149	1.158	1.083	1.014
$R_1, wR_2 [I > 2\sigma(I)]$	0.0335, 0.0784	0.0216, 0.0500	0.0466, 0.1069	0.0775, 0.1711	0.0399, 0.0835
R_1, wR_2 (all data)	0.0482, 0.0884	0.0256, 0.0523	0.0764, 0.1323	0.1602, 0.1839	0.0717, 0.0941
CCDC deposition no.	1492241	1485797	1487563	1518232	1492237

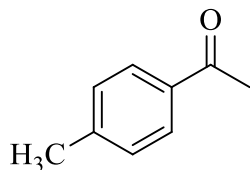
NMR data for products



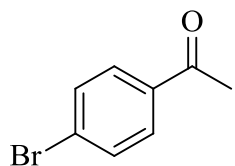
^1H NMR (ppm in CDCl_3 , 500 MHz): δ 2.56 (s, 3H, CH_3), 7.42 (t, $J = 7.5$ Hz, 2H, Ar-H), 7.52 (t, $J = 7.5$ Hz, 1H, Ar-H), 7.92 (d, $J = 7.5$ Hz, 2H, Ar-H). ^{13}C NMR (ppm in CDCl_3 , 125 MHz): δ 26.5, 128.3, 128.5, 133.1, 137.1, 198.0.



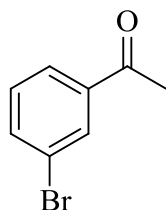
^1H NMR (ppm in CDCl_3 , 500 MHz): δ 2.56 (s, 3H, CH_3), 3.87 (s, 3H, OCH_3), 6.93 (d, $J = 8.0$ Hz, 2H, Ar-H), 7.94 (d, $J = 8.0$ Hz, 2H, Ar-H). ^{13}C NMR (ppm in CDCl_3 , 125 MHz): δ 26.3, 55.4, 113.7, 130.4, 130.6, 163.5, 196.7.



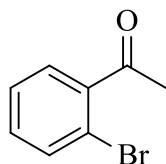
^1H NMR (ppm in CDCl_3 , 500 MHz): δ 2.37 (s, 3H, CH_3), 2.55 (s, 3H, CH_3), 7.22 (d, $J = 8.0$ Hz, 2H, Ar-H), 7.84 (d, $J = 8.0$ Hz, 2H, Ar-H). ^{13}C NMR (ppm in CDCl_3 , 125 MHz): δ 21.5, 26.4, 128.3, 129.3, 134.7, 143.8, 198.0.



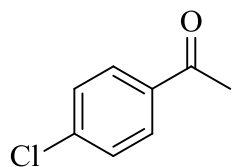
^1H NMR (ppm in CDCl_3 , 500 MHz): δ 2.60 (s, 3H, CH_3), 7.61 (d, $J = 8.5$ Hz, 2H, Ar-H), 7.83 (d, $J = 8.5$ Hz, 2H, Ar-H). ^{13}C NMR (ppm in CDCl_3 , 125 MHz): δ 26.5, 128.3, 129.8, 131.9, 135.9, 197.0.



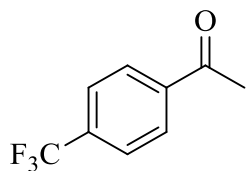
^1H NMR (ppm in CDCl_3 , 500 MHz): δ 2.57 (s, 3H, CH_3), 7.32 (t, $J = 8.0$ Hz, 1H, Ar-H), 7.66 (d, $J = 8.0$ Hz, 1H, Ar-H), 7.85 (d, $J = 8.0$ Hz, 1H, Ar-H), 8.05 (s, 1H, Ar-H). ^{13}C NMR (ppm in CDCl_3 , 125 MHz): δ 26.6, 122.9, 126.9, 130.2, 131.3, 135.9, 138.8, 196.5.



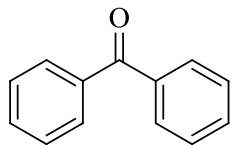
^1H NMR (ppm in CDCl_3 , 500 MHz): δ 2.63 (s, 3H, CH_3), 7.29 (t, $J = 7.5$ Hz, 1H, Ar-H), 7.36 (t, $J = 8.5$ Hz, 1H, Ar-H), 7.48 (d, $J = 8.5$ Hz, 1H, Ar-H), 7.61 (d, $J = 7.0$ Hz, 1H, Ar-H). ^{13}C NMR (ppm in CDCl_3 , 125 MHz): δ 30.3, 118.9, 127.5, 128.9, 131.8, 133.8, 141.5, 200.1.



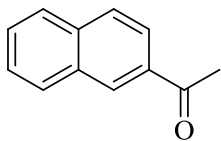
$^1\text{H NMR}$ (ppm in CDCl_3 , 500 MHz): δ 2.57(s, 3H, CH_3), 7.42 (d, $J = 9.0$ Hz, 2H, Ar-H), 7.89 (d, $J = 8.5$ Hz, 2H, Ar-H). $^{13}\text{C NMR}$ (ppm in CDCl_3 , 125 MHz): δ 26.5, 128.8, 129.7, 135.4, 139.5, 196.7.



$^1\text{H NMR}$ (ppm in CDCl_3 , 500 MHz): δ 2.67 (s, 3H, CH_3), 7.75 (d, $J = 8.0$ Hz, 2H, Ar-H), 8.08 (d, $J = 8.0$ Hz, 2H, Ar-H). $^{13}\text{C NMR}$ (ppm in CDCl_3 , 125 MHz): δ 26.7, 125.2 (q, $J = 272.5$ Hz), 125.7, 128.6, 134.3, 139.7, 196.9.



$^1\text{H NMR}$ (ppm in CDCl_3 , 500 MHz): δ 7.50 (t, $J = 7.5$ Hz, 4H, Ar-H), 7.61 (t, $J = 7.5$ Hz, 2H, Ar-H), 7.84 (d, $J = 8.5$ Hz, 4H, Ar-H). $^{13}\text{C NMR}$ (ppm in CDCl_3 , 125 MHz): δ 128.3, 130.1, 132.4, 137.6, 196.7.



¹H NMR (ppm in CDCl₃, 500 MHz): δ 2.70 (s, 3H, CH₃), 7.51-7.61 (m, 2H, Ar-H), 7.85 (t, J = 8.5 Hz, 2H, Ar-H), 7.94 (d, J = 8.0 Hz, 1H, Ar-H), 8.01 (d, J = 8.5 Hz, 1H, Ar-H), 8.44 (s, 1H, Ar-H). ¹³C NMR (ppm in CDCl₃, 125 MHz): δ 26.7, 123.9, 126.8, 127.8, 128.4, 128.5, 129.6, 130.2, 132.5, 134.5, 135.6, 198.1.