C-H Bond-activation in aromatic ketones mediated by Iridium-Tris(pyrazolyl) borate complexes

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Contents:

1) Sample ^{1}H and ^{13}C NMR spectra for new products.
2) FT-IR spectra of all complexes
3) ORTEP figures for complexes **6** and **7**
4) NMR spectra for the products of reduction catalytic transfer hydrogenation.

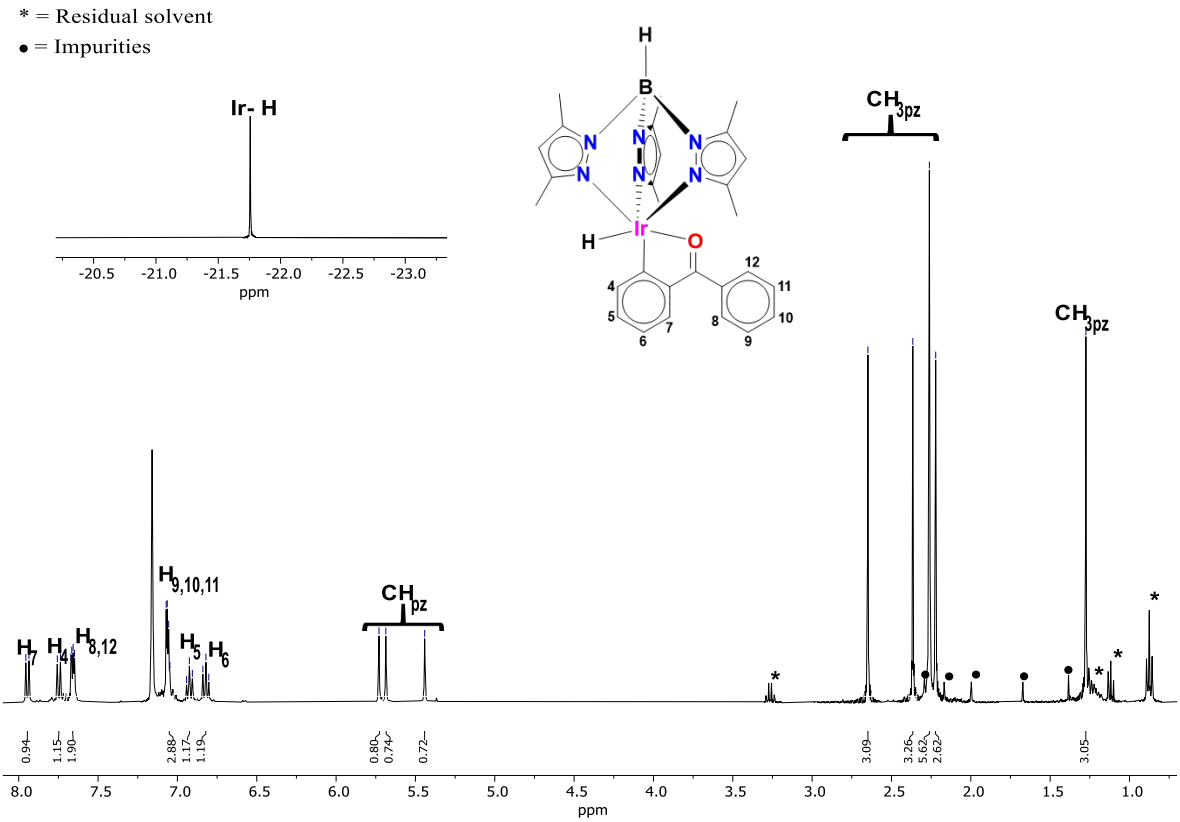


Figure S-1. ^{1}H NMR (400 MHz) spectrum for **2** in $CDCl_3$.

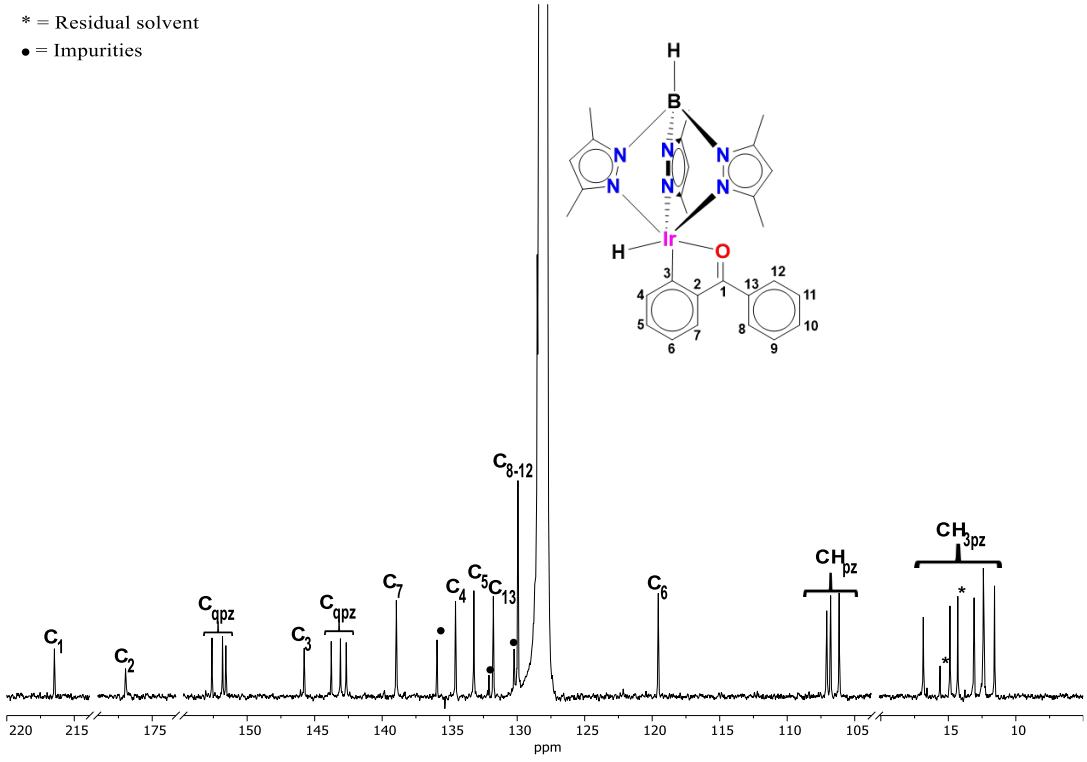


Figure S-2. ^{13}C NMR (100 MHz) spectrum for **2** in $CDCl_3$.

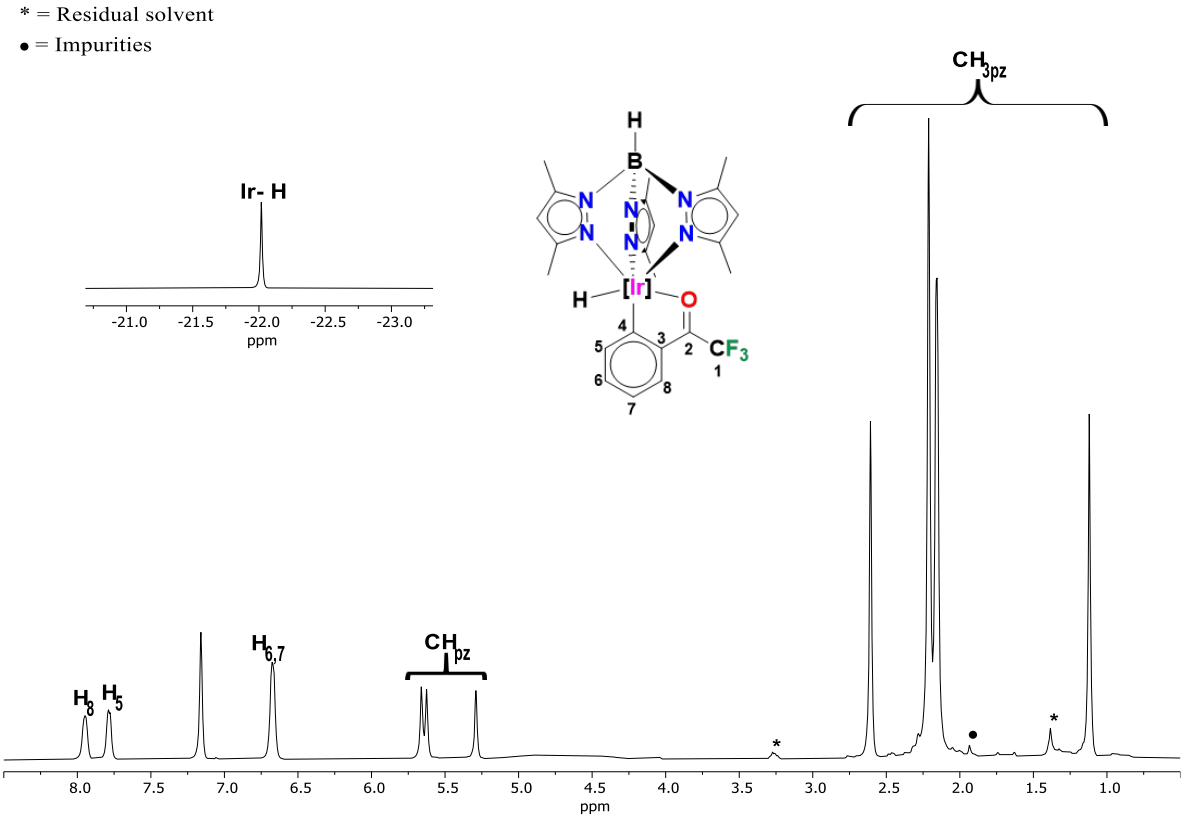


Figure S-3. ^{1}H NMR (400 MHz) spectrum for **3** in $CDCl_3$.

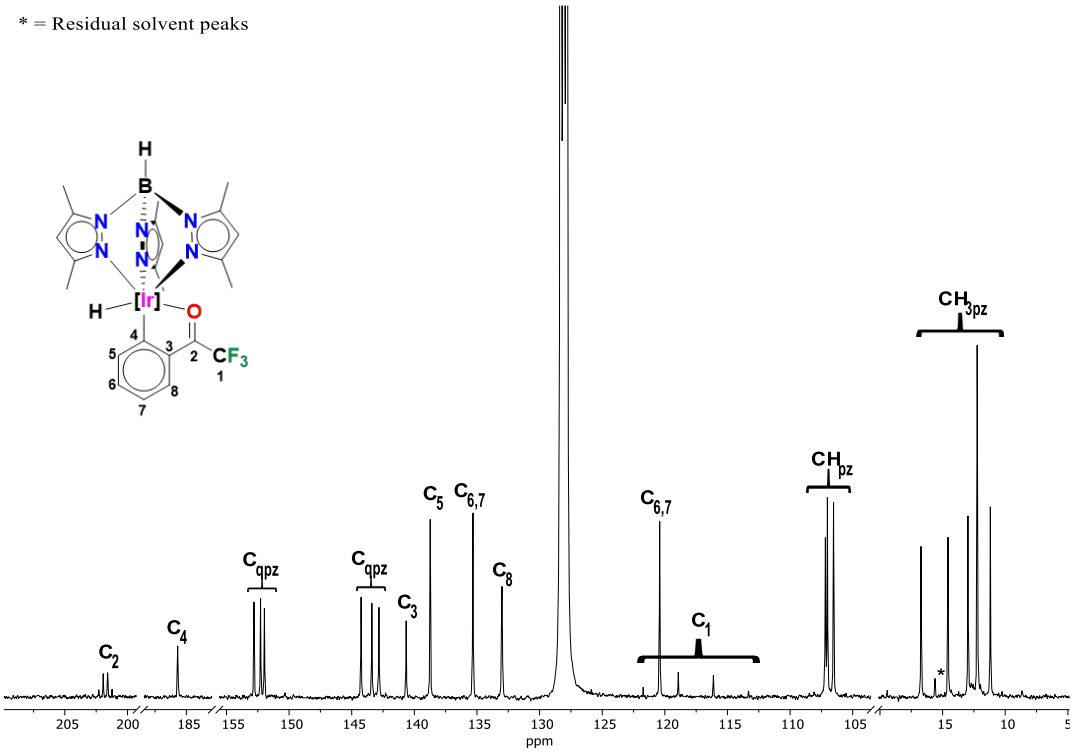


Figure S-4. ^{13}C NMR (100 MHz) spectrum for **3** in $CDCl_3$.

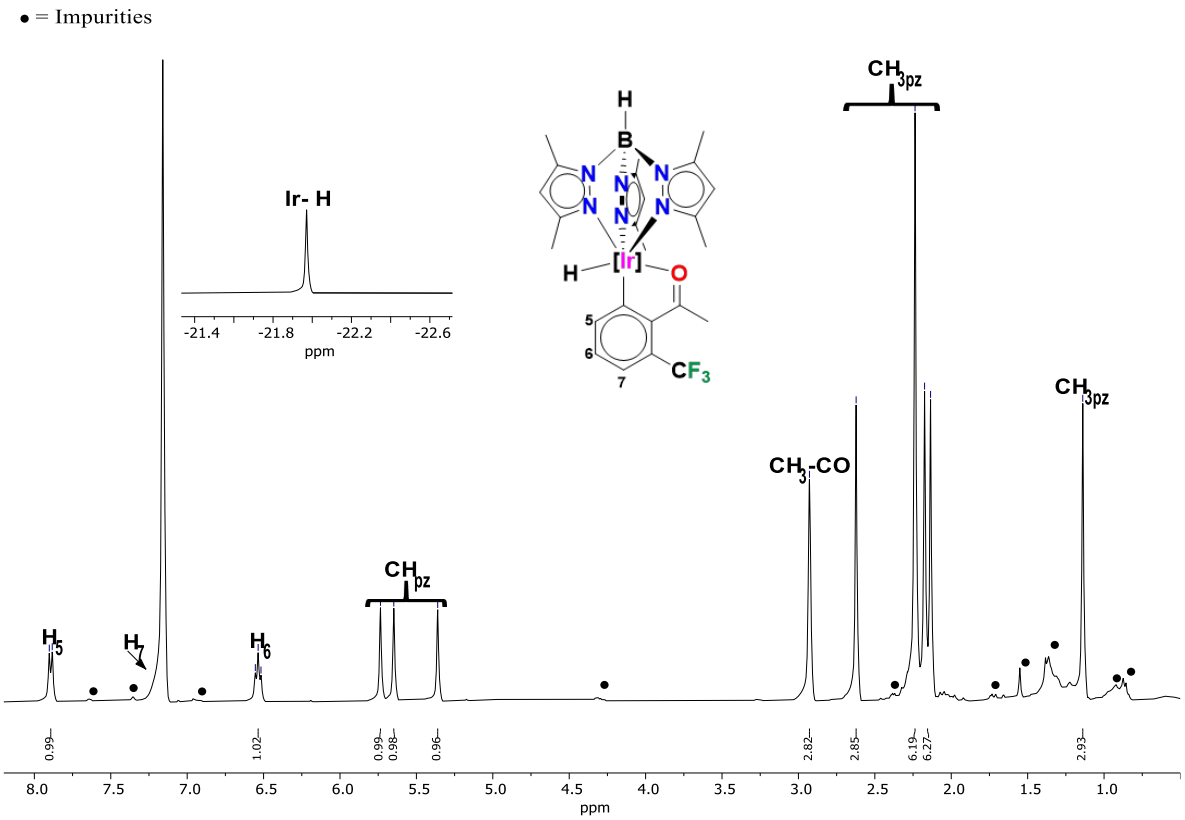


Figure S-5. ^{1}H NMR (400 MHz) spectrum for **4** in $CDCl_3$.

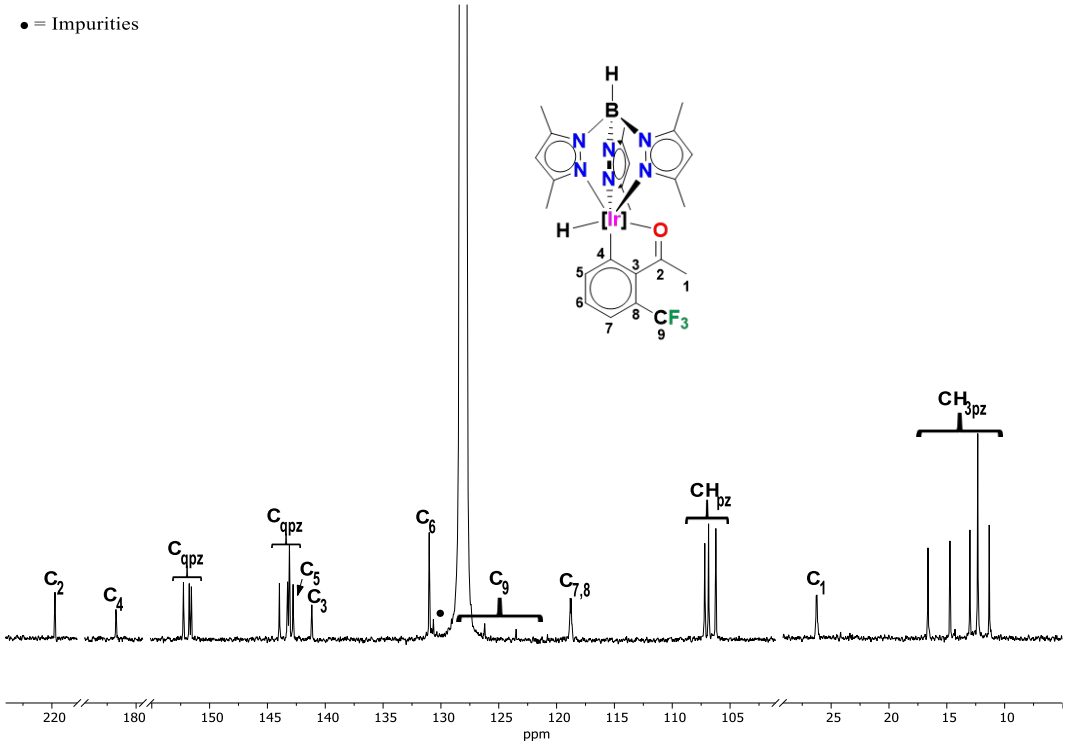


Figure S-6. ^{13}C NMR (100 MHz) spectrum for **4** in $CDCl_3$.

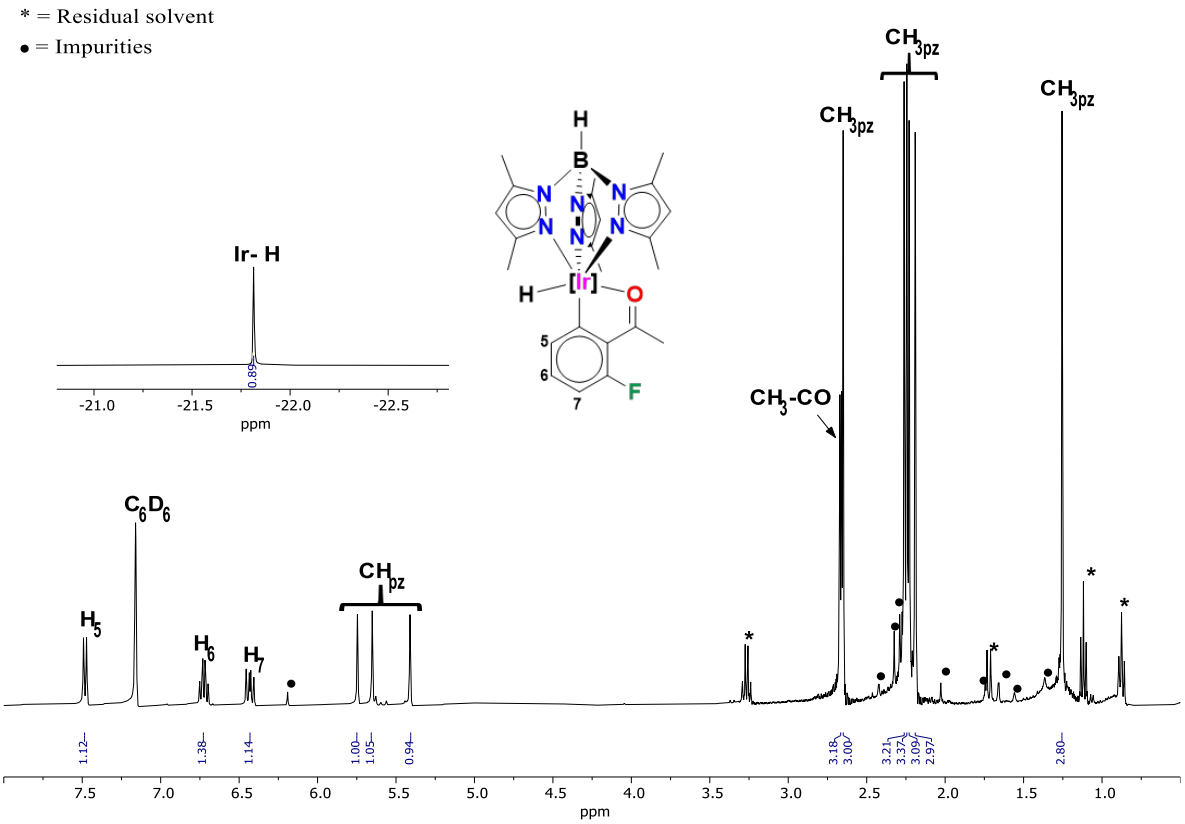


Figure S-7. ^{1}H NMR (400 MHz) spectrum for **5** in $CDCl_3$.

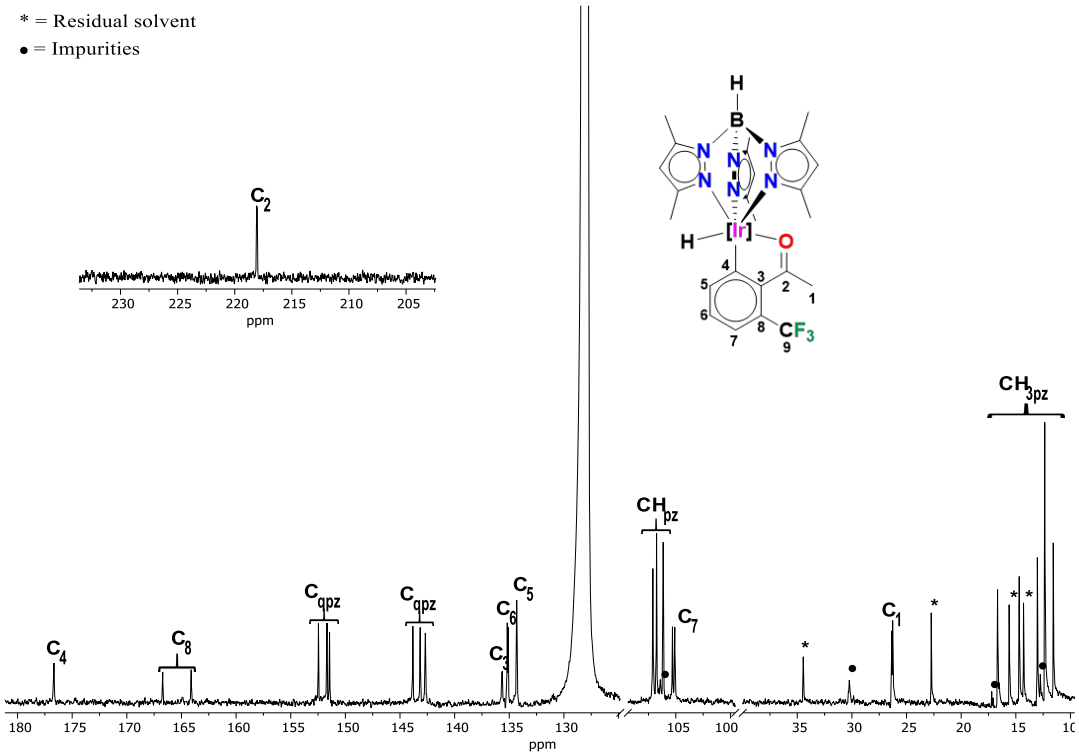


Figure S-8. ^{13}C NMR (100 MHz) spectrum for **5** in $CDCl_3$.

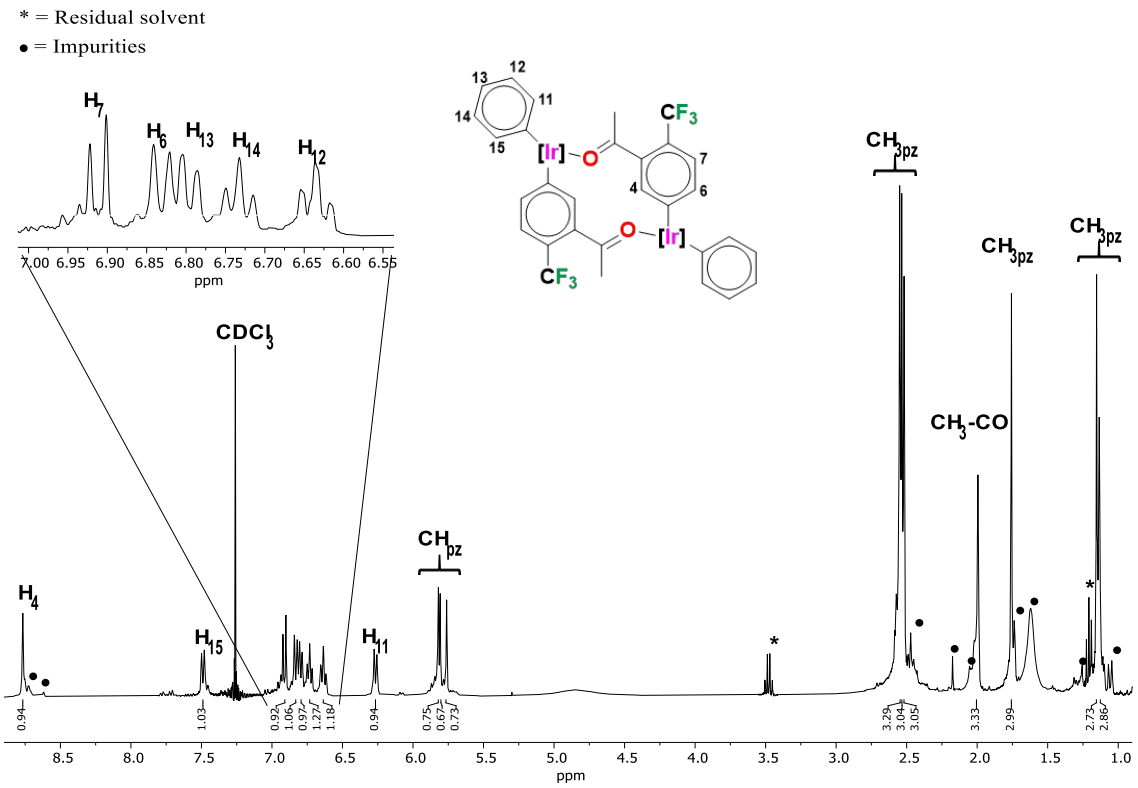


Figure S-9. ^{1}H NMR (400 MHz) spectrum for **7** in $CDCl_3$.

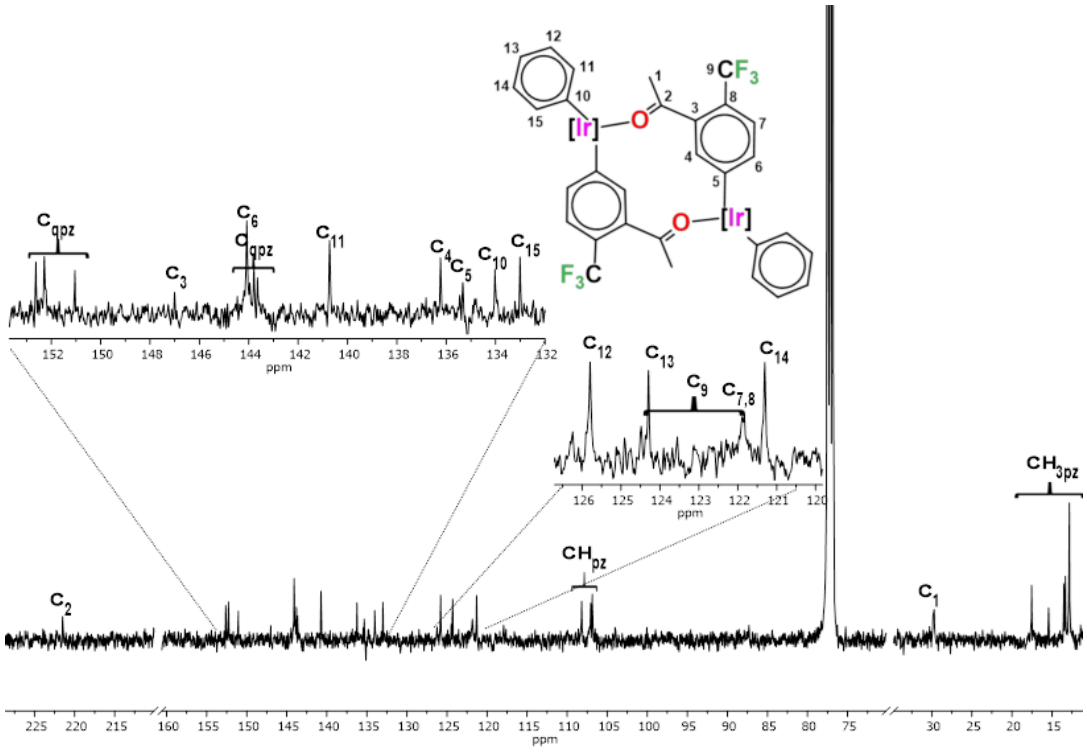


Figure S-10. ^{13}C NMR (100 MHz) spectrum for **7** in $CDCl_3$.

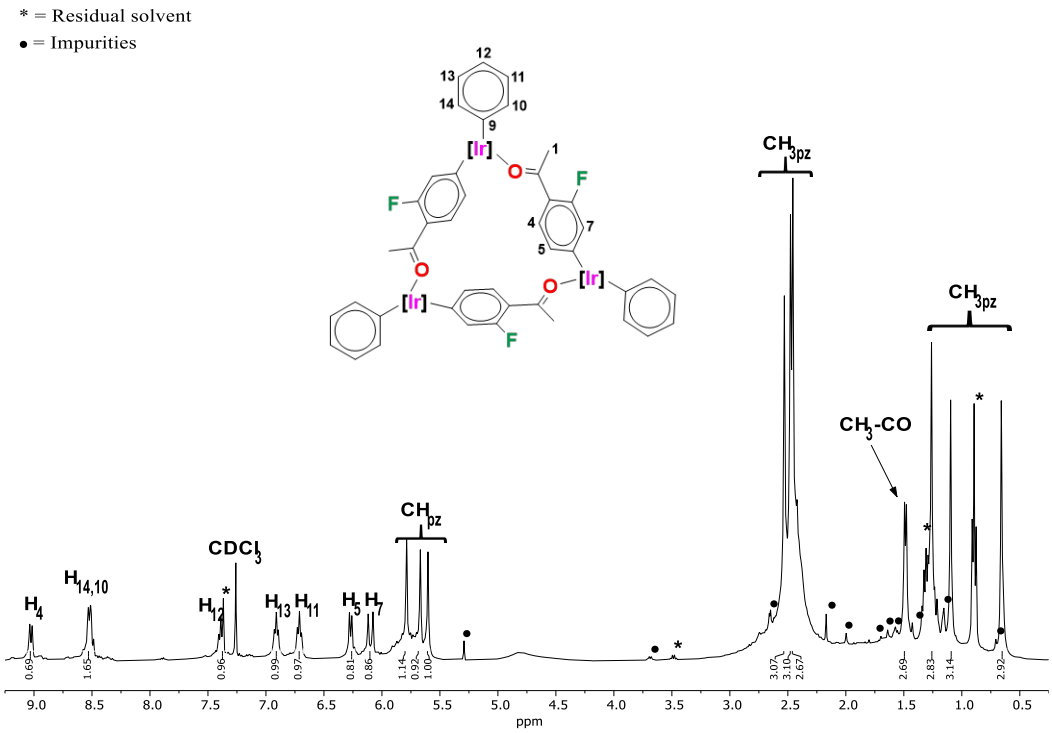


Figure S-11. ^{1}H NMR (400 MHz) spectrum for **8** in $CDCl_3$.

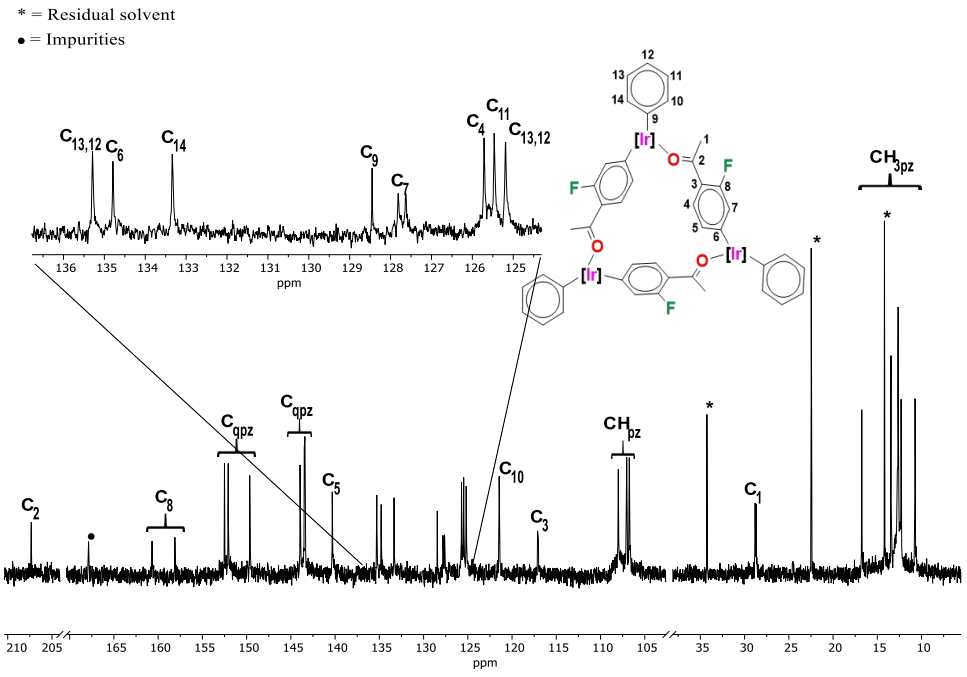


Figure S-12. ^{13}C NMR (100 MHz) spectrum for **8** in $CDCl_3$.

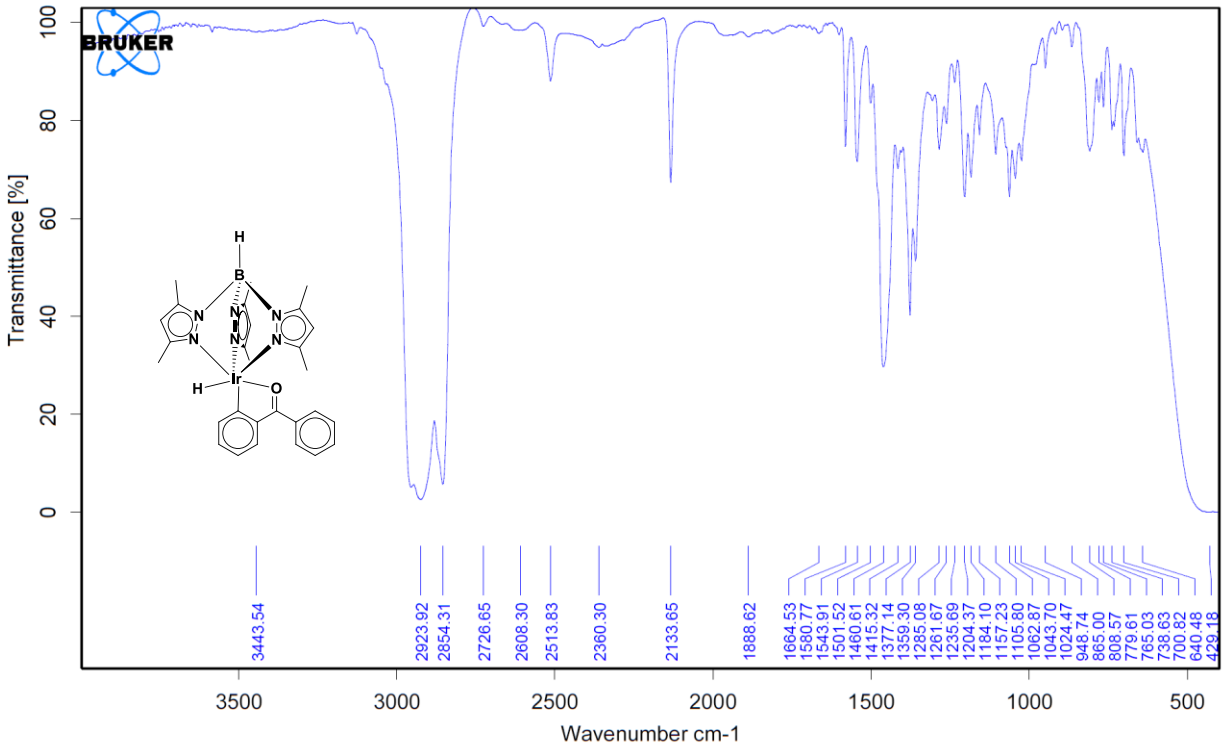


Figure S-13. Spectrum of infrared for complex **2** in nujol.

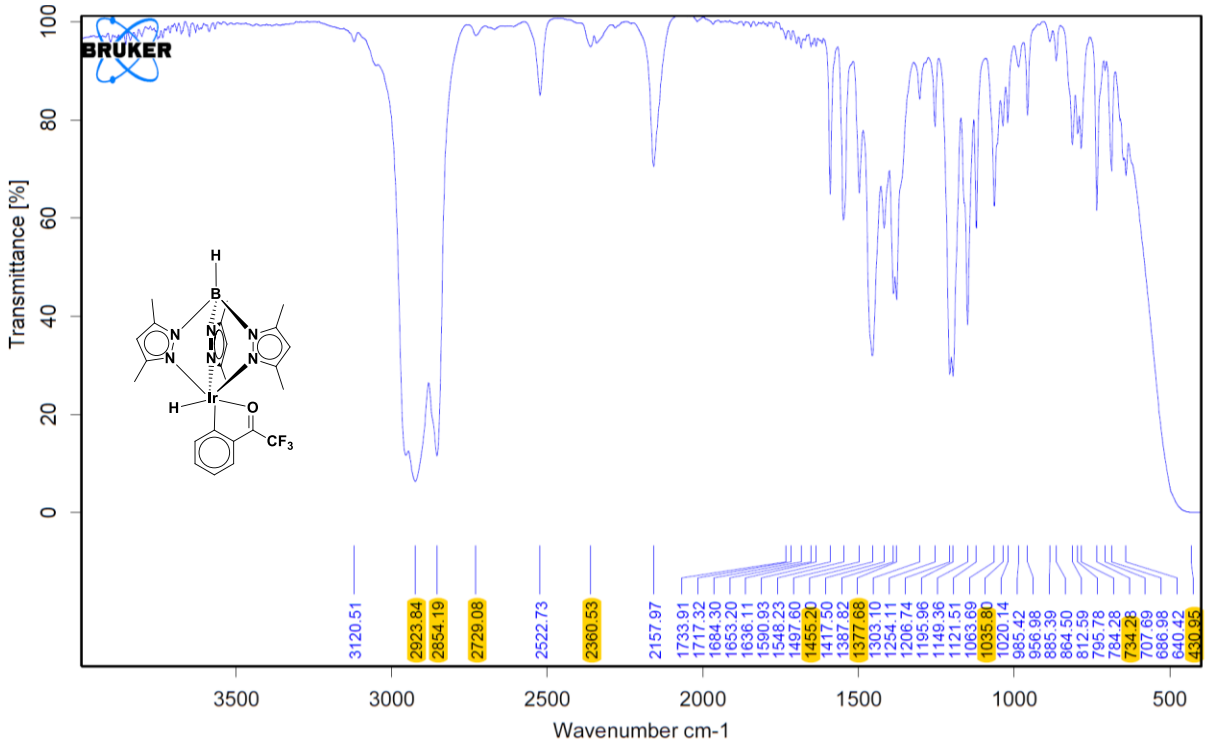


Figure S-14. Spectrum of infrared for complex **3** in nujol.

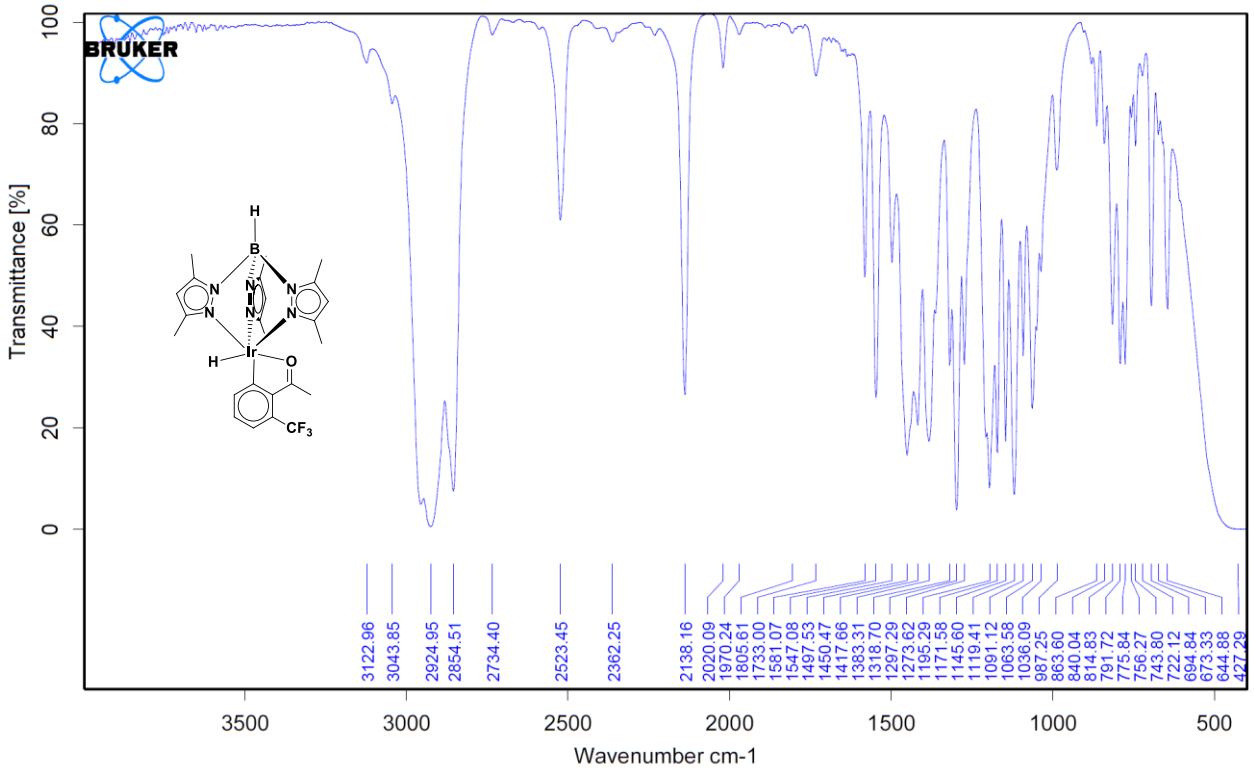


Figure S-15. Spectrum of infrared for complex **4** in nujol.

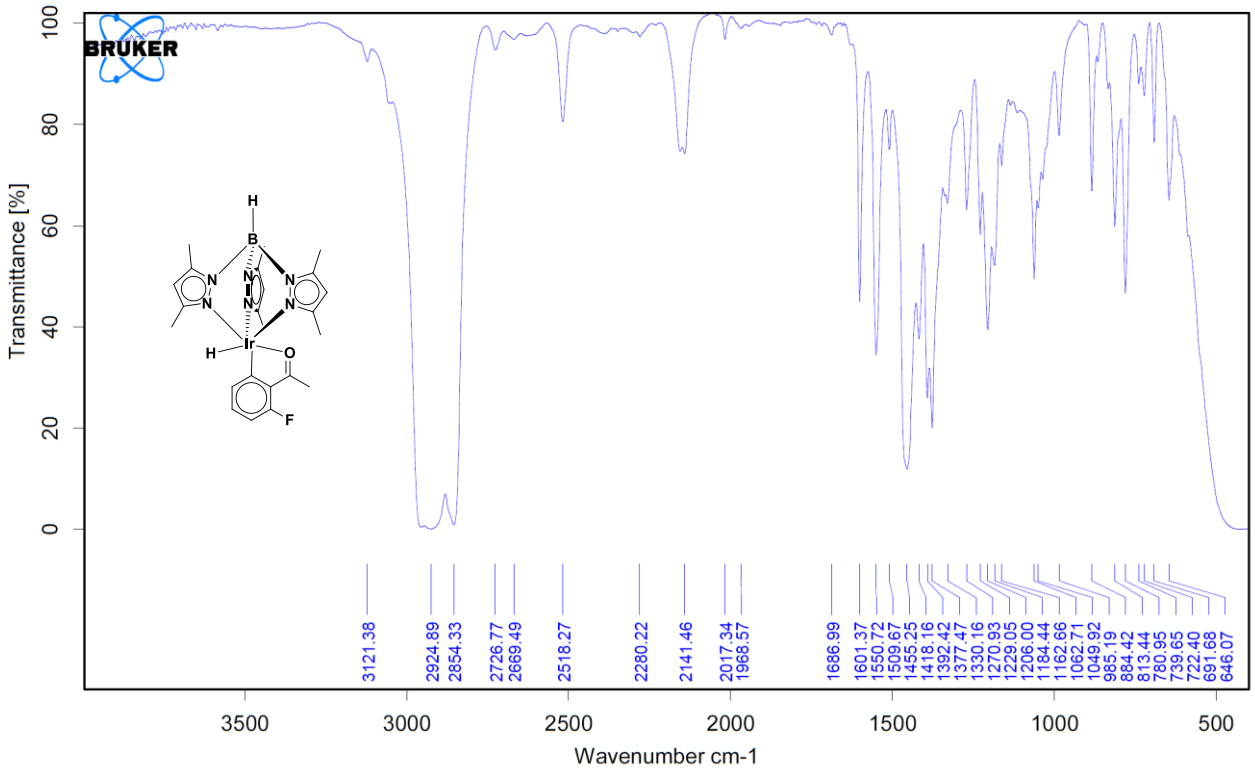


Figure S-16. Spectrum of infrared for complex **5** in nujol.

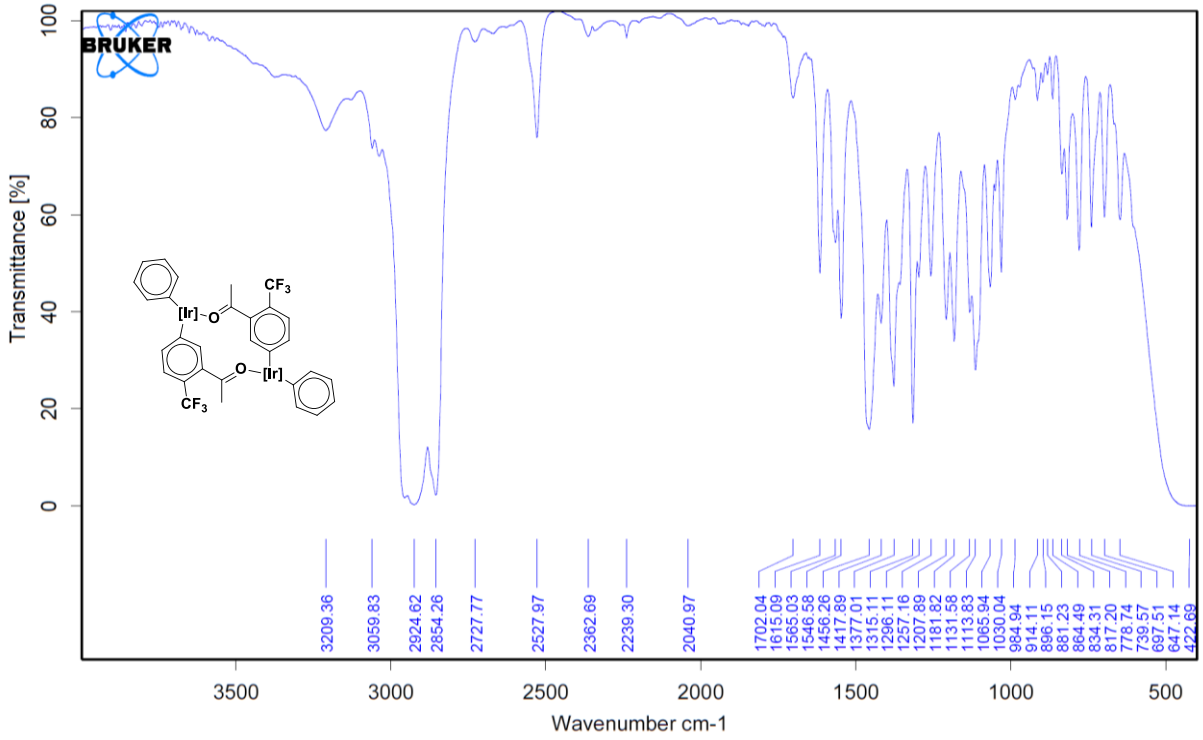


Figure S-17. Spectrum of infrared for complex **7** in nujol.

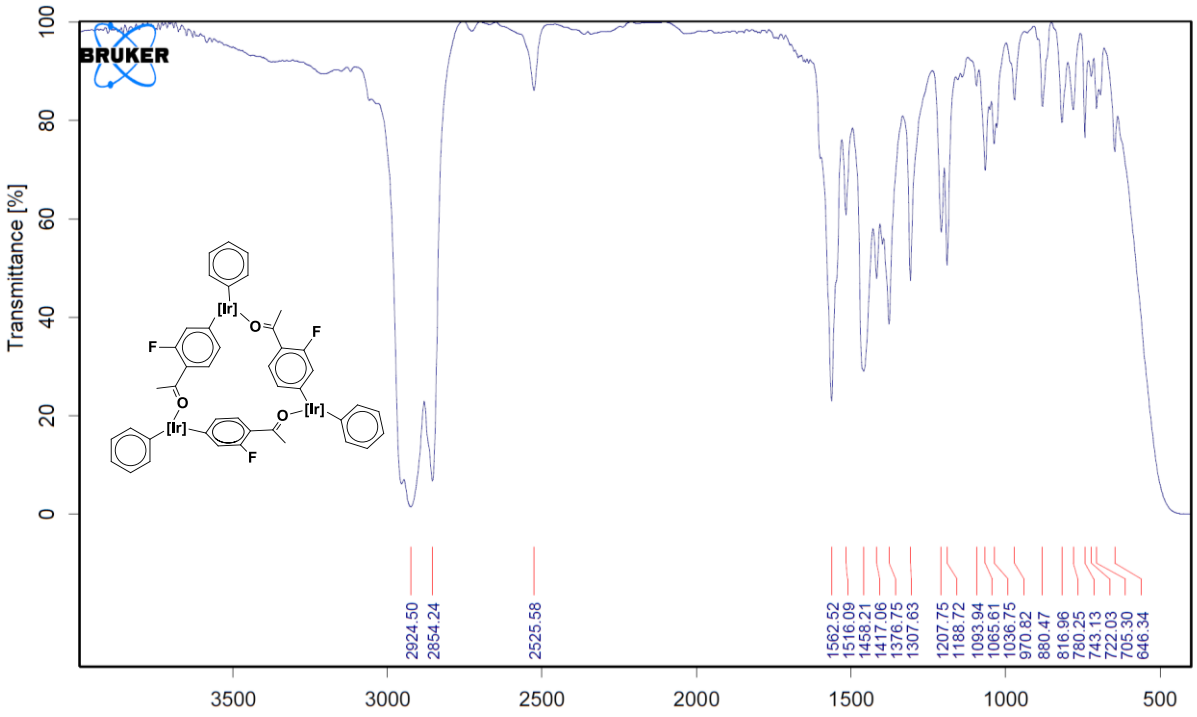


Figure S-18. Spectrum of infrared for complex **8** in nujol.

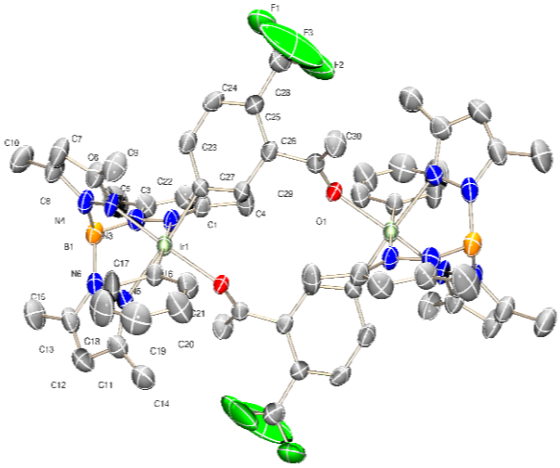


Figure S-19. ORTEP diagram of complex **7**. Ellipsoids are shown at 50 % probability level.

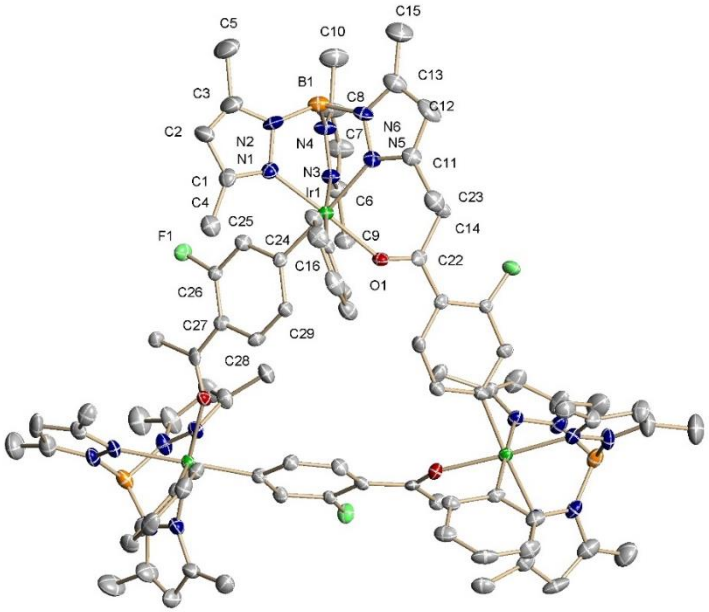
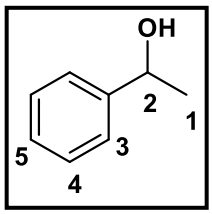


Figure S-20**.** ORTEP diagram of complex **8**. Ellipsoids are shown at 50% probability level.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, ^3J = 7.9 Hz, 2H, *H3*), 7.32 (t, ^3J = 7.9 Hz, 2H, *H4*), 7.25 (t, ^3J = 6.7 Hz, 1H, *H5*), 4.88 (q, ^3J = 6.5 Hz, 1H, *H2*), 1.83 (br. s, 1H, *OH*), 1.48 (d, ^3J = 6.5 Hz, 3H, *H1*).

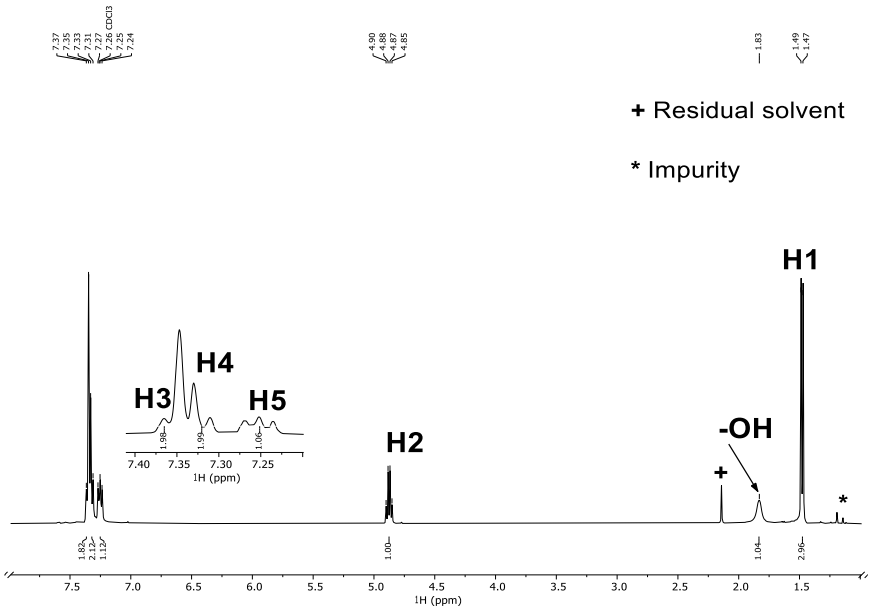
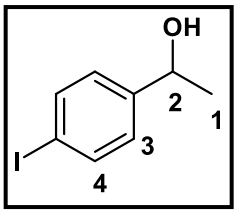


Figure S-21**.** ^{1}H NMR (400 MHz) spectrum of 1-Phenylethanol in $CDCl_3$.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, ^3J = 8.3 Hz, 2H, *H4*), 7.12 (d, ^3J = 8.4 Hz, 2H, *H3*), 4.85 (q, ^3J = 6.5 Hz, 1H, *H2*), 1.84 (br. s, 1H, *OH*), 1.47 (d, ^3J = 6.5 Hz, 3H, *H1*).

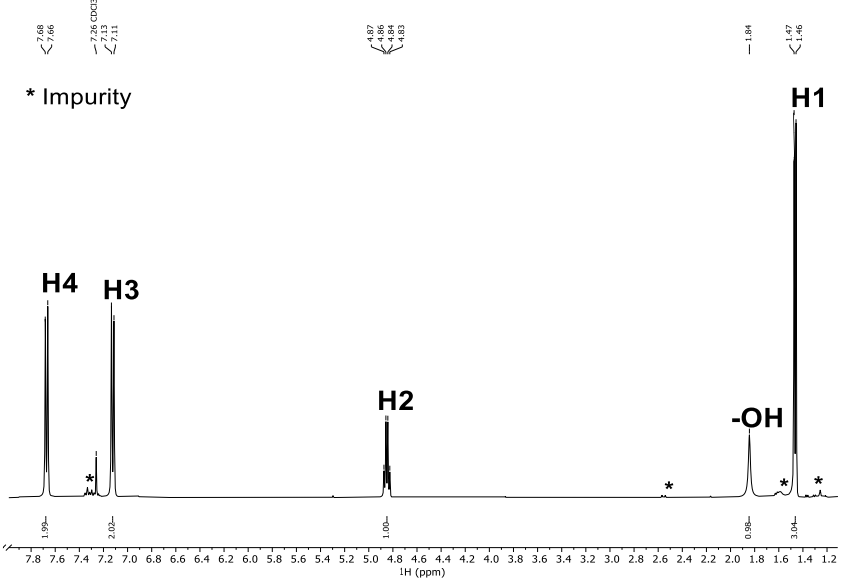
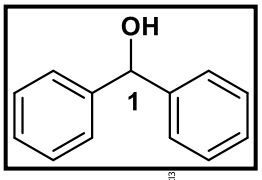


Figure S-22**.** ^{1}H NMR (400 MHz) spectrum of 1-(4-Iodophenyl)ethanol in $CDCl_3$.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 - 7.17 (m, 10H, $H_{aromatic}$), 5.75 (s, 1H, *H1*), 2.10 (br. s, 1H, *OH*).

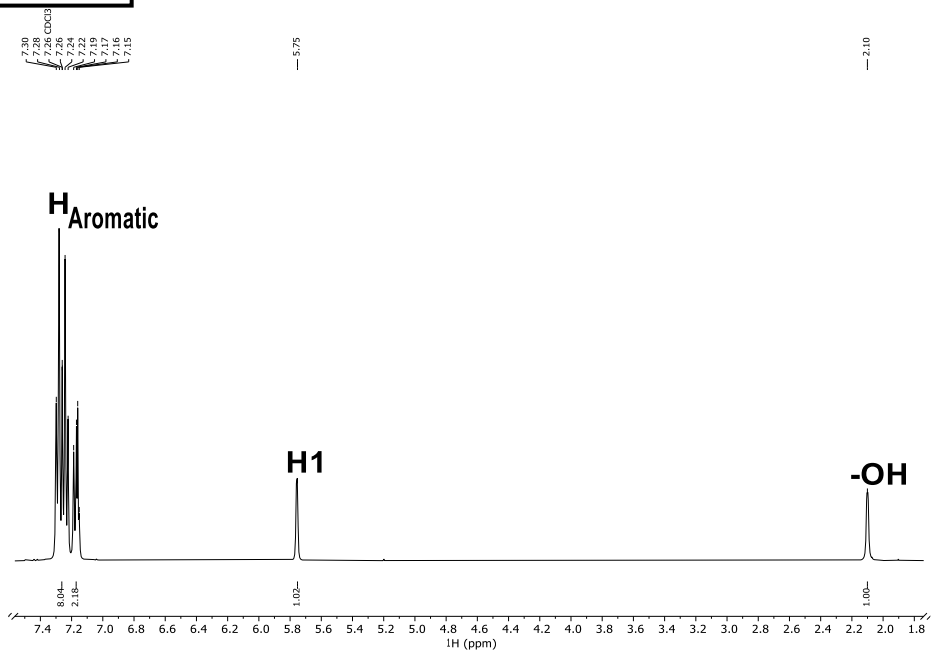
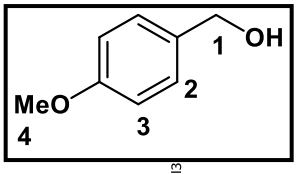


Figure S-23**.** ^{1}H NMR (400 MHz) spectrum of Diphenylmethanol in $CDCl_3$.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (d, ^3J = 8.8 Hz, 2H, *H2*), 6.81 (d, ^3J = 8.8 Hz, 2H, H3), 4.51 (s, 2H, *H1*), 3.72 (s, 3H, *H4*), 2.00 (br. s, 1H, O*H*).

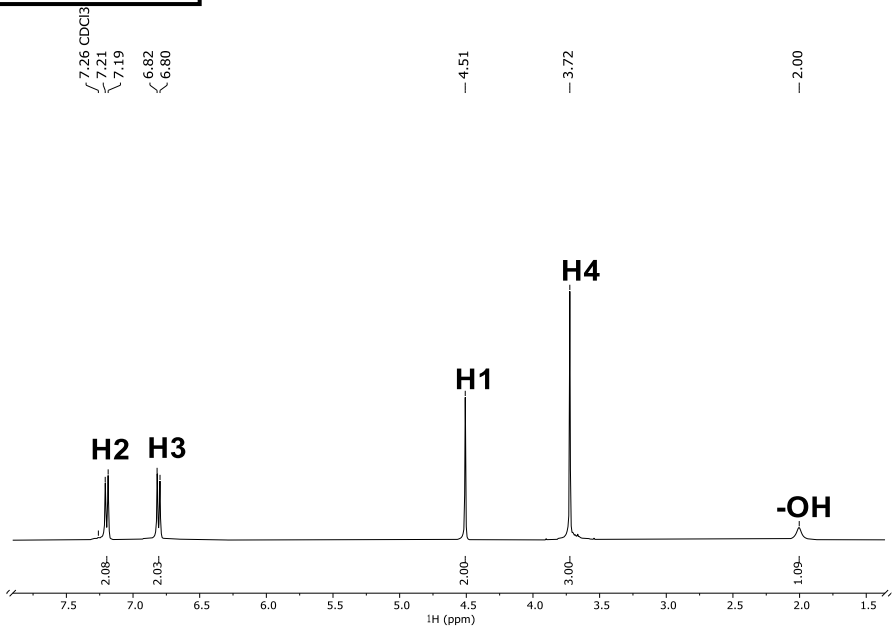
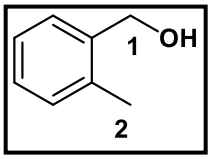


Figure S-24. ^{1}H NMR (400 MHz) spectrum of 4-Methoxybenzyl alcohol in $CDCl_3$.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (m, 1H, $H_{aromatic}$), 7.24 (m, 3H, $H_{aromatic}$), 4.72 (s, 2H, *H1*), 2.40 (s, 3H, *H2*), 1.94 (br. s, 1H, *OH*).

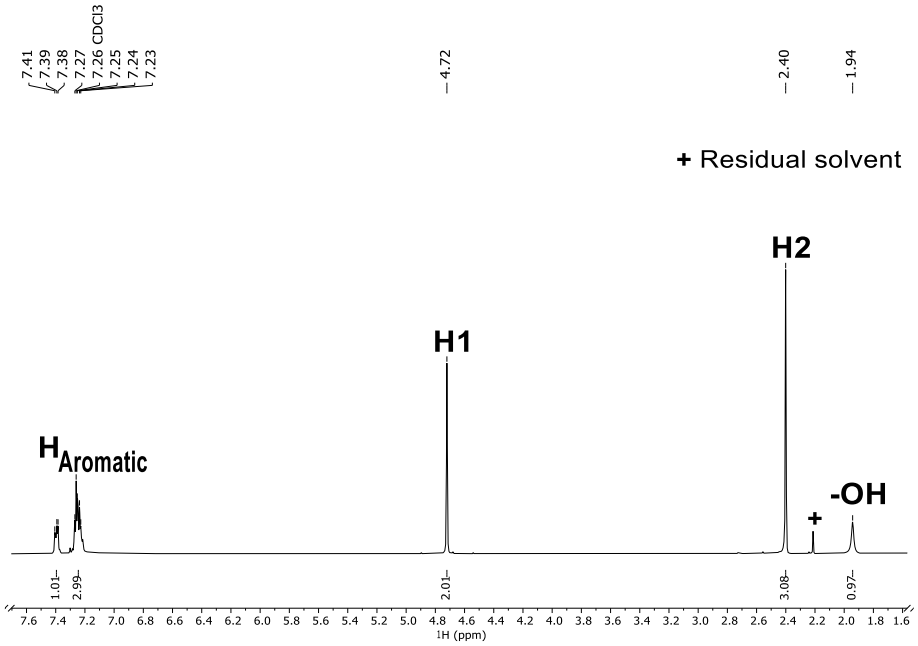
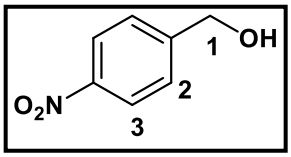


Figure S-25. ^{1}H NMR (400 MHz) spectrum of 2-Methylbenzyl alcohol in $CDCl_3$.



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, ^3J = 8.8 Hz, 2H, *H3*), 7.53 (d, ^3J = 8.7 Hz, 2H, *H2*), 4.83 (s, 2H, *H1*), 2.11 (br. s, 1H, O*H*).

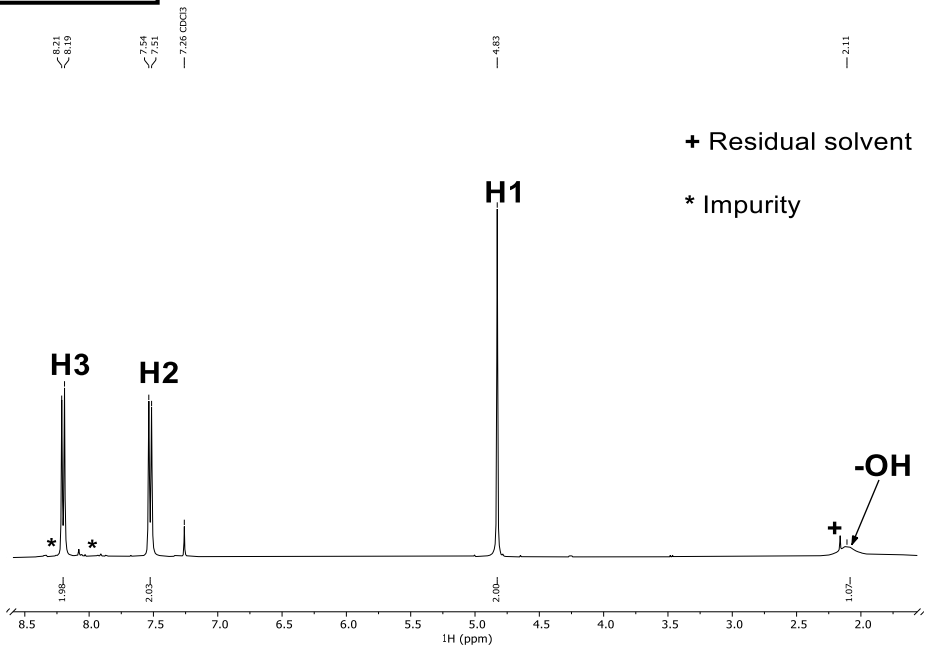
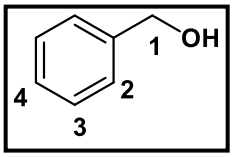


Figure S-26. ^{1}H NMR (400 MHz) spectrum of 4-Nitrobenzylalcohol in $CDCl_3$.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (m, 5H, $H_{aromatic}$), 4.59 (s, 2H, *H1*), 1.81 (br. s, 1H, O*H*).

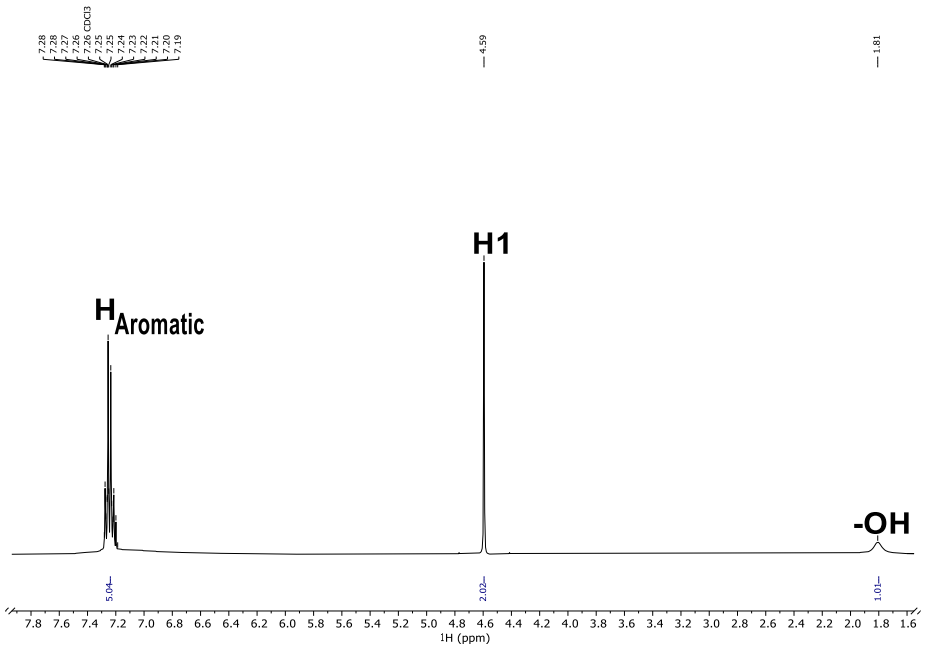
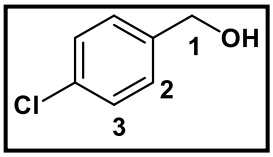


Figure S-27. ^{1}H NMR (400 MHz) spectrum of Benzyl alcohol in $CDCl_3$.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (m, 4H, *H2*, *H3*), 4.67 (s, 2H, *H1*), 1.72 (br. s, 1H, O*H*).

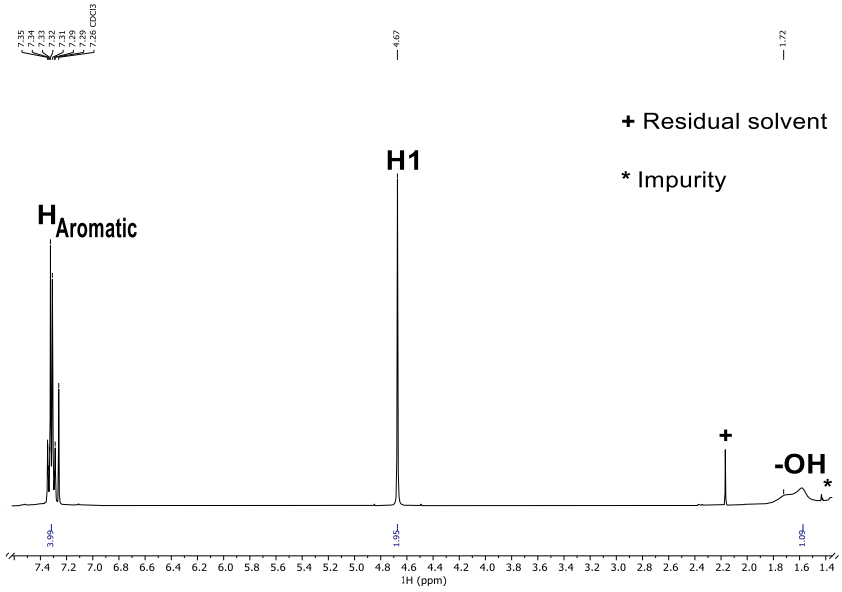


Figure S-28. ^{1}H NMR (400 MHz) spectrum of 4-Chlorobenzyl alcohol in $CDCl_3$.