

Supporting Information

New Type of 2,6-Bis(imidazo[1,2-*a*]pyridin-2-yl)pyridine-Based Ruthenium Complexes: Active Catalysts for Transfer Hydrogenation of Ketones

Ke Li, Jun-Long Niu, Ming-Ze Yang, Zhen Li, Li-Yuan Wu, Xin-Qi Hao*, Mao-Ping
Song*

College of Chemistry and Molecular Engineering, Henan Key Laboratory of Chemical Biology
and Organic Chemistry, Zhengzhou University, Zhengzhou 450001, People's Republic of China

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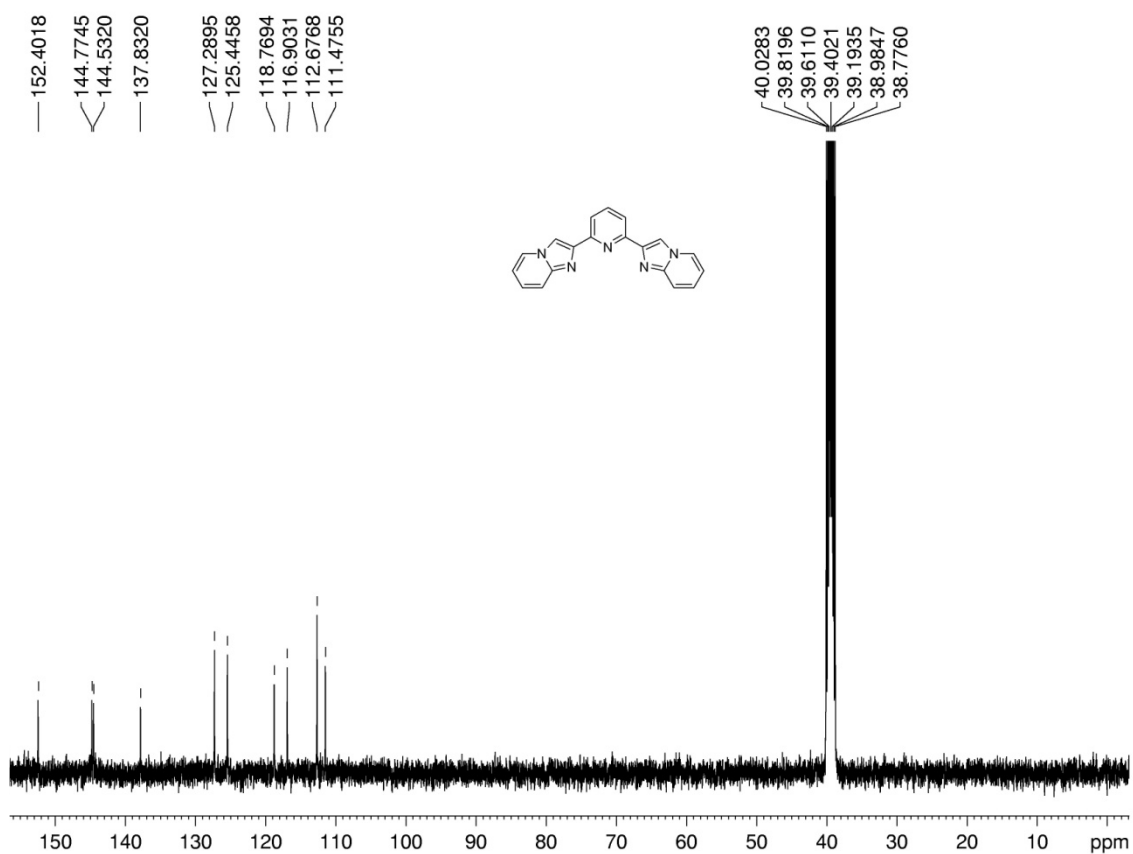
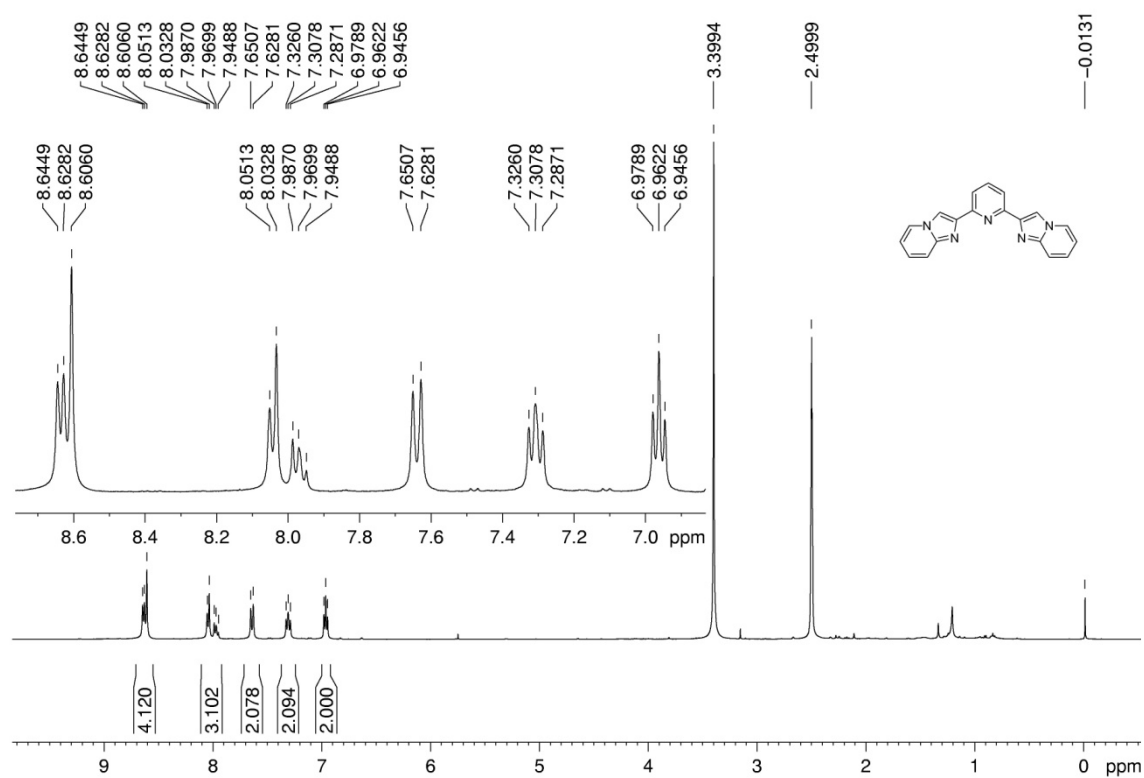
*Tel./Fax: (+86)-371-6776-3869.

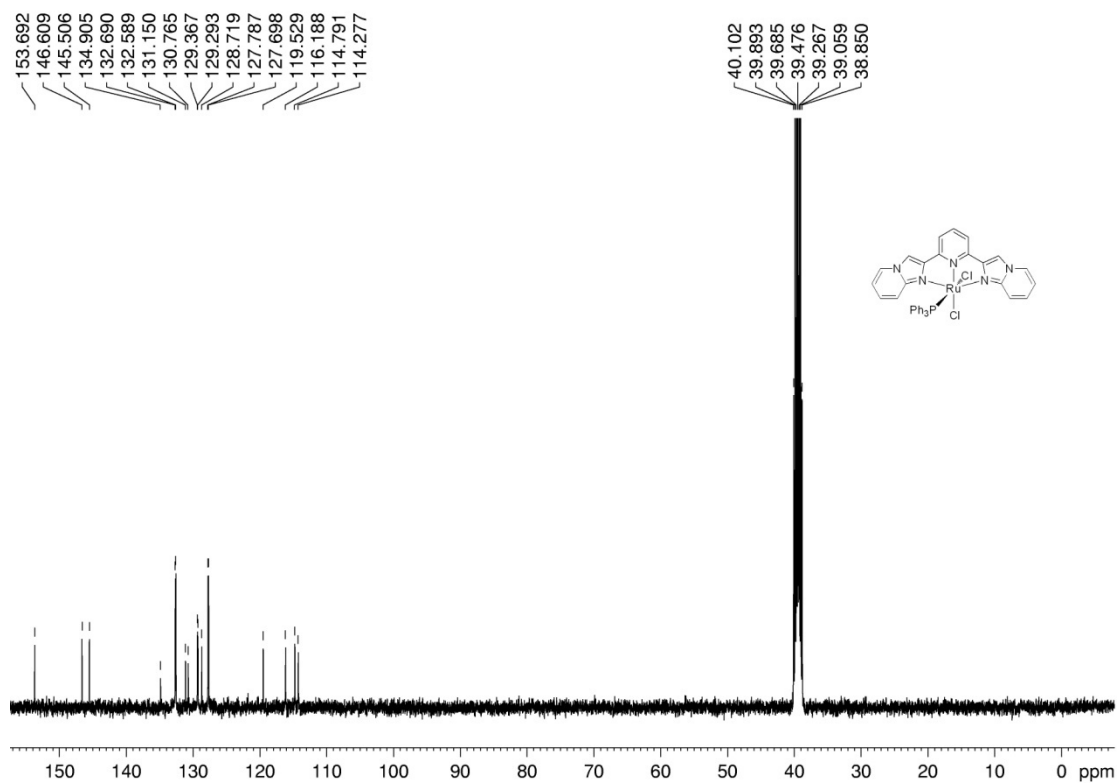
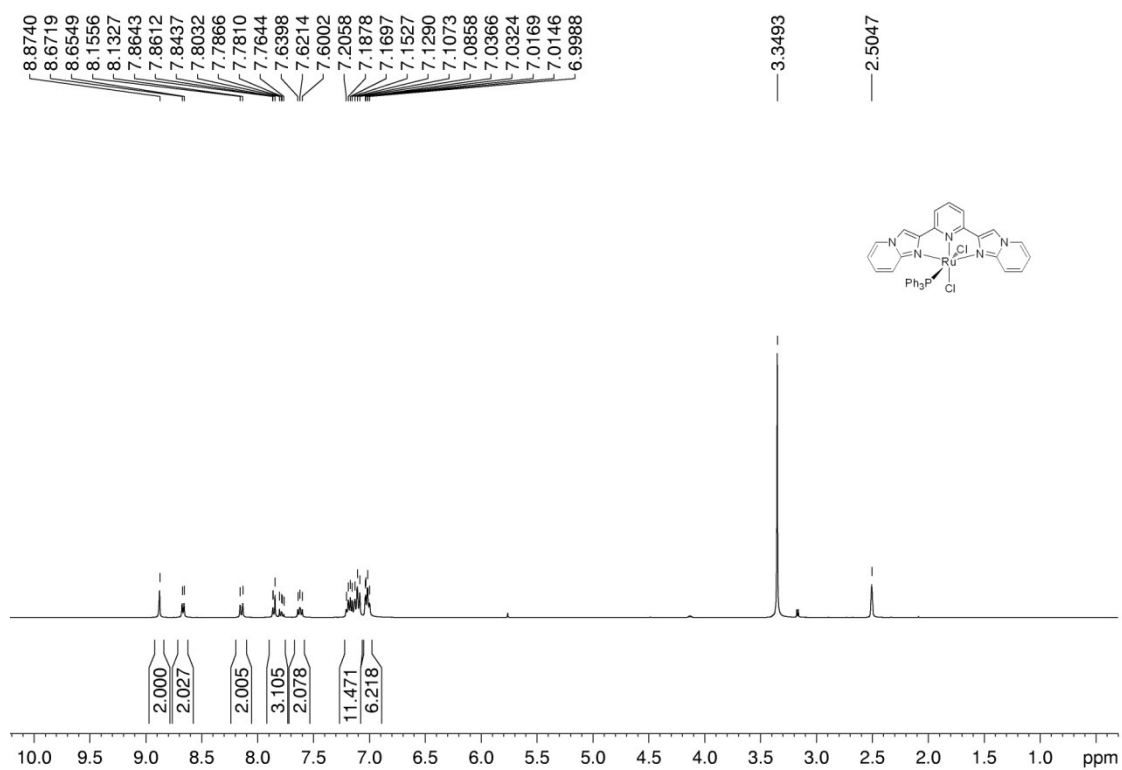
E-mail: mpsong@zzu.edu.cn (M.-P. Song), xqhao@zzu.edu.cn (X.-Q. Hao)

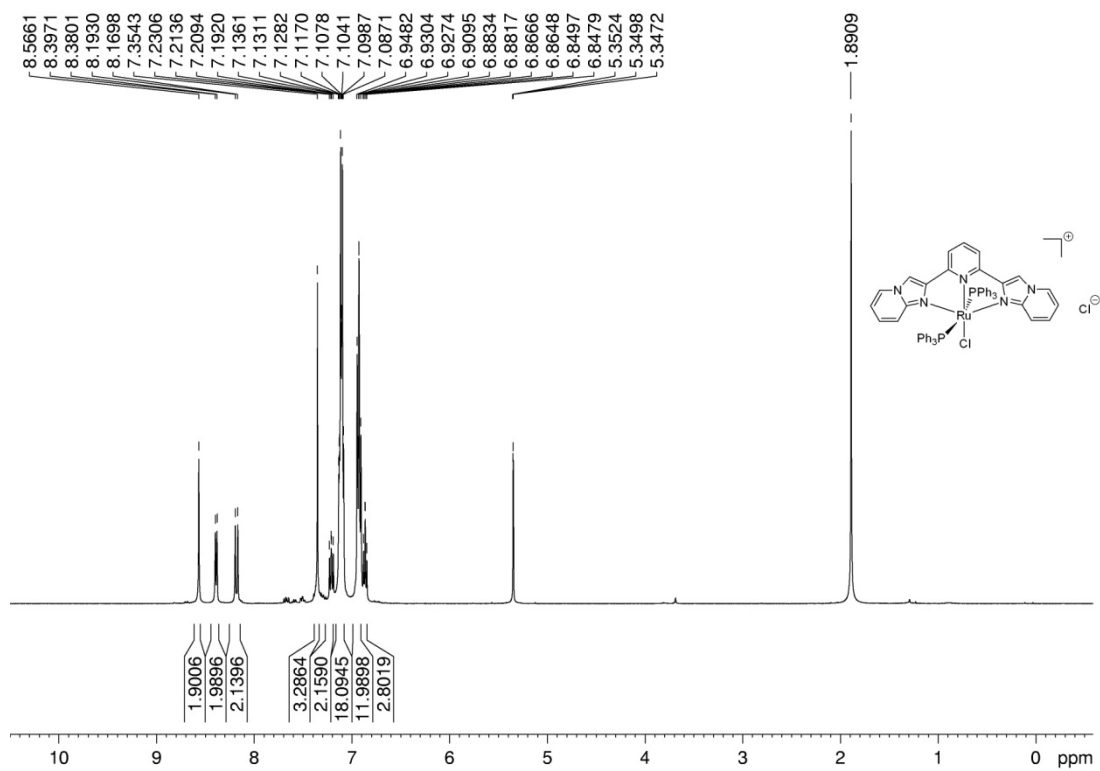
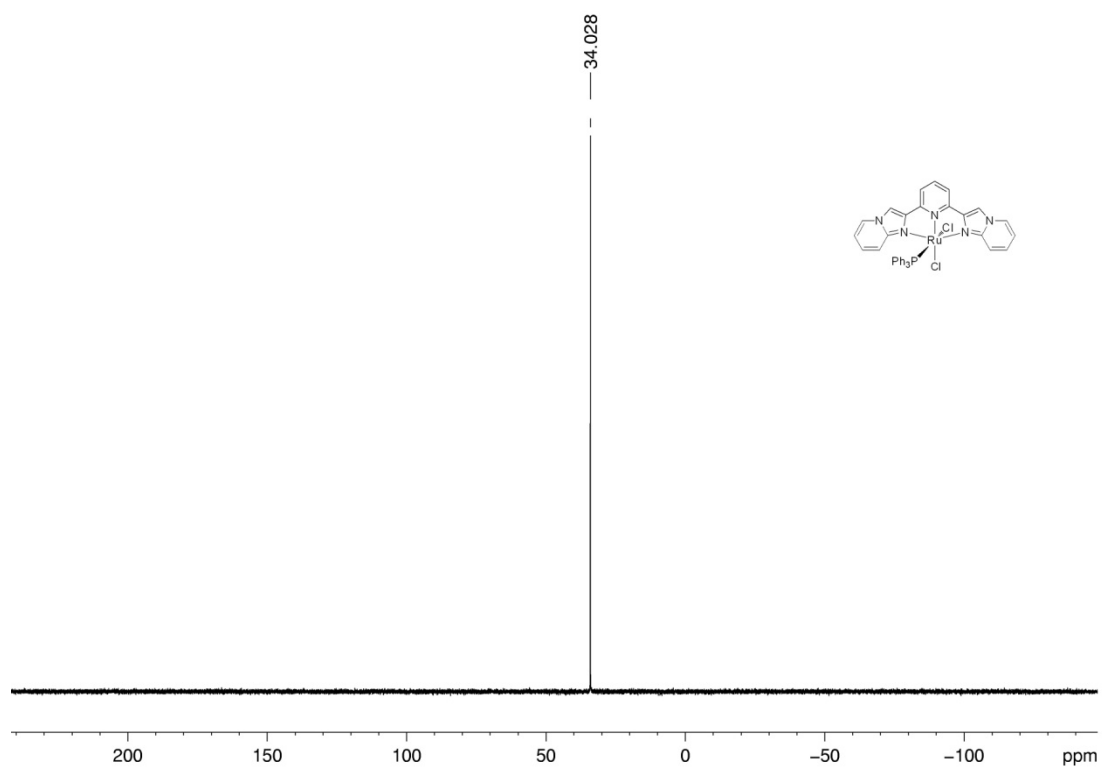
Table S1. Summary of Crystal Structure Determination for Complexes 4 and 5

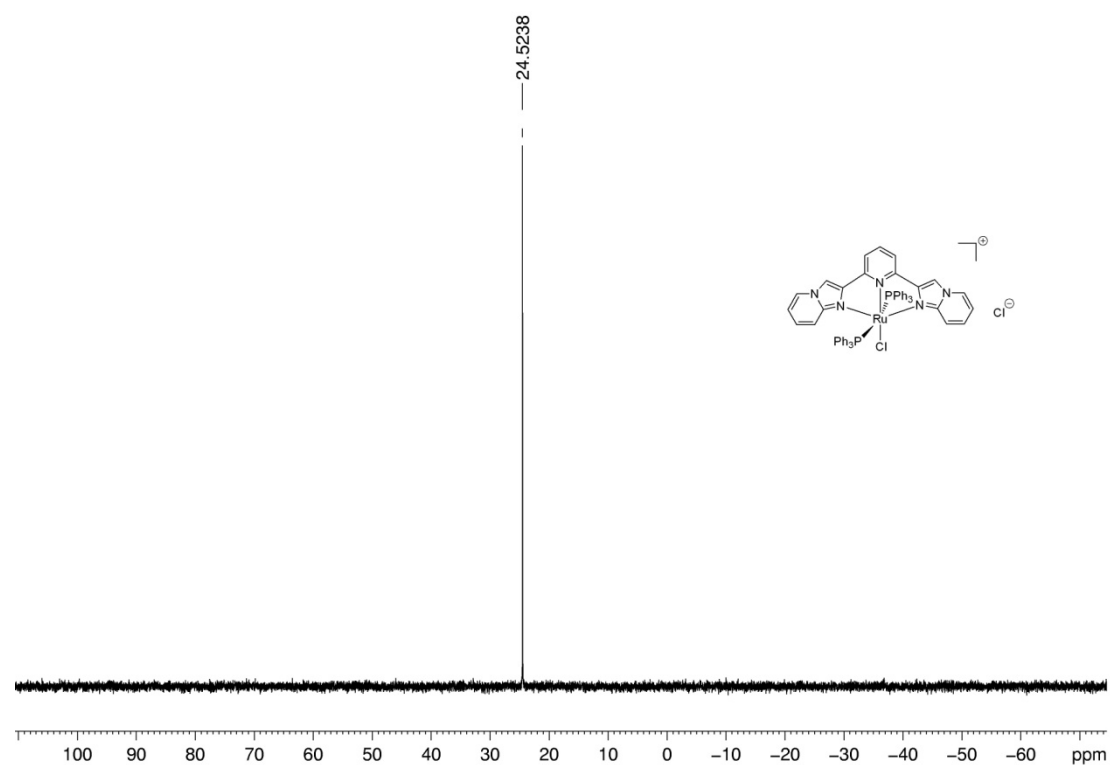
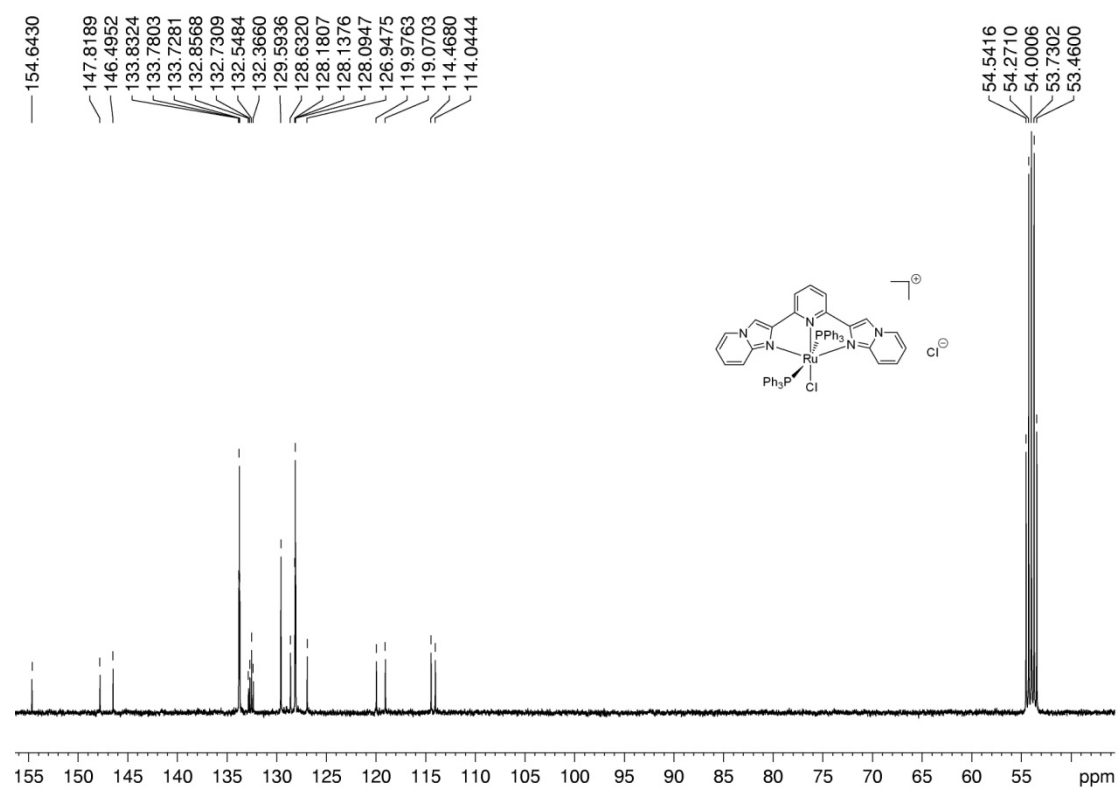
formula	C ₃₇ H ₂₈ Cl ₂ N ₅ PRu	C ₅₈ H ₄₉ Cl ₈ N ₅ P ₂ Ru
<i>Mr.</i>	745.58	1262.63
Temp (K)	291.15	291.15
Cryst syst	tetragonal	orthorhombic
Space group	I4 ₁ /a	C222 ₁
Cryst size/mm ³	0.2 × 0.2 × 0.2	0.20 × 0.20 × 0.18
<i>a</i> /Å	32.3373(9)	12.4002(3)
<i>b</i> /Å	32.3373(9)	19.0341(6)
<i>c</i> /Å	15.1351(7)	24.7514(12)
<i>α</i> /°	90.00	90.00
<i>β</i> /°	90.00	90.00
<i>γ</i> /°	90.00	90.00
<i>V</i> /Å ³	15826.7(9)	5842.0(4)
<i>Z</i>	16	4
<i>D</i> _{calc} g/cm ³	1.252	1.436
<i>μ</i> /mm ⁻¹	5.062	0.731
<i>θ</i> range/°	7.74 to 133.80	6.30 to 52.74
F(000)	6048.0	2568.0
Index ranges	-36 ≤ <i>h</i> ≤ 38, -38 ≤ <i>k</i> ≤ 14, -17 ≤ <i>l</i> ≤ 17	-15 ≤ <i>h</i> ≤ 15, -23 ≤ <i>k</i> ≤ 21, -30 ≤ <i>l</i> ≤ 30
Reflections collected	14644	24148
Independent reflections	7022 [<i>R</i> _{int} = 0.0333]	5969 [<i>R</i> _{int} = 0.0426]
Data/restraints/parameters	7022/54/415	5969/1/338
Goodness-of-fit on <i>F</i> ²	1.018	1.042
Final <i>R</i> indexes [<i>I</i> ≥ 2σ (<i>I</i>)]	<i>R</i> ₁ = 0.0452, <i>wR</i> ₂ = 0.1238	<i>R</i> ₁ = 0.0438, <i>wR</i> ₂ = 0.1042
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0613, <i>wR</i> ₂ = 0.1359	<i>R</i> ₁ = 0.0508, <i>wR</i> ₂ = 0.1082
Largest diff. Peak / hole / e Å ⁻³	0.59/-0.26	0.49/-0.32

Copies of the NMR Spectra of Compounds **3-5**.

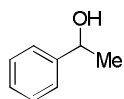




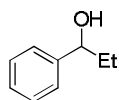




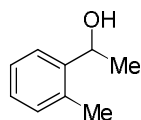
Characterization Data of Compounds the Catalysis Products.



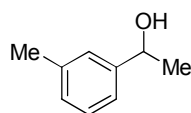
^1H NMR (400 MHz, CDCl_3): δ 7.36-7.31 (m, 4H), 7.27-7.23 (m, 1H), 4.85 (q, $J = 6.4$ Hz, 1H), 2.26 (brs, 1H), 1.46 (d, $J = 6.4$ Hz, 3H).



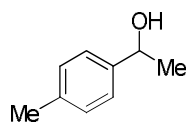
^1H NMR (400 MHz, CDCl_3): δ 7.34-7.28 (m, 4H), 7.26-7.22 (m, 1H), 4.52 (t, $J = 6.4$ Hz, 1H), 2.41 (brs, 1H), 1.81-1.66 (m, 2H), 0.87 (t, $J = 7.4$ Hz, 3H).



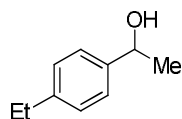
^1H NMR (400 MHz, CDCl_3): δ 7.51 (dd, $J = 0.8, 7.6$ Hz, 1H), 7.25 (dt, $J = 1.2, 7.2$ Hz, 1H), 7.19 (dt, $J = 1.2, 7.2$ Hz, 1H), 7.15 (d, $J = 7.2$ Hz, 1H), 5.10 (q, $J = 6.4$ Hz, 1H), 2.35 (s, 4H), 1.46 (d, $J = 6.4$ Hz, 3H).



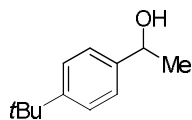
^1H NMR (400 MHz, CDCl_3): δ 7.25 (t, $J = 7.6$ Hz, 1H), 7.20 (s, 1H), 7.17 (d, $J = 7.6$ Hz, 1H), 7.10 (d, $J = 7.6$ Hz, 1H), 4.84 (q, $J = 6.4$ Hz, 1H), 2.38 (s, 3H), 2.22 (brs, 1H), 1.49 (d, $J = 6.4$ Hz, 3H).



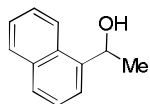
^1H NMR (400 MHz, CDCl_3): δ 7.26 (d, $J = 8.0$ Hz, 2H), 7.16 (d, $J = 8.0$ Hz, 2H), 4.85 (q, $J = 6.4$ Hz, 1H), 2.35 (s, 3H), 2.09 (s, 1H), 1.48 (d, $J = 6.4$ Hz, 3H).



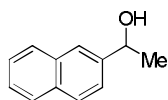
^1H NMR (400 MHz, CDCl_3): δ 7.29 (d, $J = 8.0$ Hz, 2H), 7.19 (d, $J = 8.0$ Hz, 2H), 4.85 (q, $J = 6.4$ Hz, 1H), 2.66 (q, $J = 7.6$ Hz, 2H), 2.21 (brs, 1H), 1.48 (d, $J = 6.4$ Hz, 2H), 1.25 (t, $J = 7.6$ Hz, 3H).



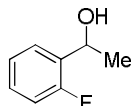
^1H NMR (400 MHz, CDCl_3): δ 7.39 (dt, $J = 2.0, 8.4$ Hz, 2H), 7.32 (dt, $J = 2.0, 8.4$ Hz, 2H), 4.88 (dq, $J = 2.8, 6.4$ Hz, 1H), 1.93 (brs, 1H), 1.50 (d, $J = 6.4$ Hz, 3H), 1.34 (s, 9H).



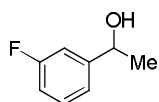
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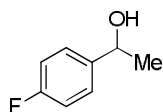
^1H NMR (400 MHz, CDCl_3): δ 7.86-7.82 (m, 3H), 7.79 (s, 1H), 7.52-7.47 (m, 3H), 5.05-5.00 (m, 1H), 2.31 (brs, 1H), 1.58 (d, $J = 6.4$ Hz, 3H).



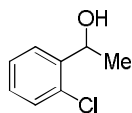
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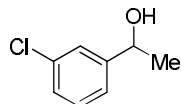
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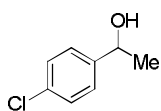
^1H NMR (400 MHz, CDCl_3): δ 7.31-7.26 (m, 2H), 7.00 (tt, $J = 2.0, 8.8$ Hz, 2H), 4.82 (q, $J = 6.4$ Hz, 1H), 2.66 (brs, 1H), 1.43 (d, 6.4 Hz, 3H).



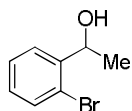
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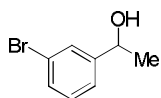
^1H NMR (400 MHz, CDCl_3): δ 7.35 (s, 1H), 7.28-7.20 (m, 3H), 4.84 (q, $J = 6.4$ Hz, 1H), 2.32 (brs, 1H), 1.45 (d, $J = 6.4$ Hz, 3H).



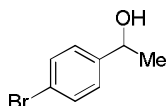
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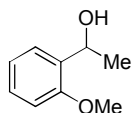
^1H NMR (400 MHz, CDCl_3): δ 7.56 (dd, $J = 1.6, 7.6$ Hz, 1H), 7.50 (dd, $J = 1.2, 8.0$ Hz, 1H), 7.32 (dt, $J = 1.2, 7.6$ Hz, 1H), 7.10 (dt, $J = 1.6, 7.6$ Hz, 1H), 5.21 (q, $J = 6.4$ Hz, 1H), 2.47 (brs, 1H), 1.45 (d, $J = 6.4$ Hz, 3H).



^1H NMR (400 MHz, CDCl_3): δ 7.48 (s, 1H), 7.36 (d, $J = 7.6$ Hz, 1H), 7.22 (d, $J = 7.6$ Hz, 1H), 7.17 (t, $J = 7.6$ Hz, 1H), 4.76 (q, $J = 6.4$ Hz, 1H), 2.97 (brs, 1H), 1.41 (dd, $J = 2.8, 6.4$ Hz, 3H).

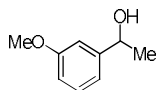


^1H NMR (400 MHz, CDCl_3): δ 7.43 (d, $J = 8.4$ Hz, 2H), 7.18 (d, $J = 8.4$ Hz, 2H), 4.78 (q, $J = 6.0$ Hz, 1H), 2.72 (brs, 1H), 1.41 (dd, $J = 0.8, 6.4$ Hz, 3H).

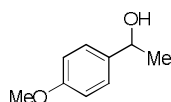


^1H NMR (400 MHz, CDCl_3): δ 7.36 (dd, $J = 1.6, 7.6$ Hz, 1H), 7.25 (dt, $J = 1.6, 7.6$ Hz,

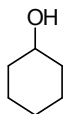
1H), 6.97 (dt, $J = 0.8, 7.6$ Hz, 1H), 6.87 (d, $J = 8.0$ Hz, 1H), 5.10 (q, $J = 6.4$ Hz, 1H), 3.84 (s, 3H), 2.94 (brs, 1H), 1.50 (d, $J = 6.4$ Hz, 3H).



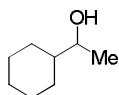
^1H NMR (400 MHz, CDCl_3): δ 7.24 (t, $J = 8.0$ Hz, 1H), 6.93-6.91 (m, 2H), 6.81-6.78 (m, 1H), 4.82 (q, $J = 6.4$ Hz, 1H), 3.79 (s, 3H), 2.53 (brs, 1H), 1.46 (d, $J = 6.4$ Hz, 3H).



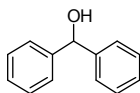
^1H NMR (400 MHz, CDCl_3): δ 7.26 (d, $J = 8.4$ Hz, 2H), 6.86 (d, $J = 8.8$ Hz, 2H), 4.79 (q, $J = 6.4$ Hz, 1H), 3.78 (s, 3H), 2.67 (brs, 1H), 1.44 (d, $J = 6.4$ Hz, 3H).



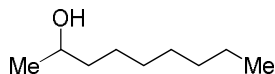
^1H NMR (400 MHz, CDCl_3): δ 3.60-3.54 (m, 1H), 2.00 (brs, 1H), 1.87-1.84 (m, 2H), 1.73-1.69 (m, 2H), 1.54-1.49 (m, 1H), 1.30-1.11 (m, 5H).



^1H NMR (400 MHz, CDCl_3): δ 3.55-3.48 (m, 1H), 1.84-1.63 (m, 6H), 1.29-1.08 (m, 4H), 1.13 (d, $J = 6.4$ Hz, 3H), 1.03-0.88 (m, 2H).



^1H NMR (400 MHz, CDCl_3): δ 7.40-7.28 (m, 10H), 5.82 (d, $J = 2.8$ Hz, 1H), 2.48 (brs, 1H).



^1H NMR (400 MHz, CDCl_3): δ 3.81-3.76 (m, 1H), 1.42-1.41 (m, 4H), 1.29 (brs, 9H), 1.19 (dd, $J = 6.2, 1.9$ Hz, 3H), 0.90-0.87 (m, 3H).

Copies of the NMR Spectra of the Catalysis Products.

