

Supplementary Information

N-Heterocyclic carbene-palladium-PEPPSI complexes and their catalytic activity in the direct C-H bond activation of heteroarenes derivatives with aryl bromides: Synthesis, antimicrobial and antioxidant activities

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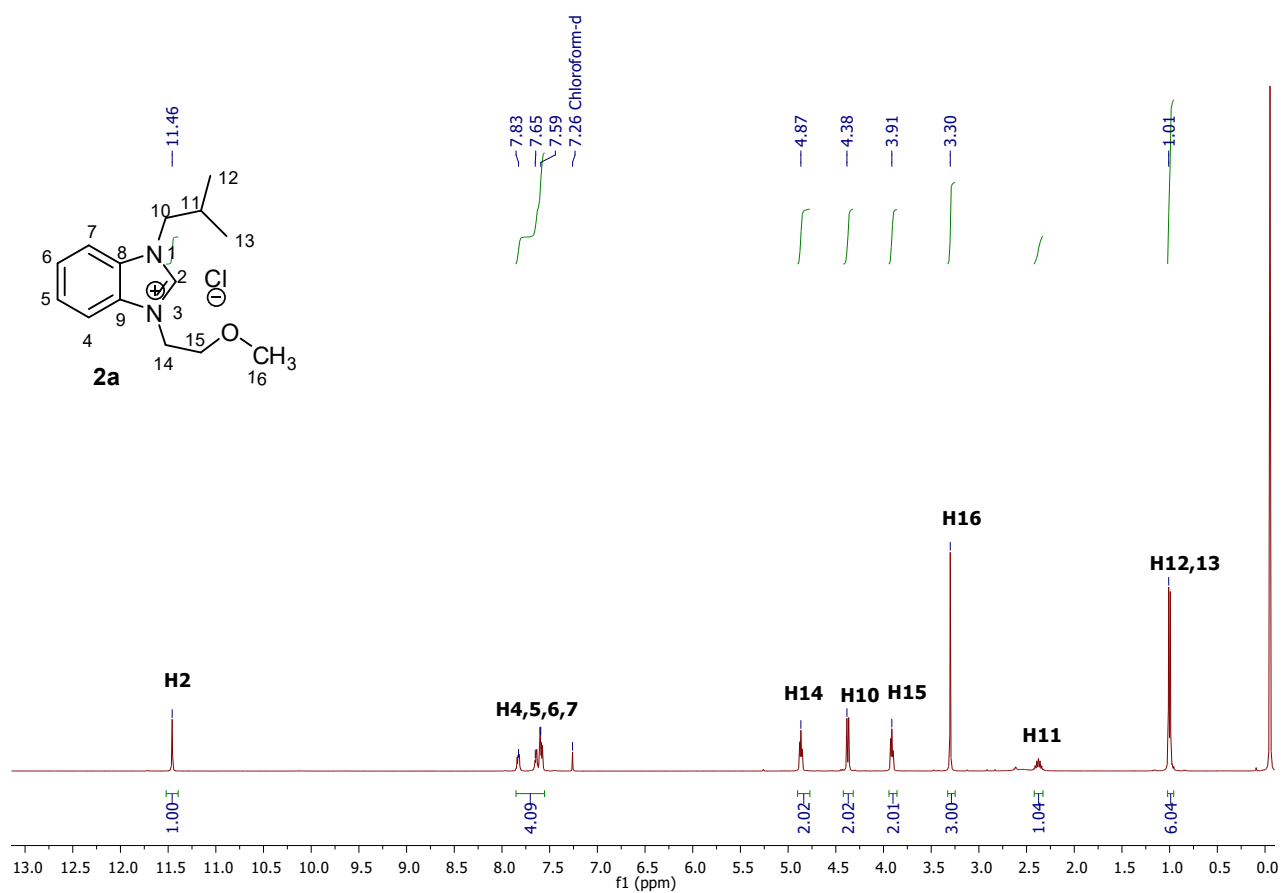


Figure 1. ^1H -NMR spectra of benzimidazolium salt **2a** in CDCl_3

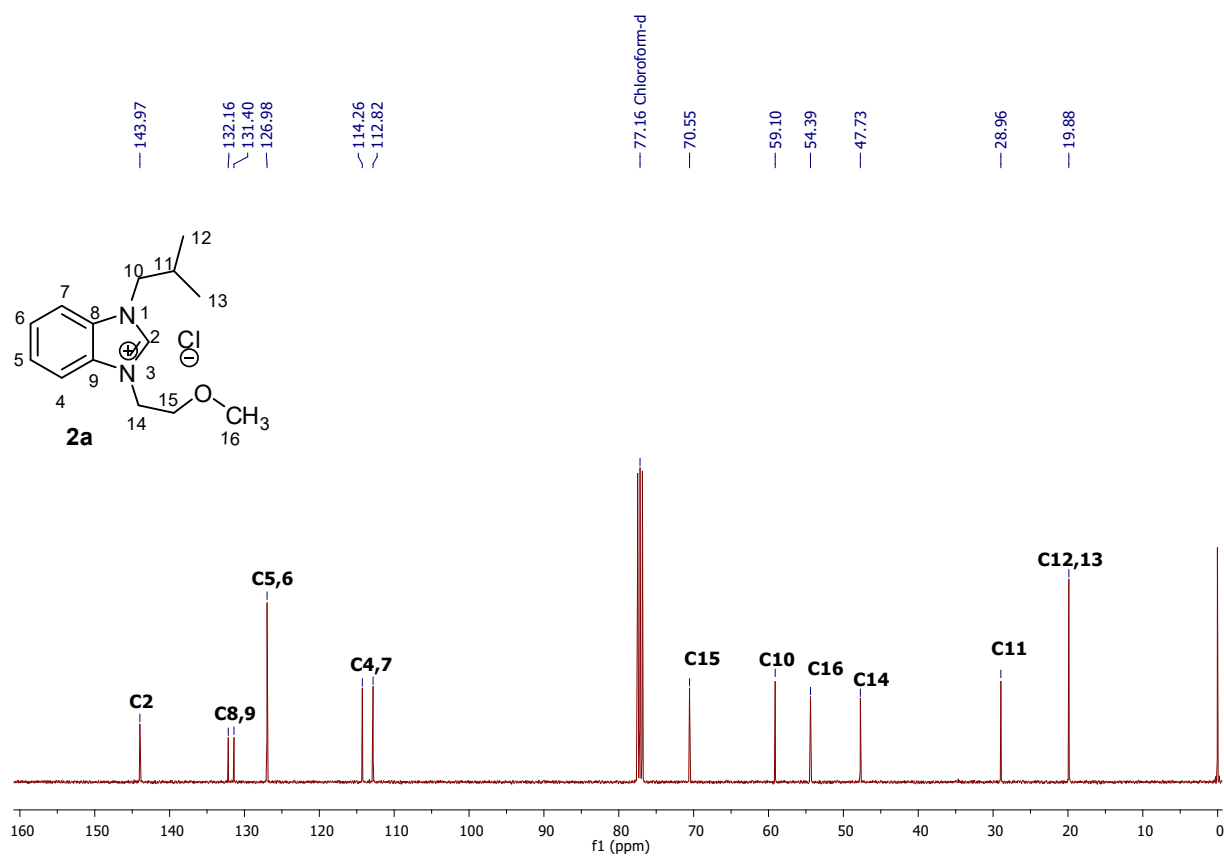


Figure 2. ¹³C-NMR spectra of benzimidazolium salt **2a** in CDCl₃

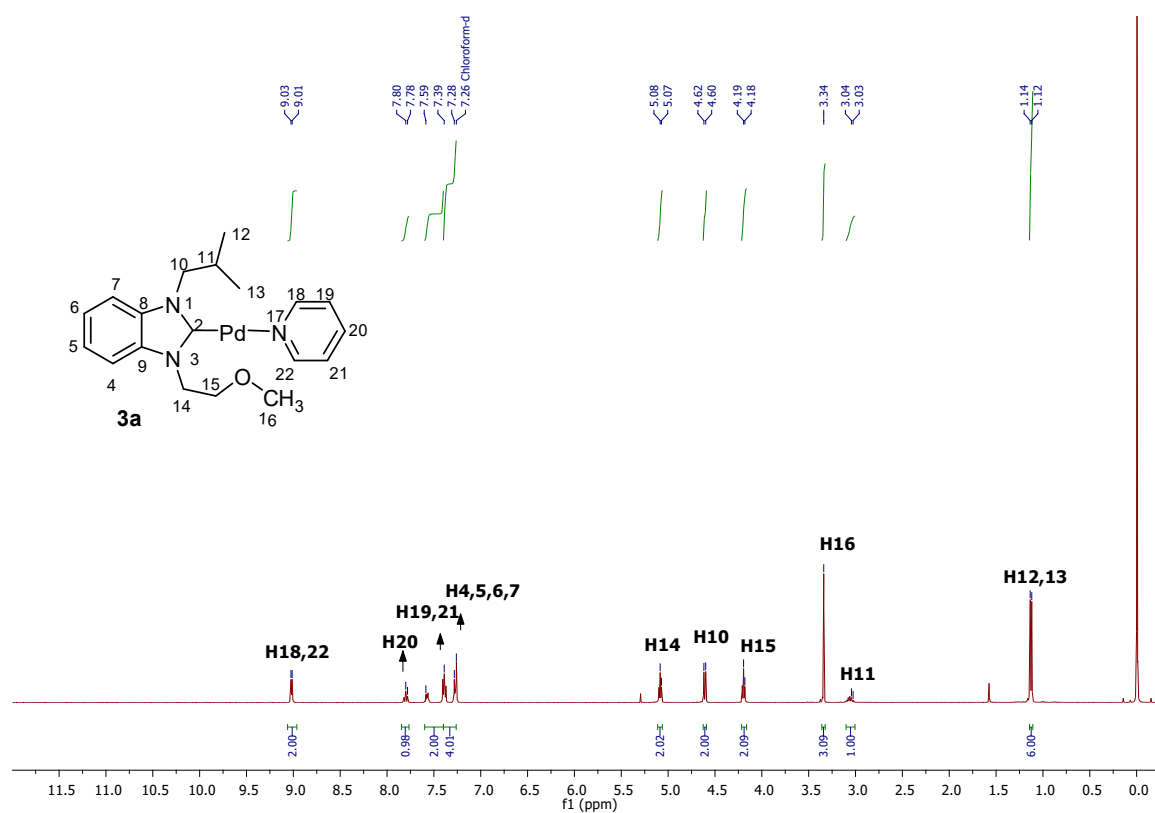


Figure 3. ¹H-NMR spectra of Pd-PEPPSI complex **3a** in CDCl₃

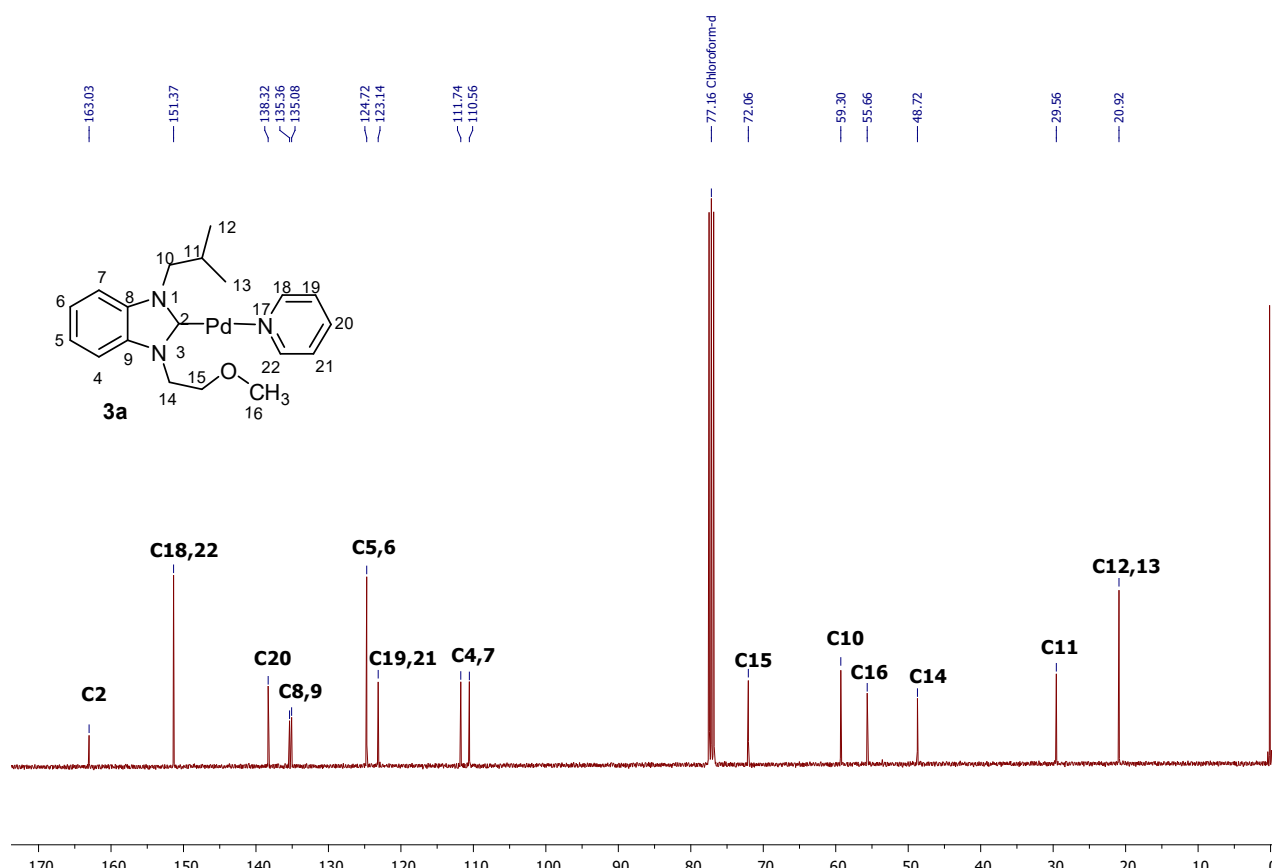


Figure 4. ^{13}C -NMR spectra of Pd-PEPPSI complex **3a** in CDCl_3

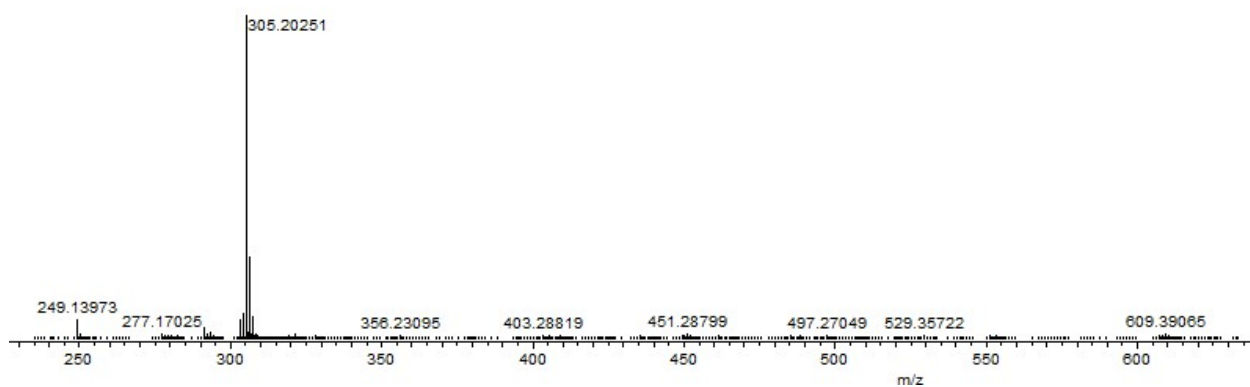


Figure 5. DART MS spectrum (DART-TOF-MS) of complex **3e**.

The fragmentation leading to the $m/z = 305$ can occur via the mechanism of fragmentation given in **Figure 6**.

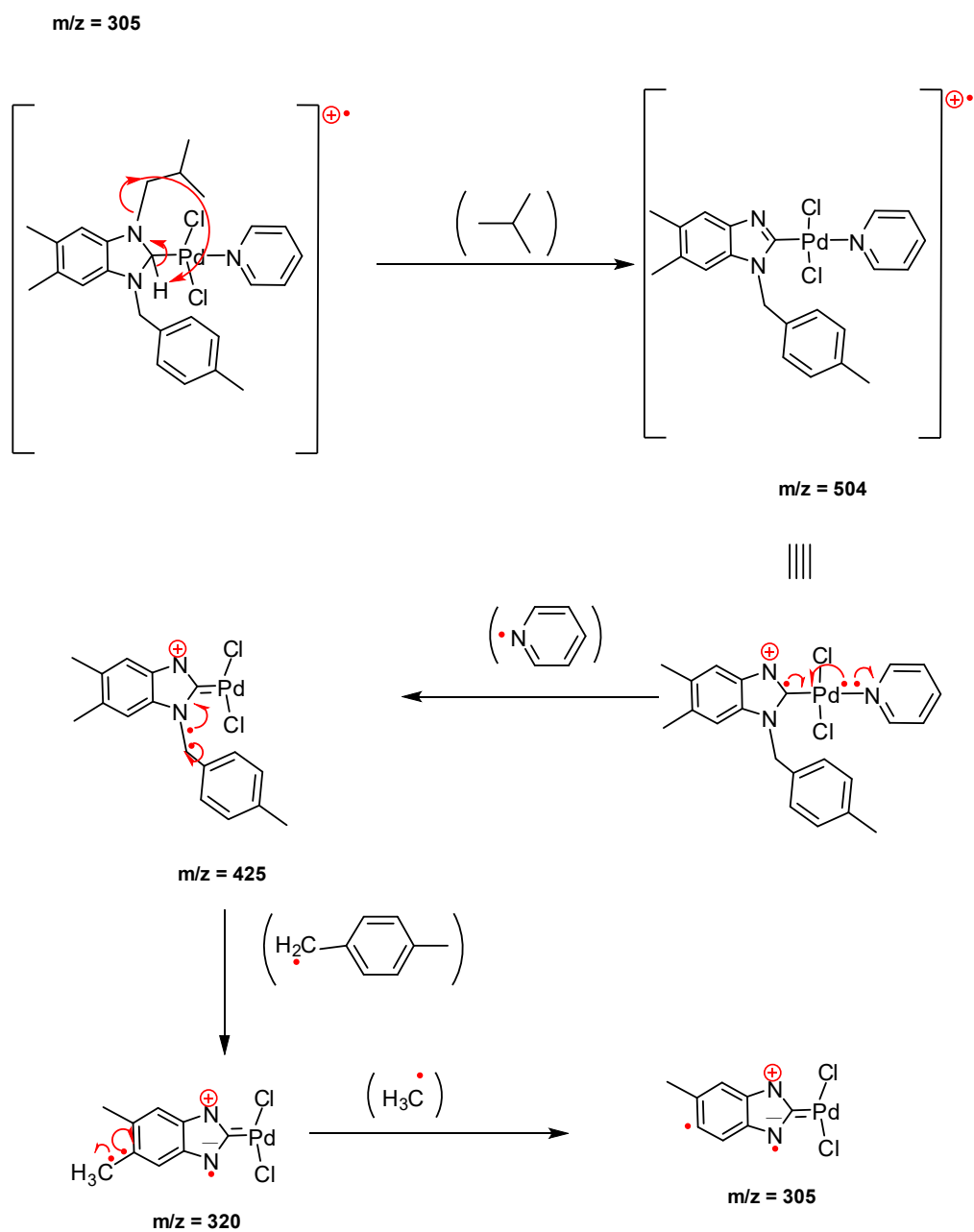


Figure 6. Mechanism of fragmentation leading to the peak $m/z = 305$ with isotope ^{35}Cl .

NMR an IR Data of benzimidazol salts 2a-g

2a NMR spectra are reported in the literature [49a]

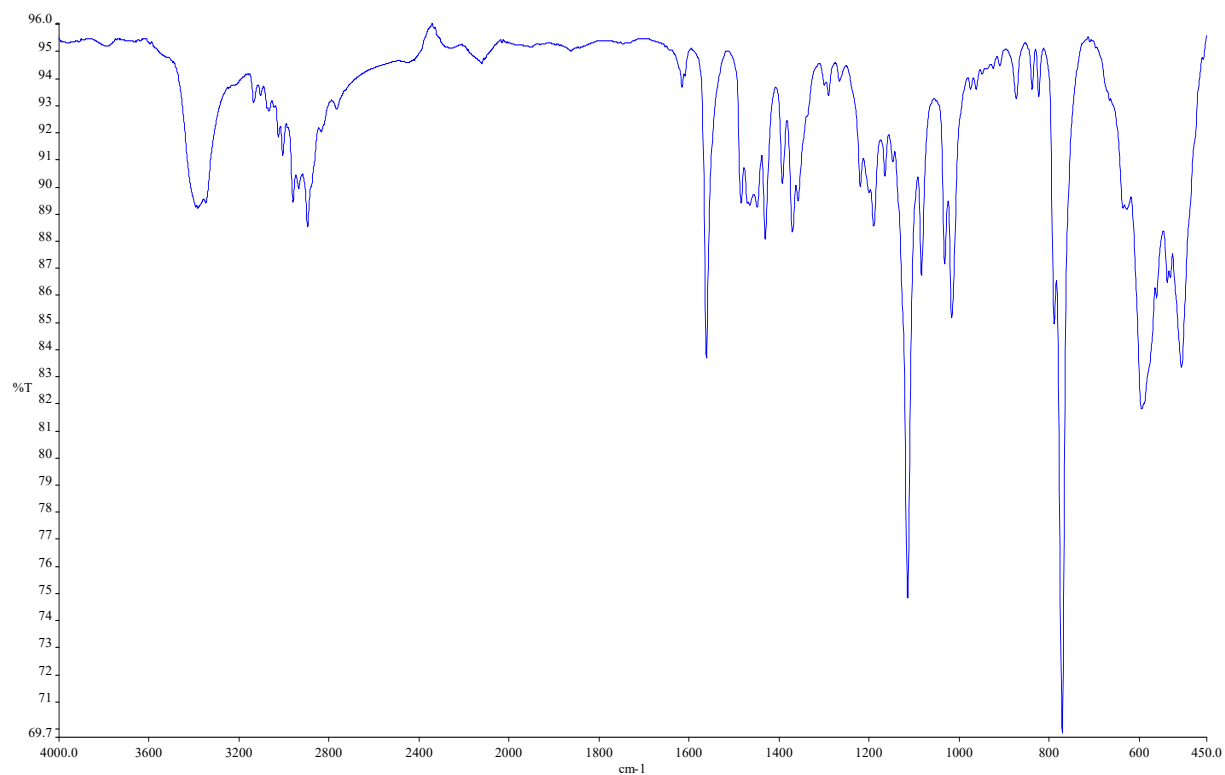


Figure S1. IR spectra on ATR unit of salt 2a

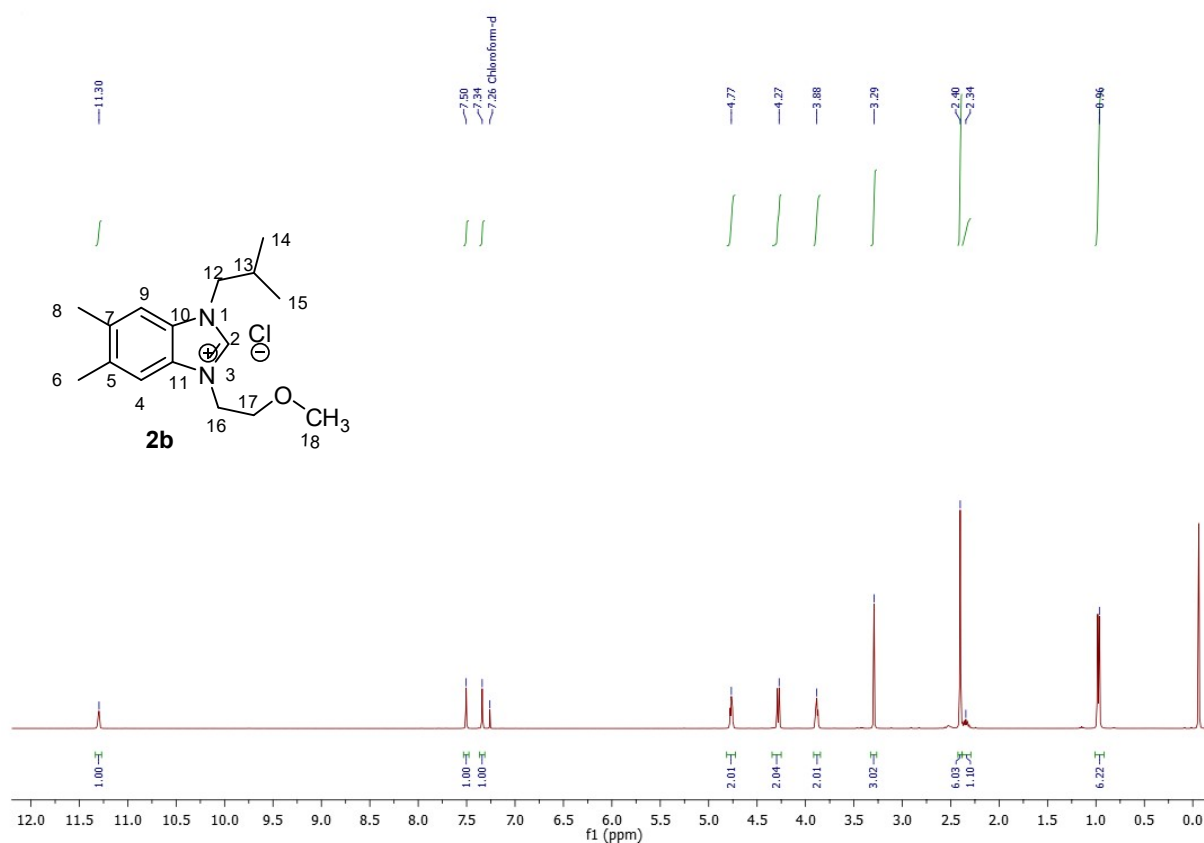


Figure S2. ¹H NMR spectrum (400 MHz, CDCl₃) of salt **2b**

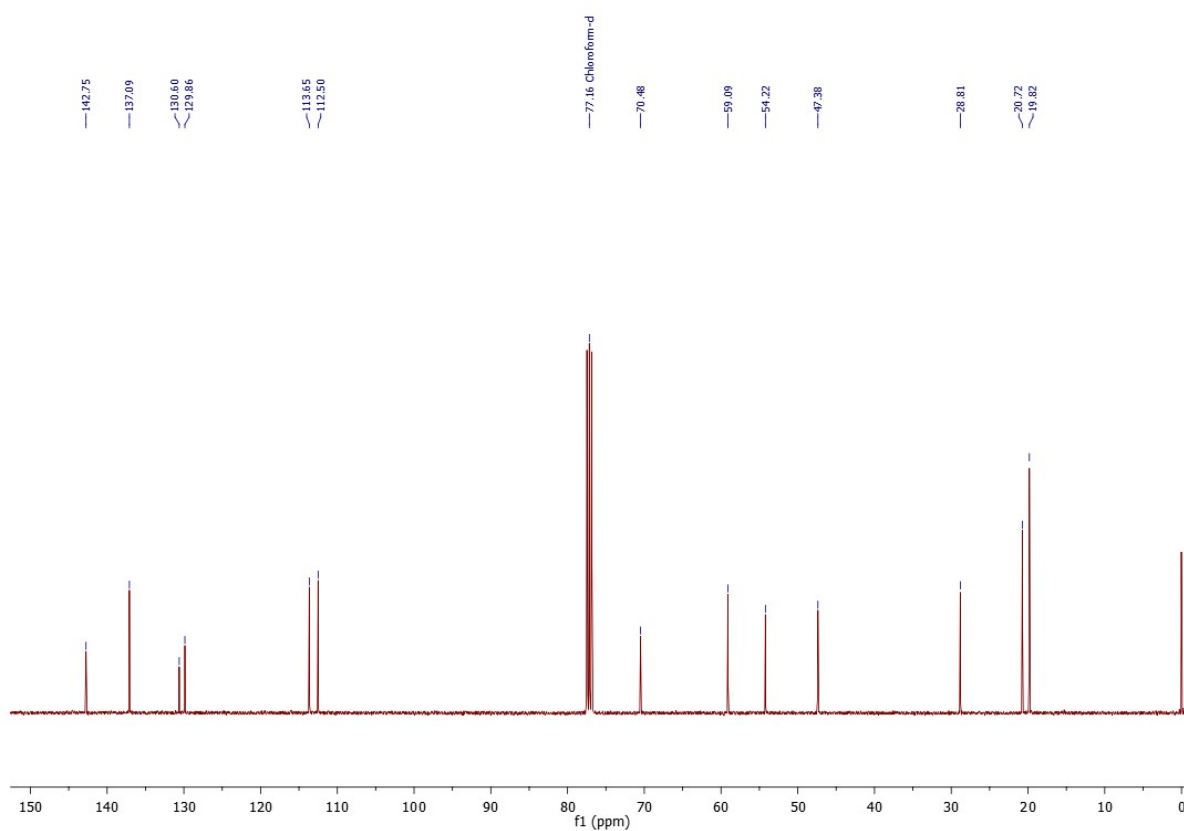


Figure S3. ^{13}C NMR spectrum (100 MHz, CDCl_3) of salt 2b.

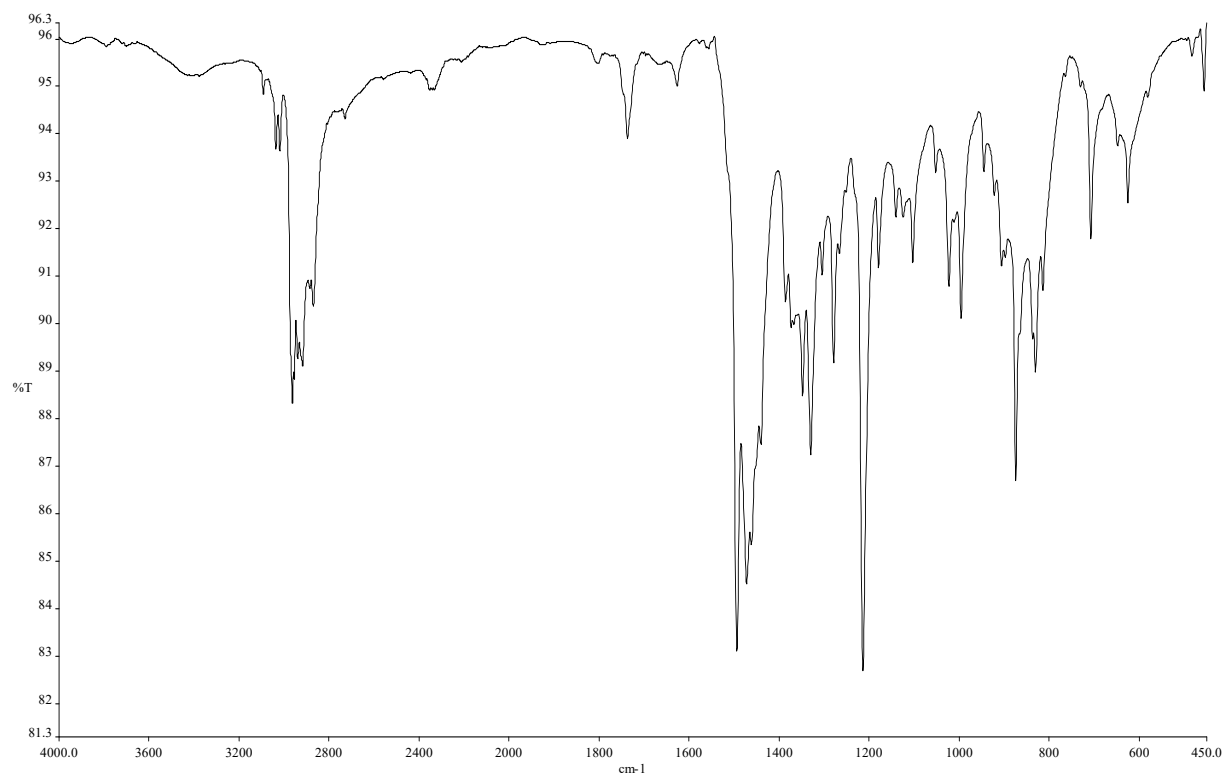


Figure S4. IR spectra on ATR unit of salt 2b

2c NMR spectra are reported in the literature [49a]

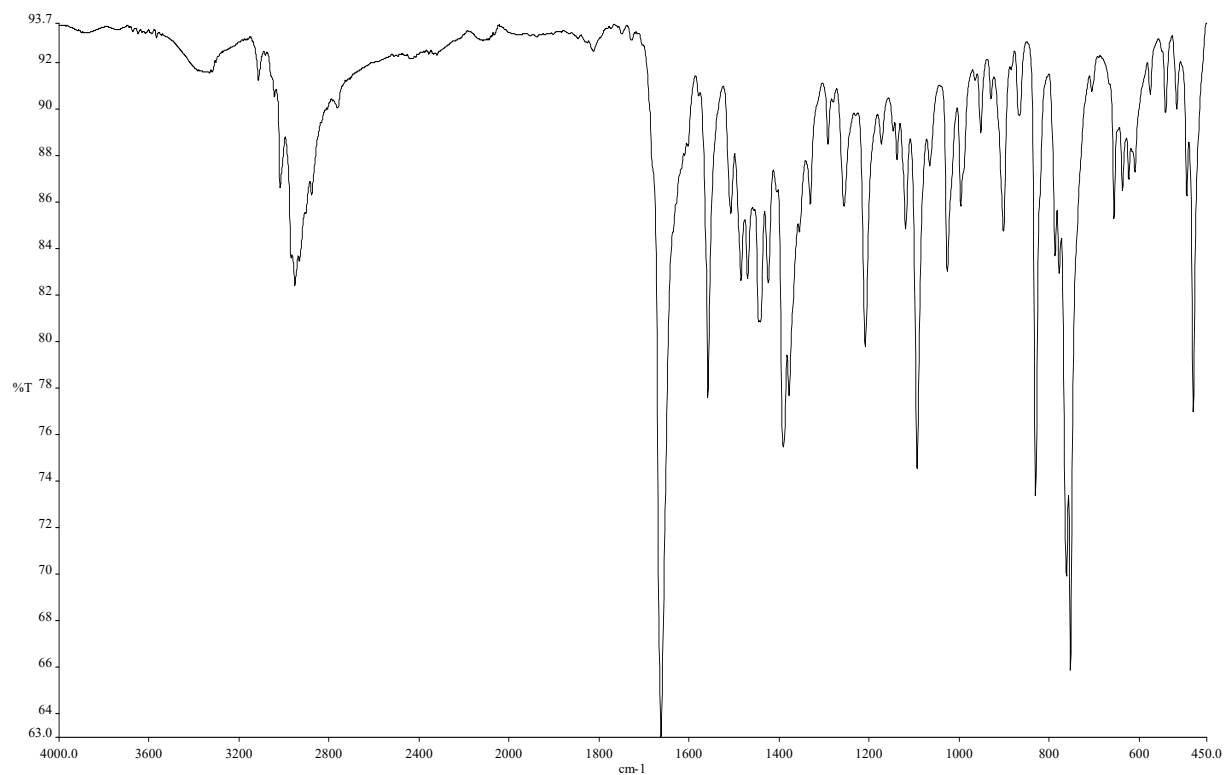


Figure S5. IR spectra on ATR unit of salt 2c

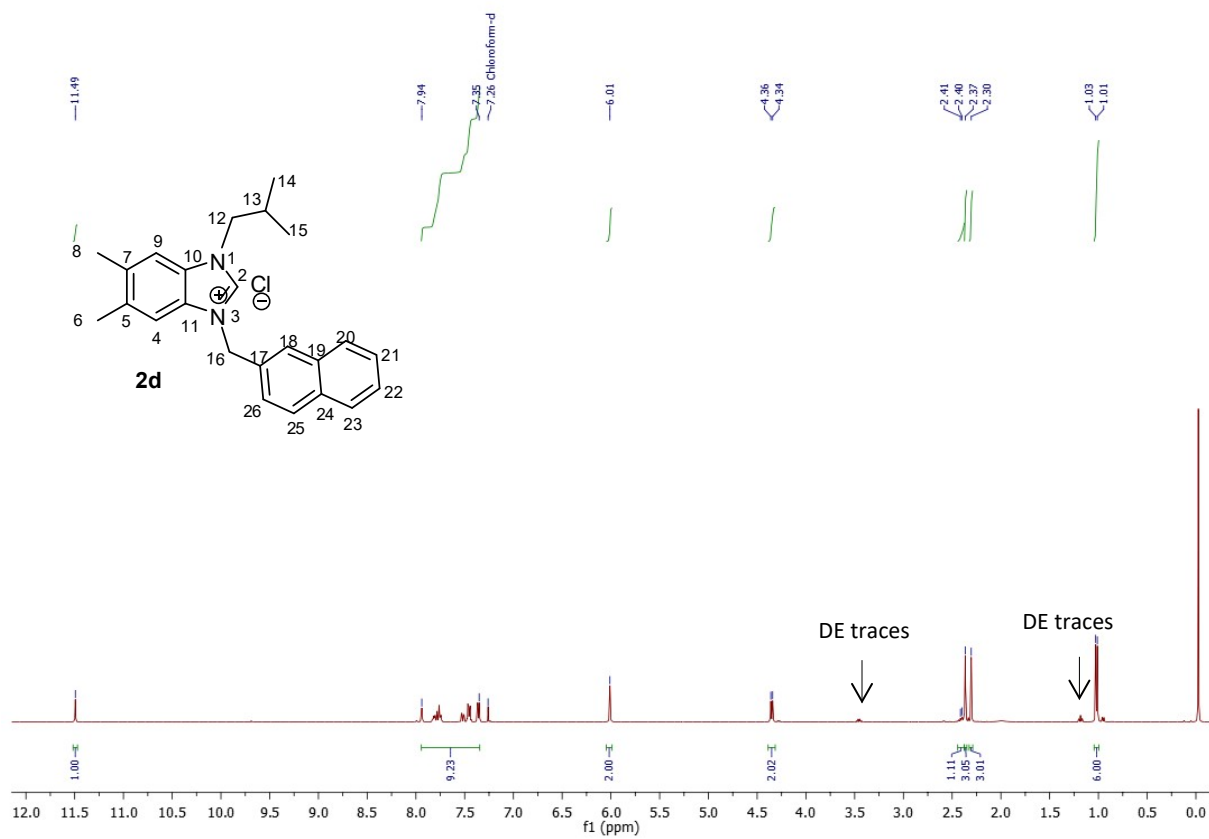


Figure S6. ¹H NMR spectrum (400 MHz, CDCl₃) of salt 2d

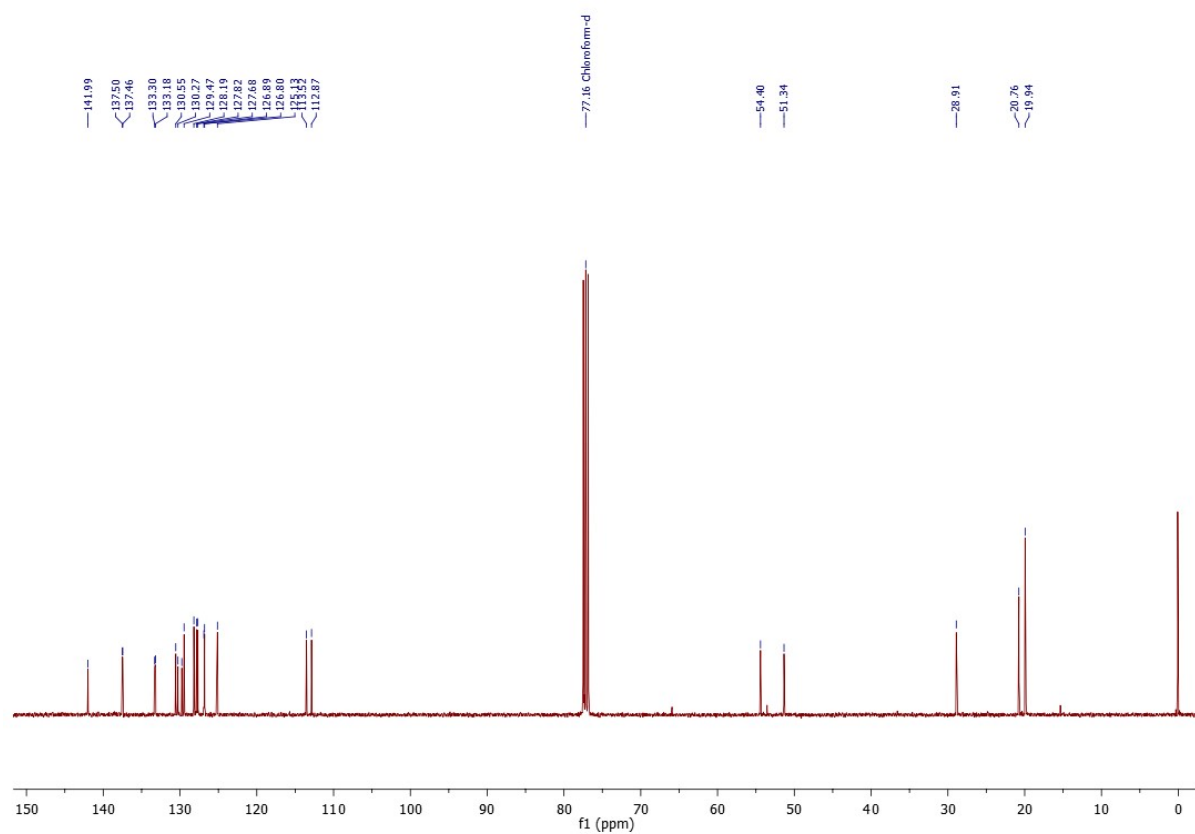


Figure S7. ^{13}C NMR spectrum (100 MHz, CDCl_3) of salt 2d.

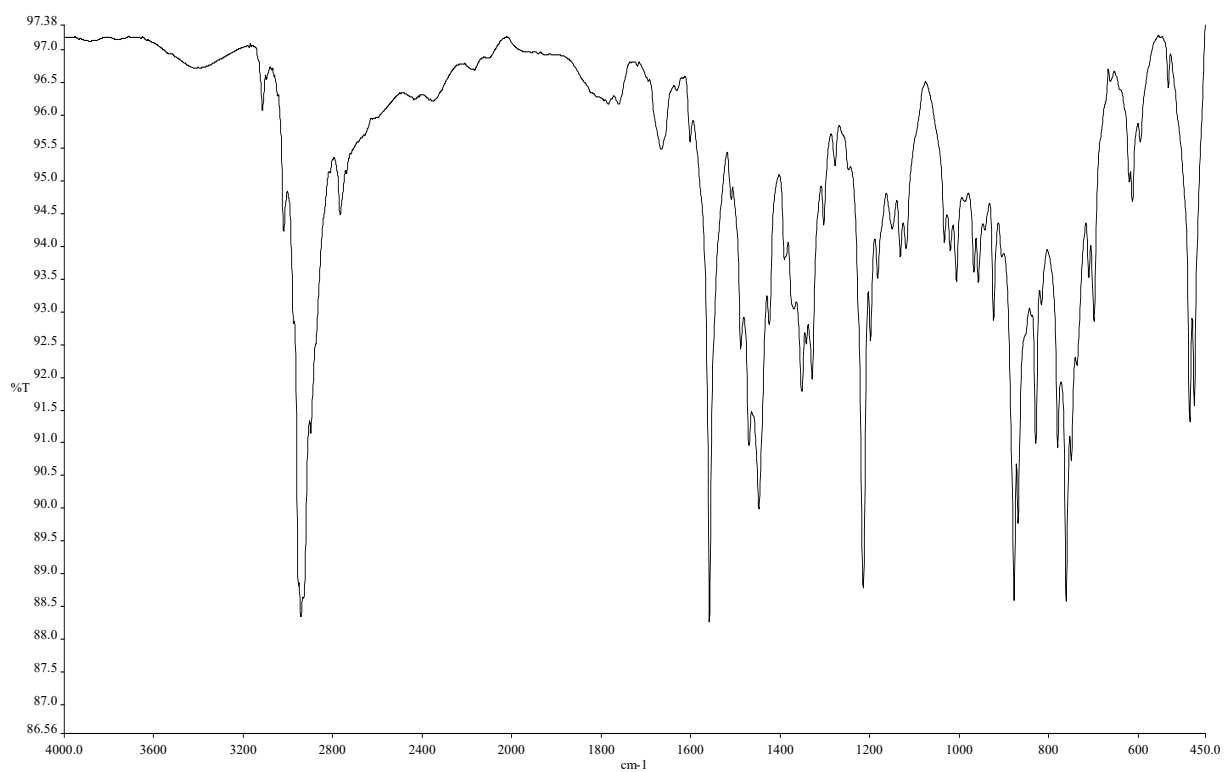


Figure S8. IR spectra on ATR unit of salt 2d

2e NMR spectra are reported in the literature [49a]

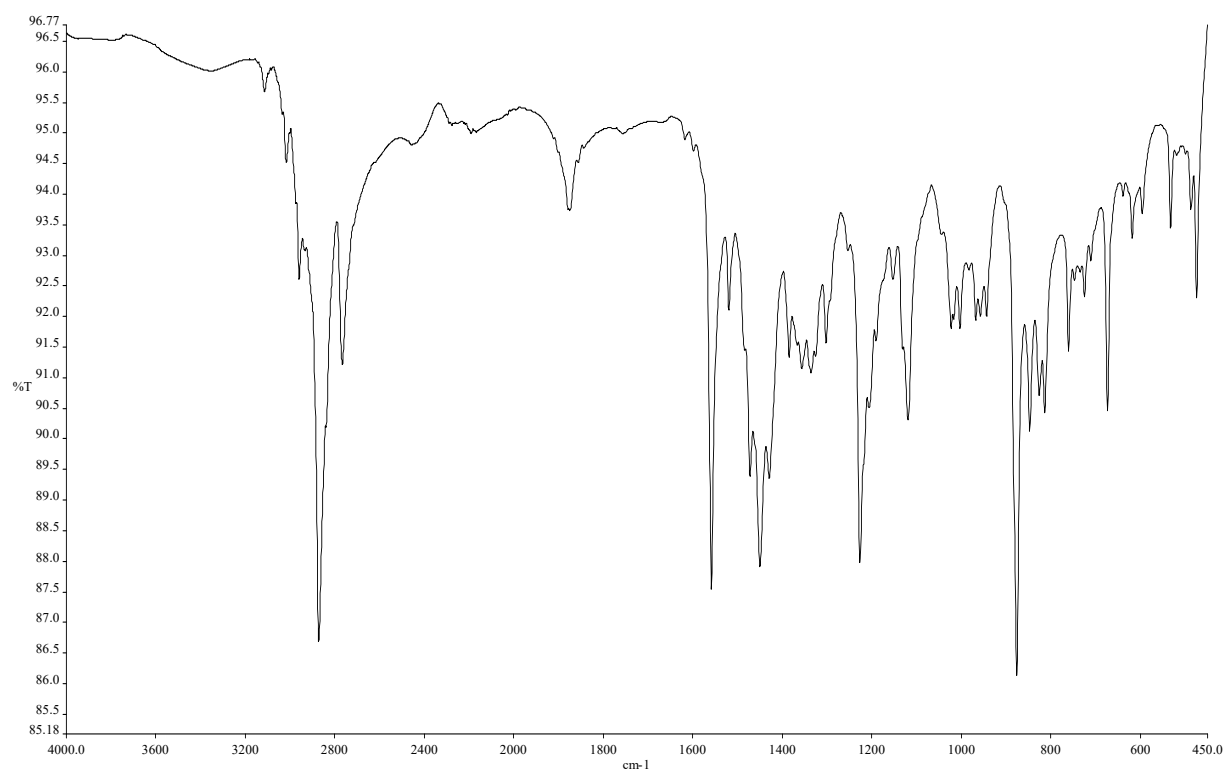


Figure S9. IR spectra on ATR unit of salt 2e

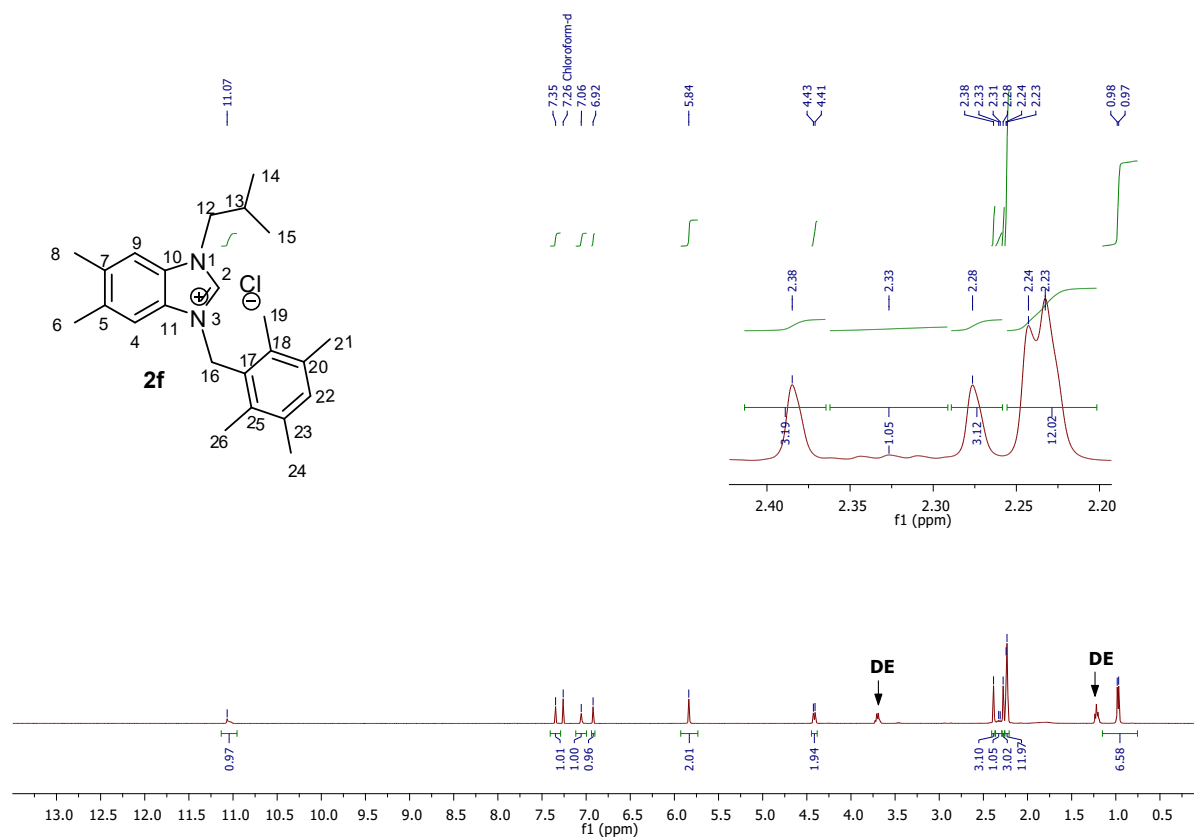


Figure S10. ¹H NMR spectrum (400 MHz, CDCl₃) of salt 2f.

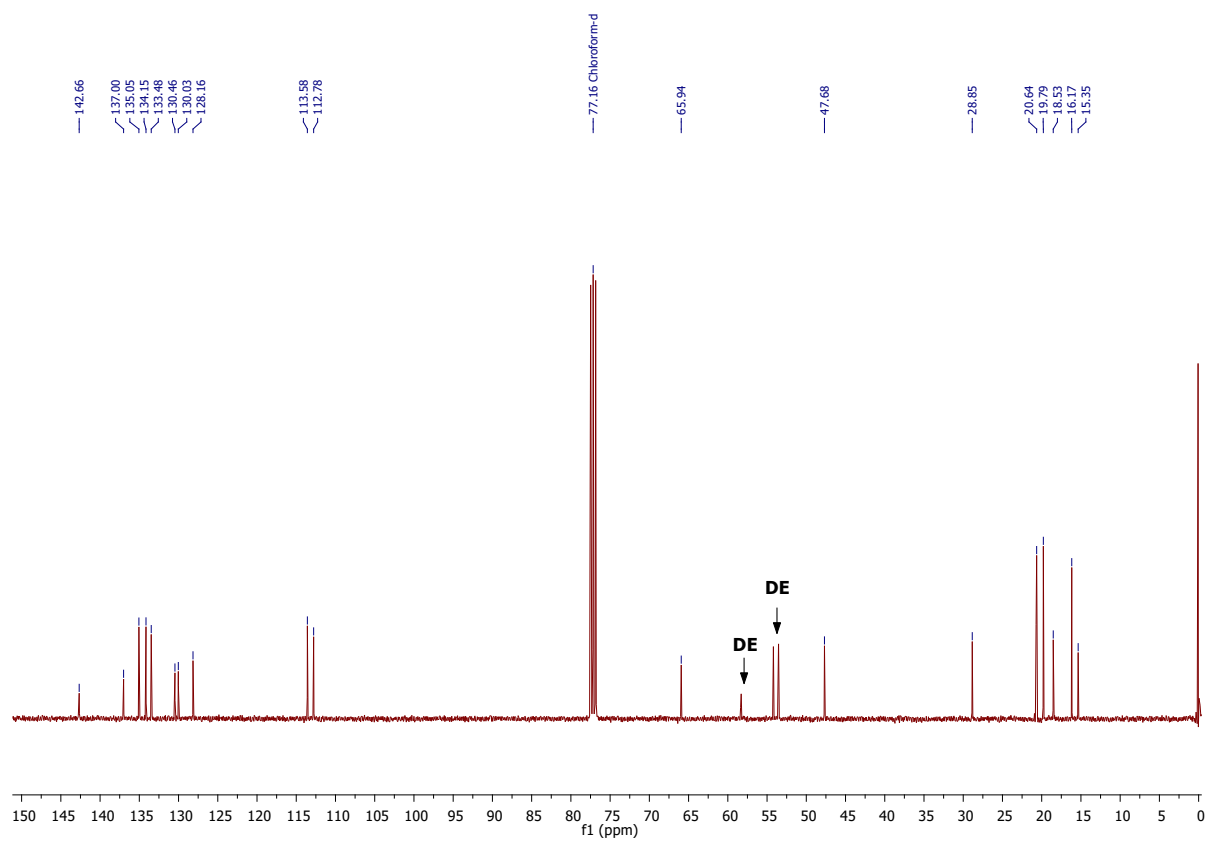


Figure S11. ^{13}C NMR spectrum (100 MHz, CDCl_3) of salt 2f

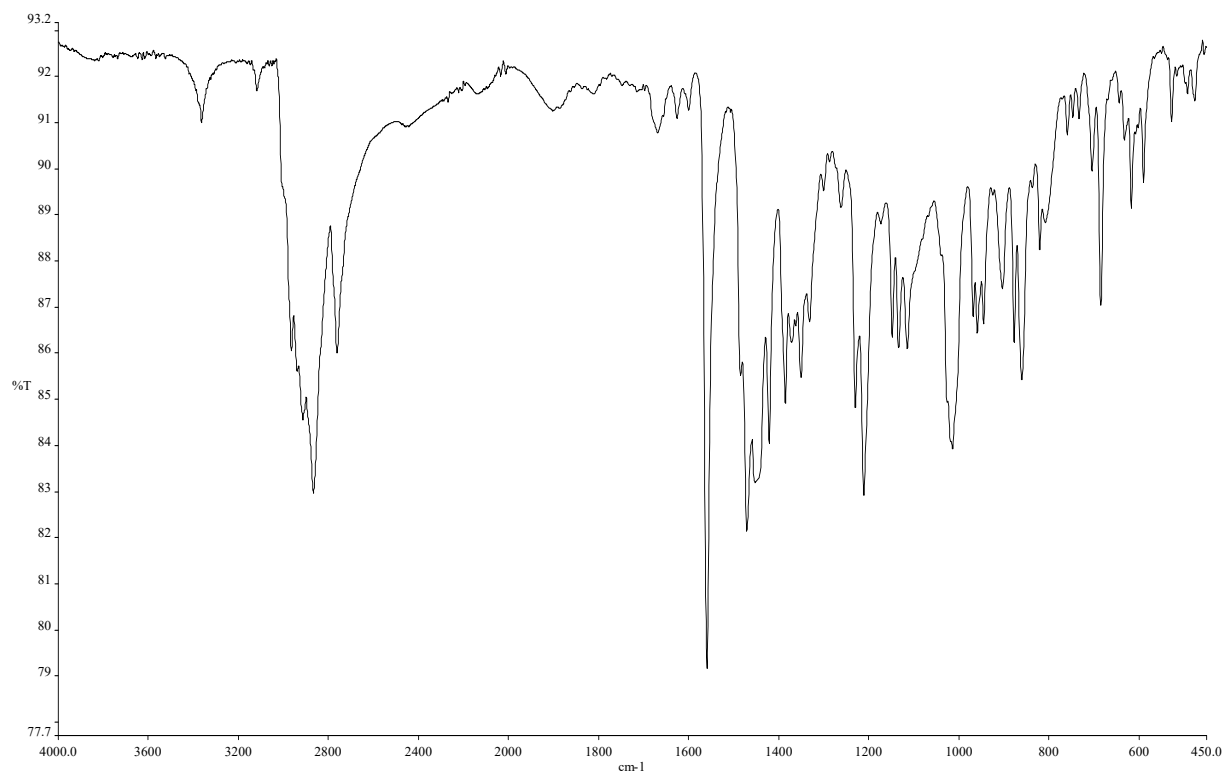


Figure S12. IR spectra on ATR unit of salt 2f

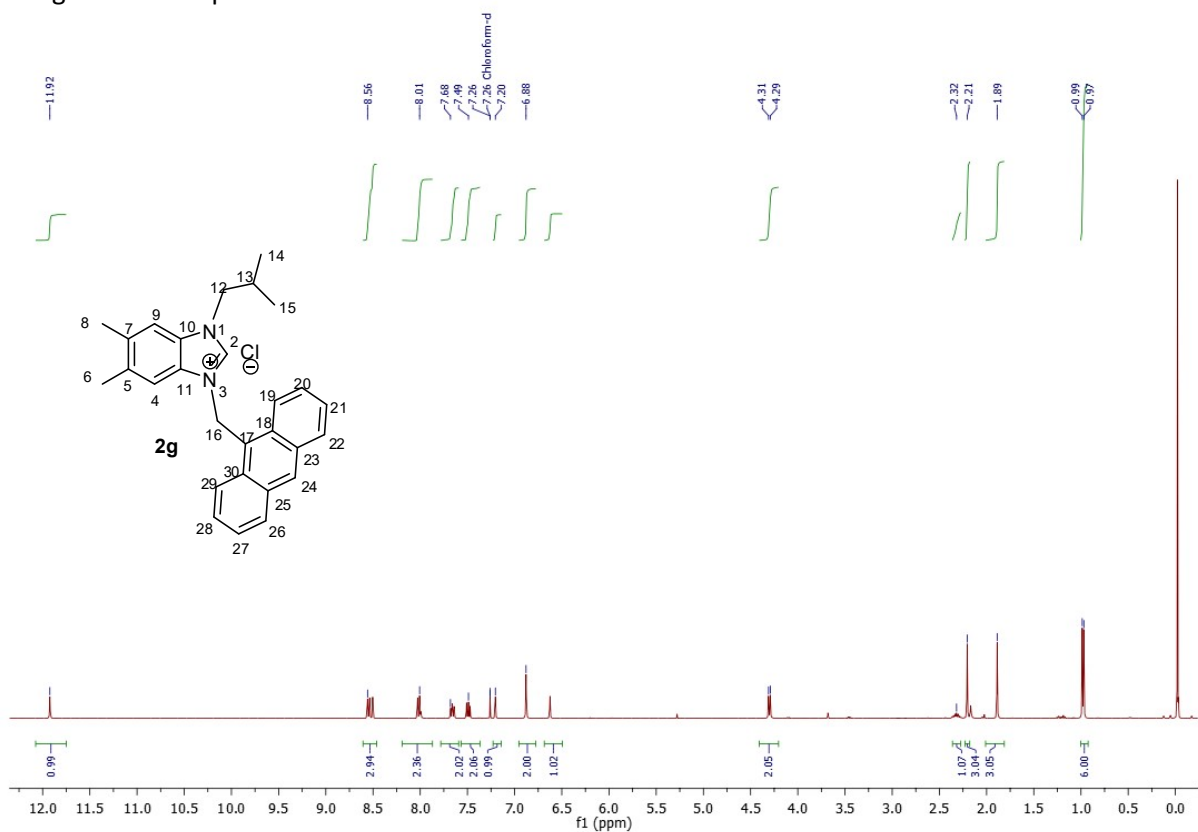


Figure S13. ^1H NMR spectrum (400 MHz, CDCl_3) of salt 2g.

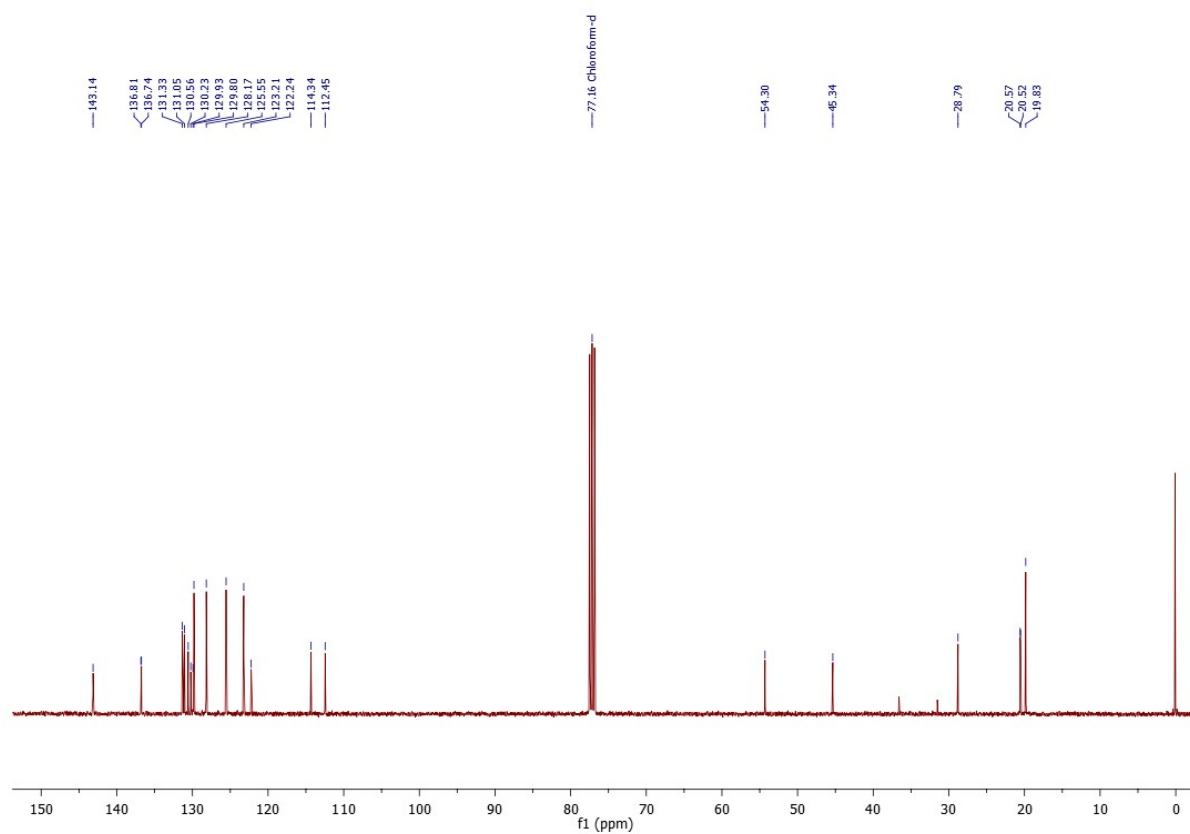


Figure S14. ^{13}C NMR spectrum (100 MHz, CDCl_3) of salt 2g

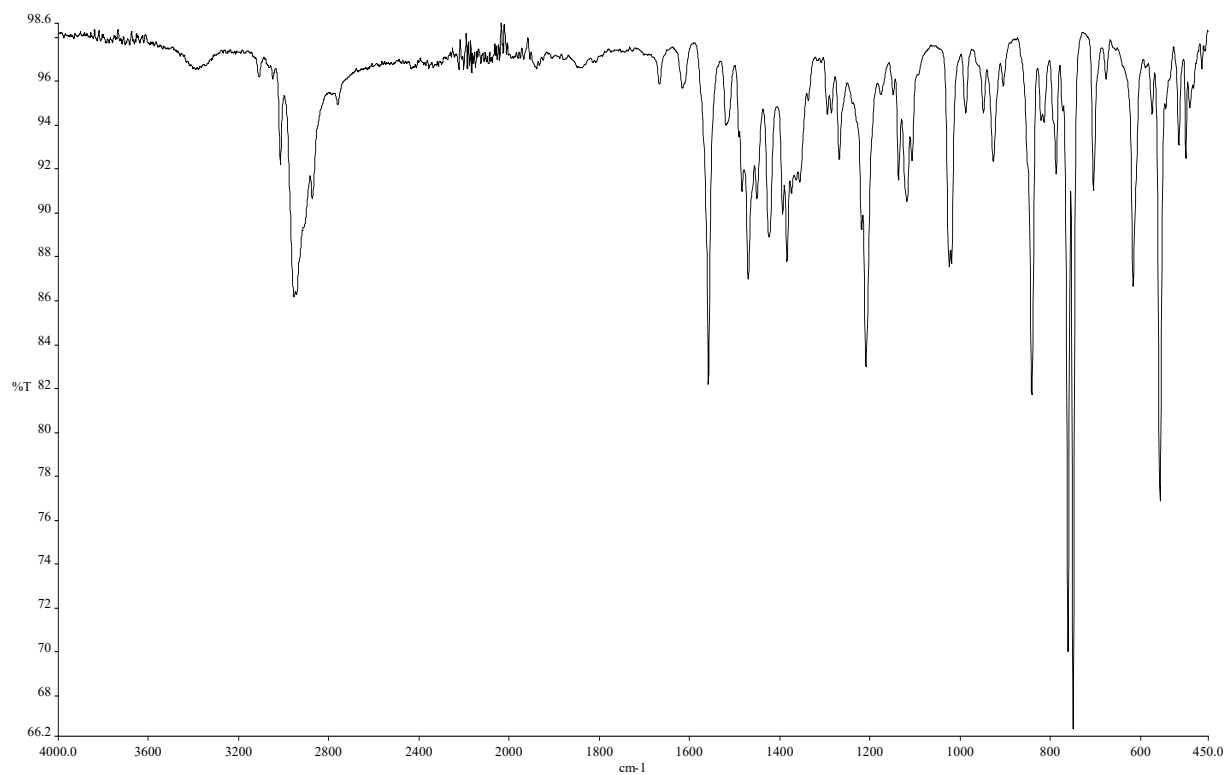


Figure S15. IR spectra on ATR unit of salt 2g

NMR an IR Data of Pd-PEPPSI complexes 3a-g

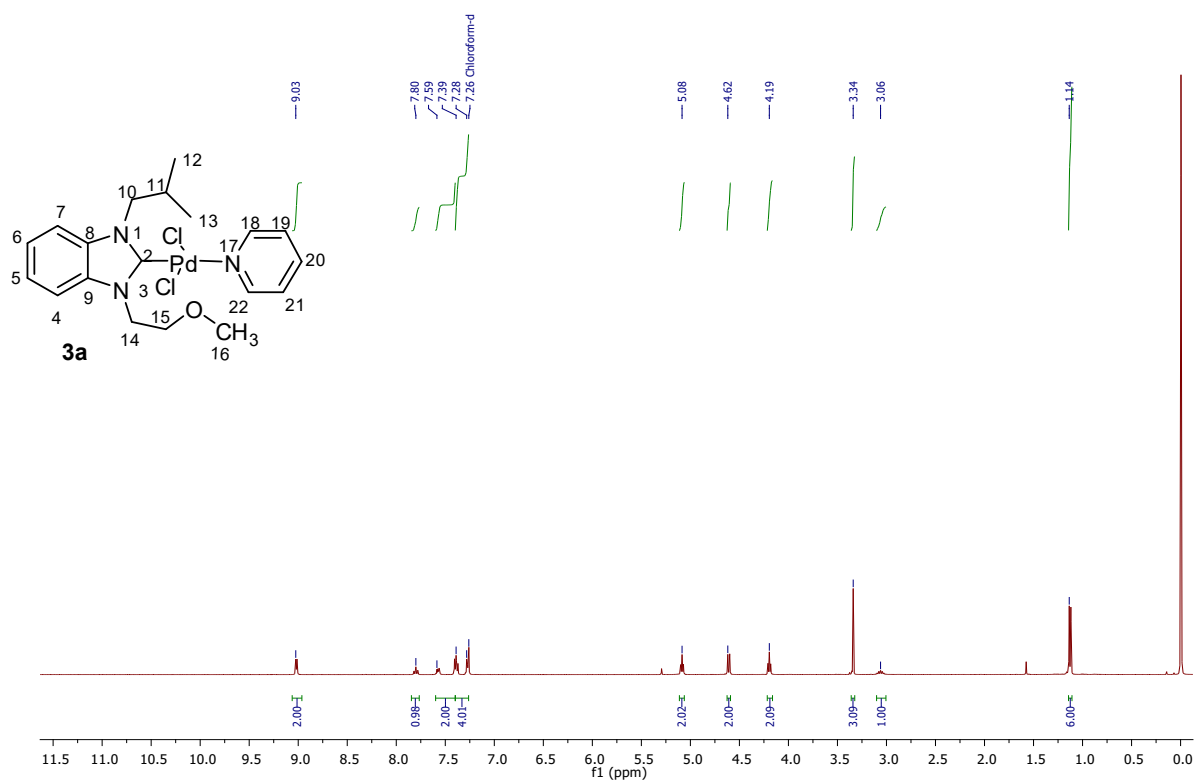


Figure S16. ¹³C NMR spectrum (400 MHz, CDCl₃) of Pd-PEPPSI complex 3a.

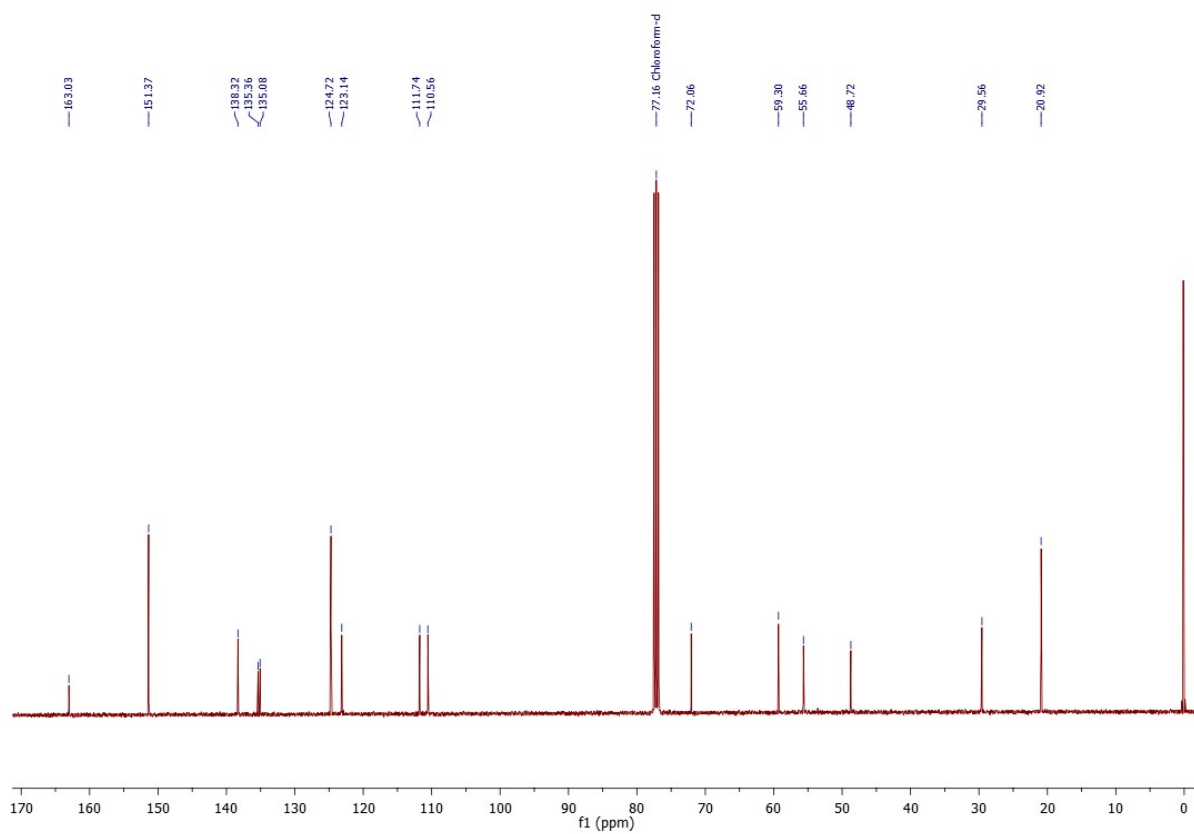


Figure S17. ^{13}C NMR spectrum (100 MHz, CDCl_3) of Pd-PEPPSI complex **3a**

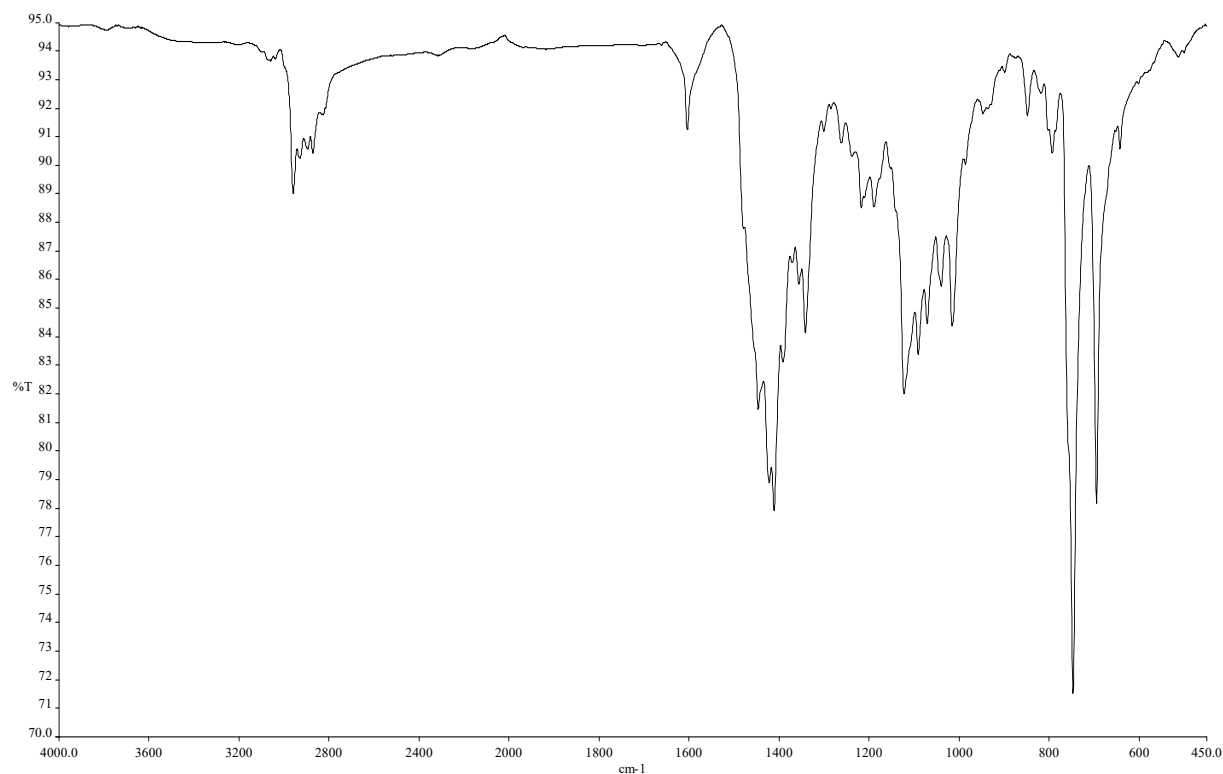


Figure S18. IR spectra on ATR unit of Pd-PEPPSI complex **3a**.

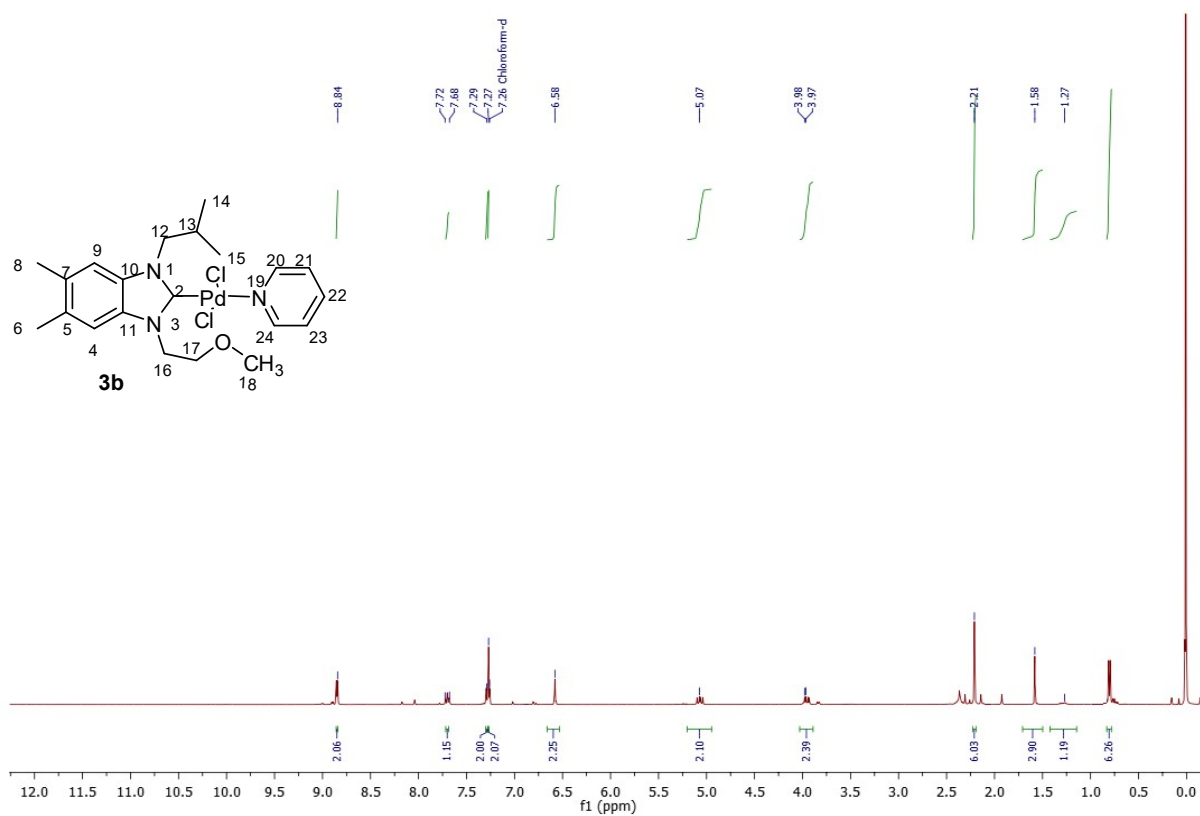


Figure S19. ^1H NMR spectrum (400 MHz, CDCl_3) of Pd-PEPPSI complex 3b.

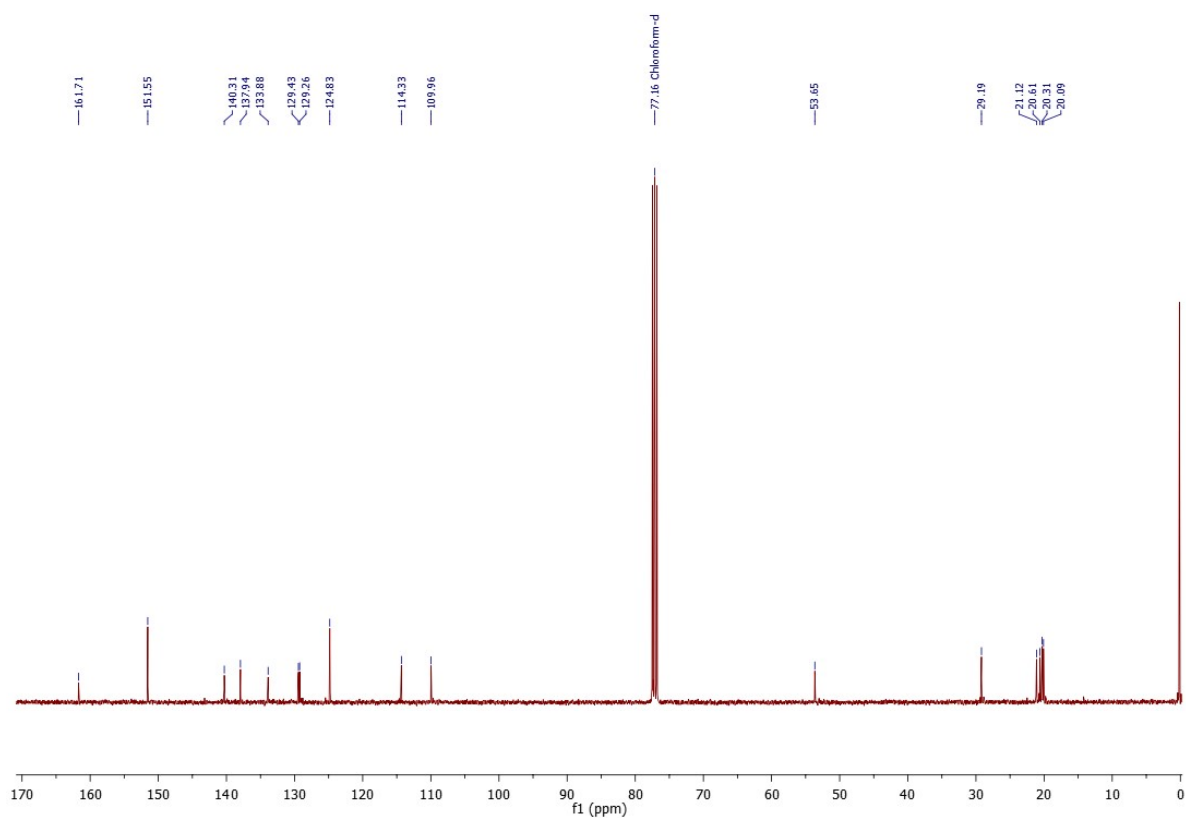


Figure S20. ^{13}C NMR spectrum (100 MHz, CDCl_3) of Pd-PEPPSI complex 3b

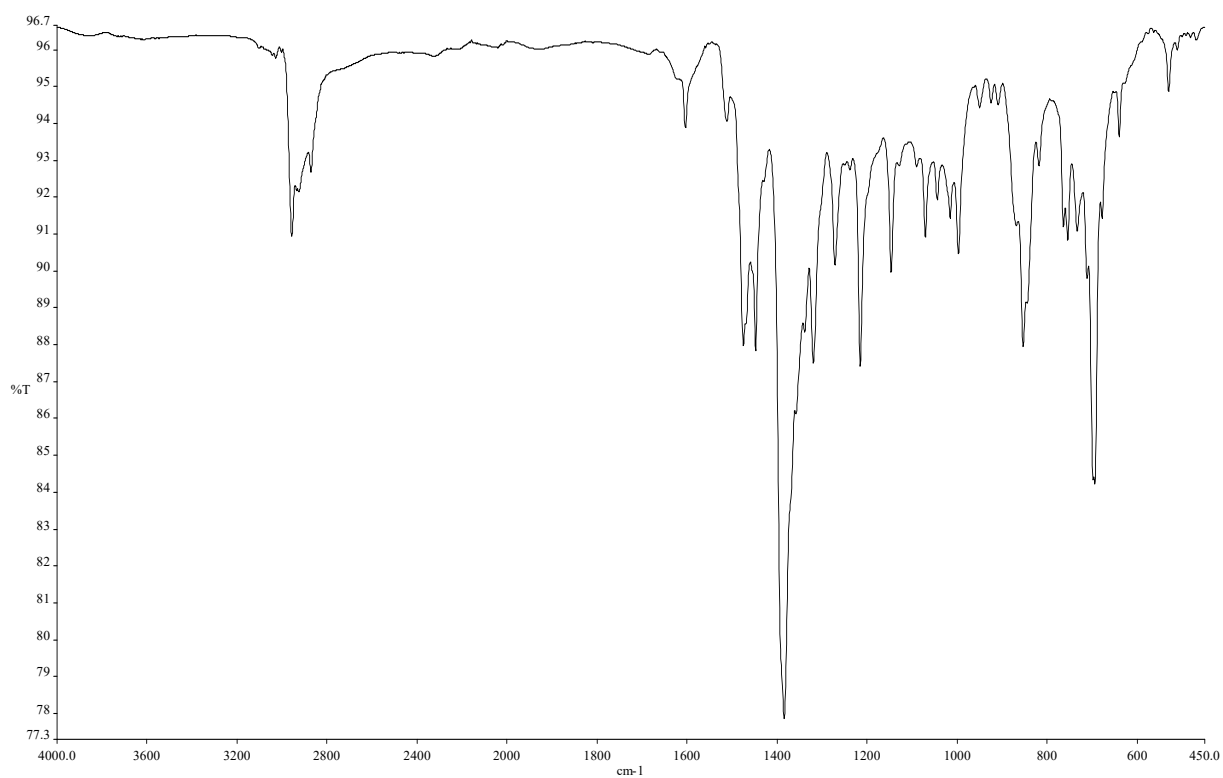


Figure S21. IR spectra on ATR unit of Pd-PEPPSI complex 3b.

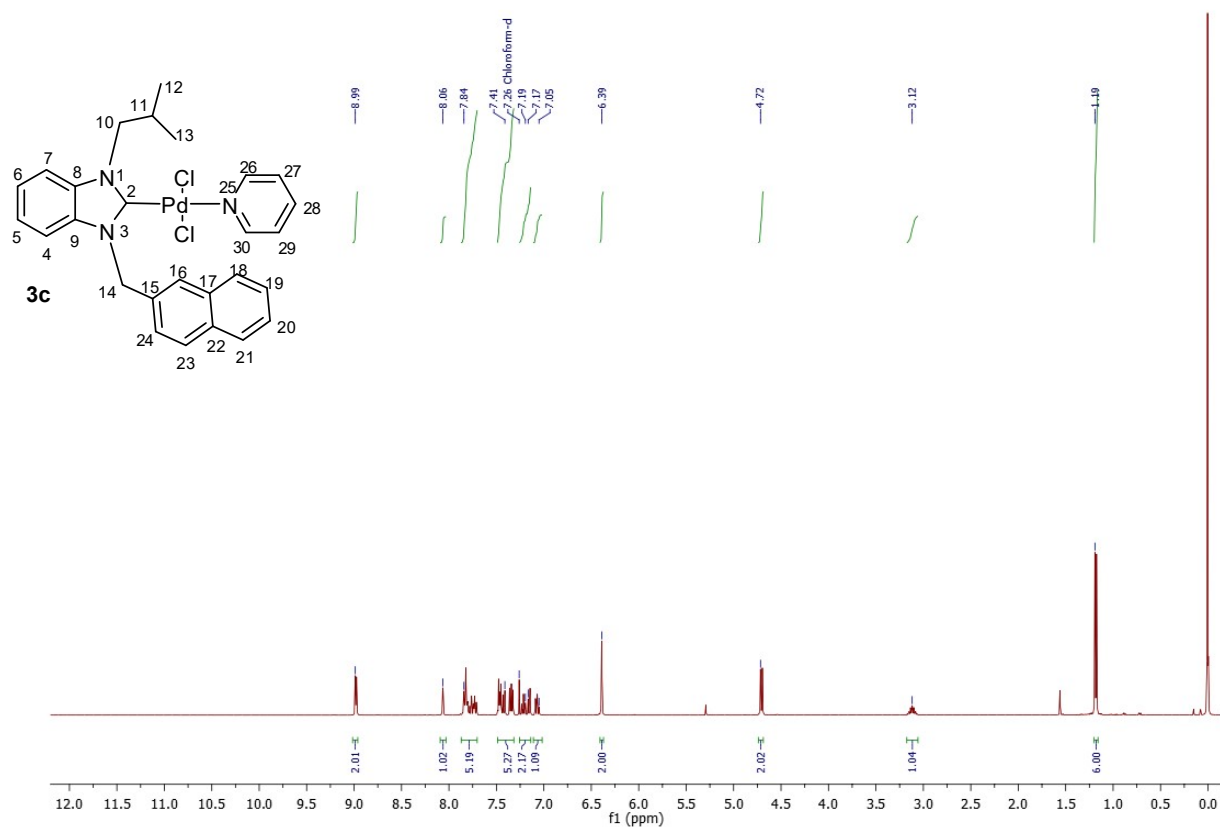


Figure S22. ^{13}C NMR spectrum (400 MHz, CDCl_3) of Pd-PEPPSI complex 3c.

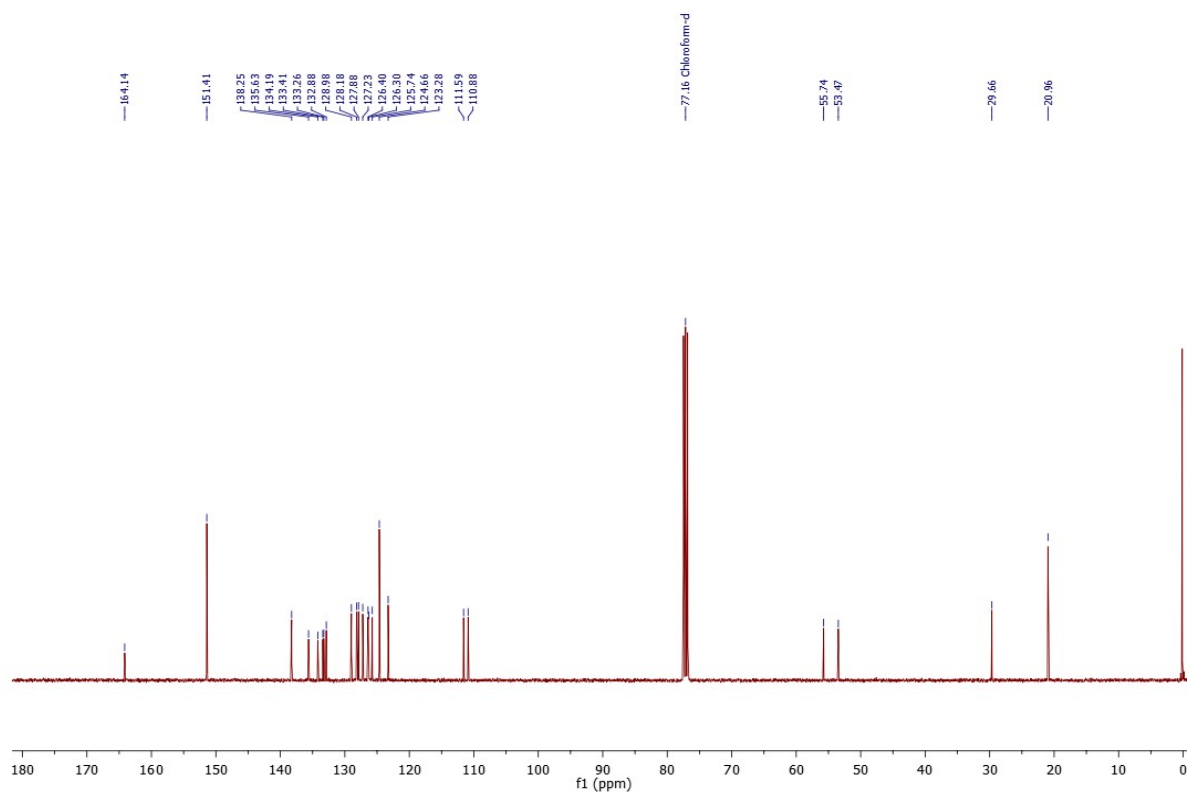


Figure S23. ^{13}C NMR spectrum (100 MHz, CDCl_3) of Pd-PEPPSI complex **3c**

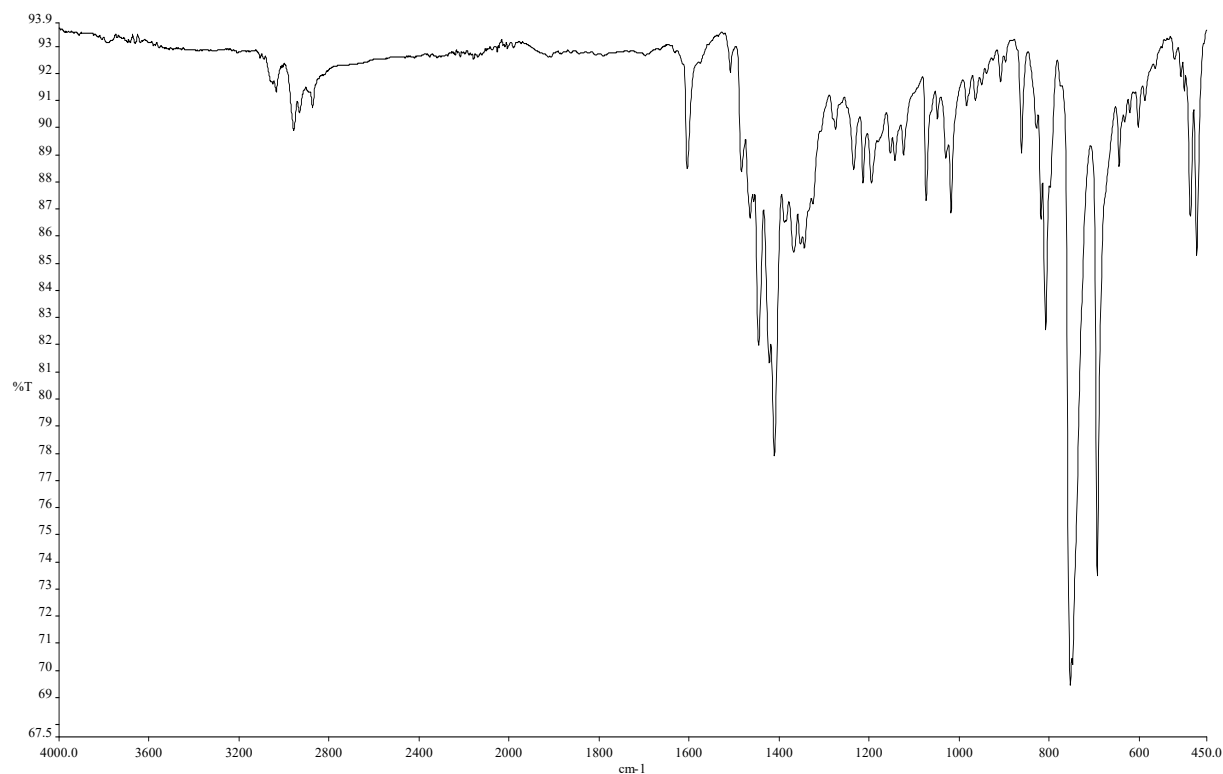


Figure S24. IR spectra on ATR unit of Pd-PEPPSI complex **3c**.

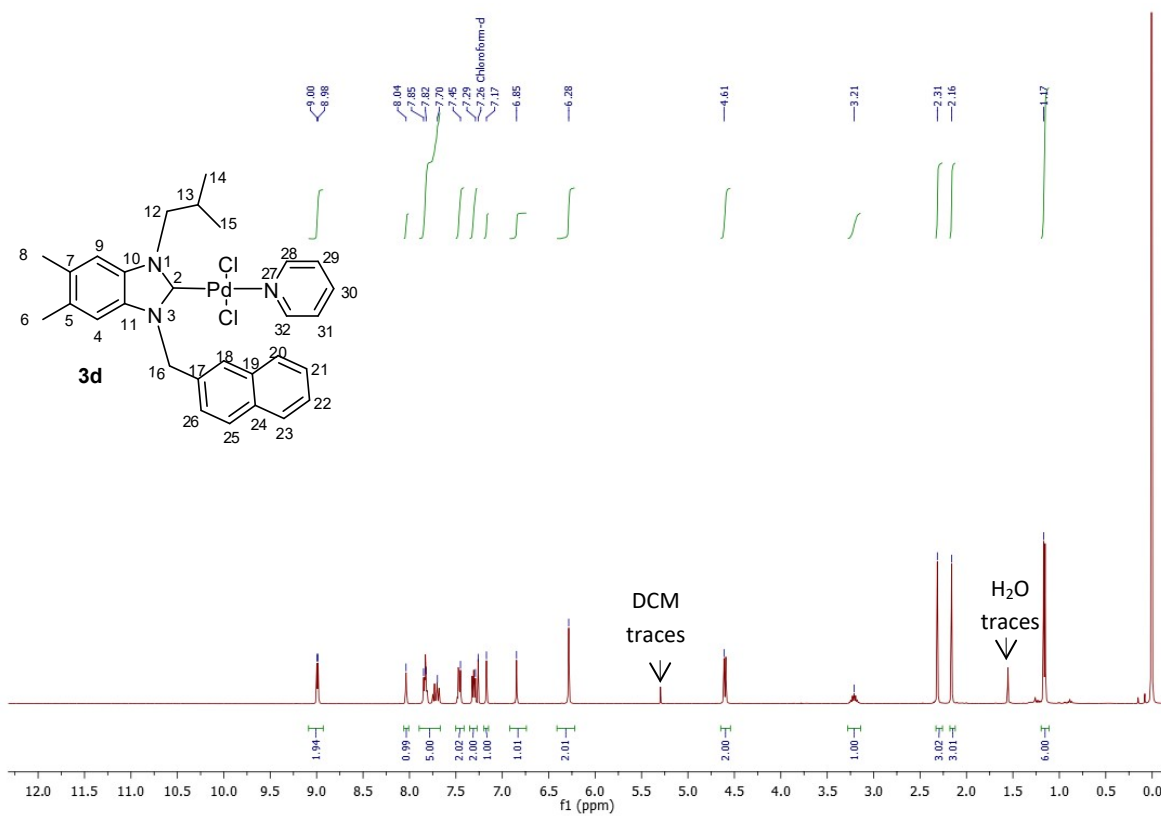


Figure S25. ^1H NMR spectrum (400 MHz, CDCl_3) of Pd-PEPPSI complex 3d.

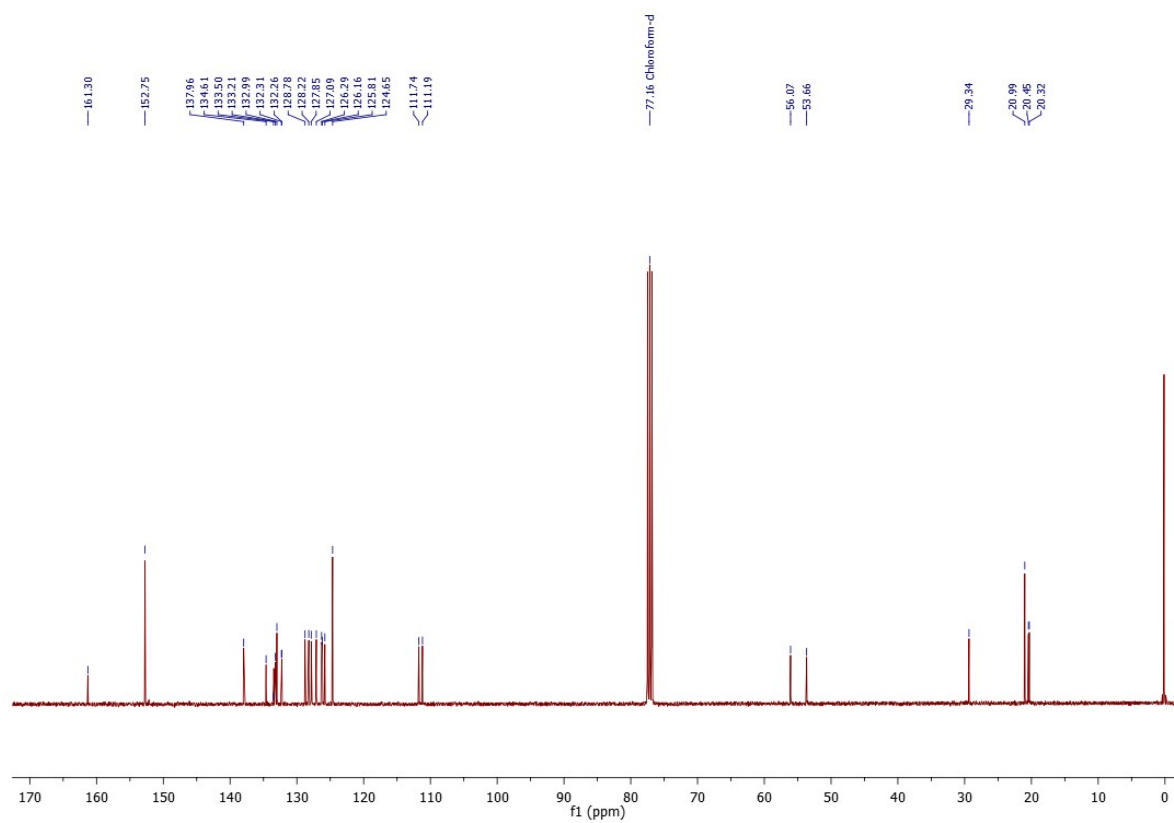


Figure S26. ^{13}C NMR spectrum (100 MHz, CDCl_3) of Pd-PEPPSI complex 3d

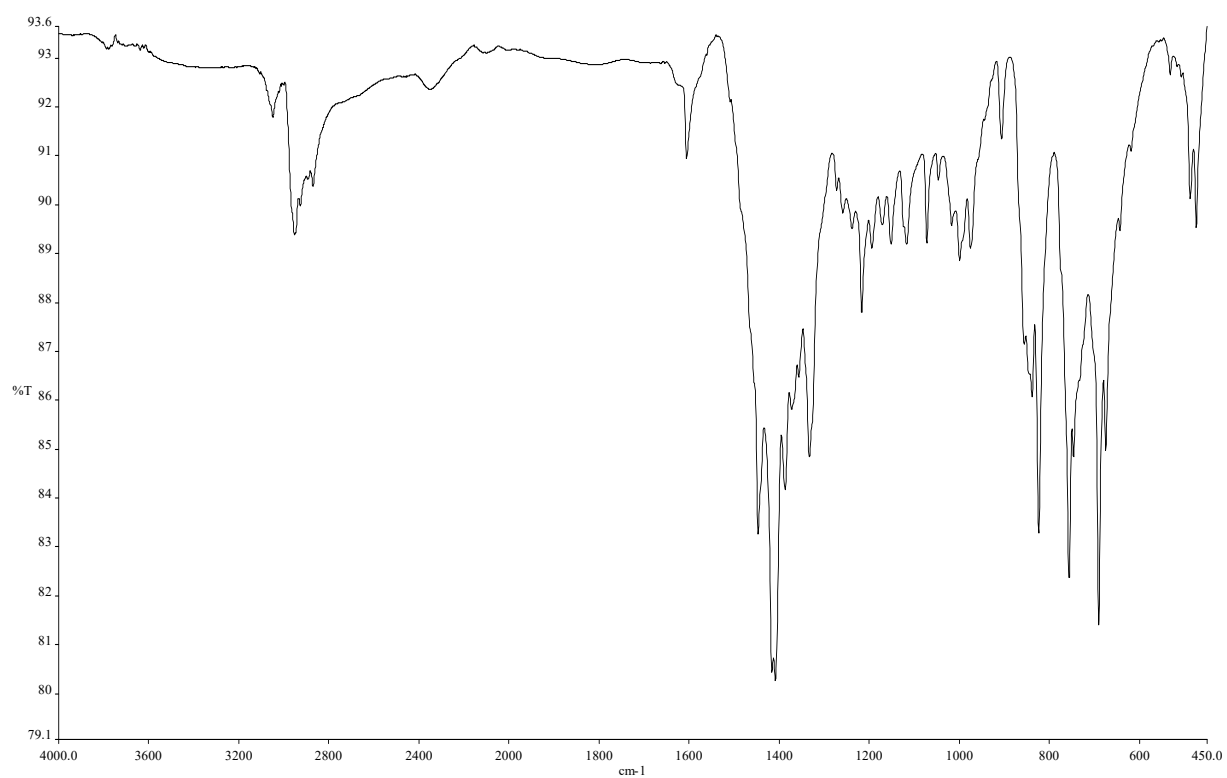


Figure S27. IR spectra on ATR unit of Pd-PEPPSI complex 3d.

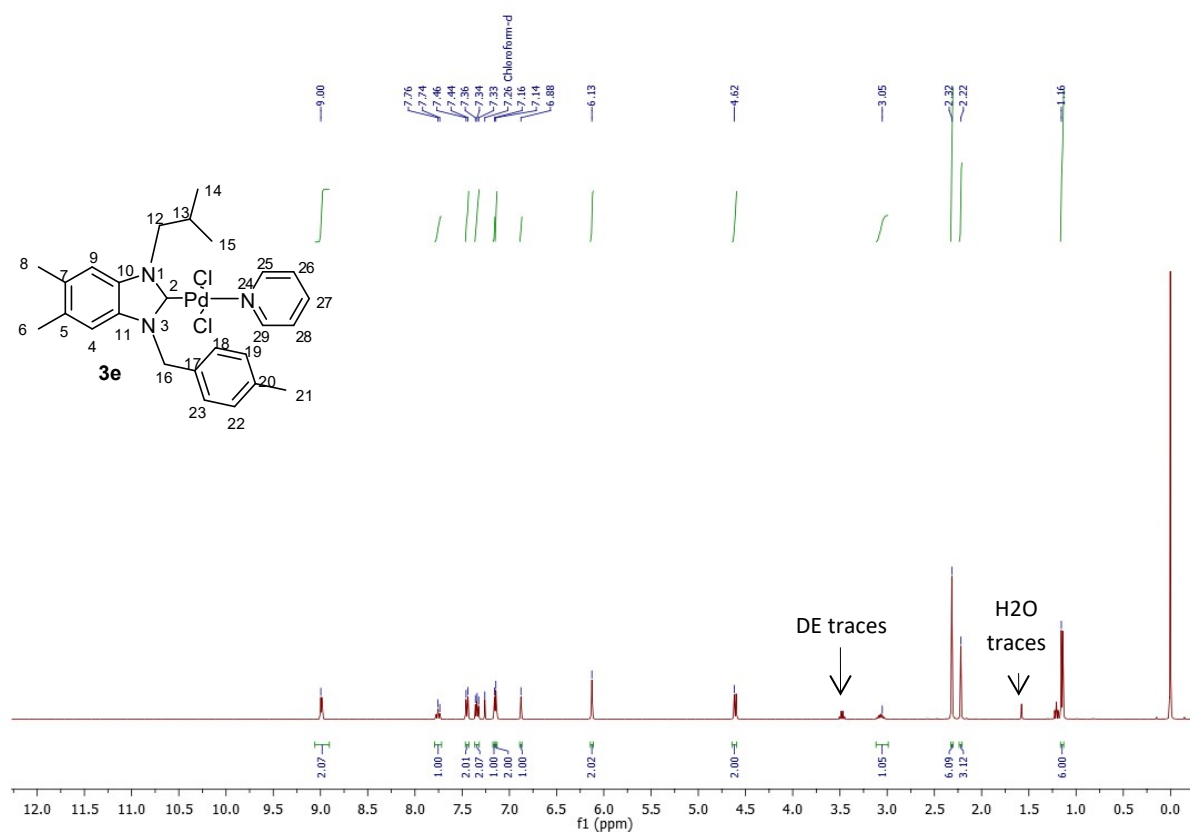


Figure S28. ¹H NMR spectrum (400 MHz, CDCl₃) of Pd-PEPPSI complex 3e.

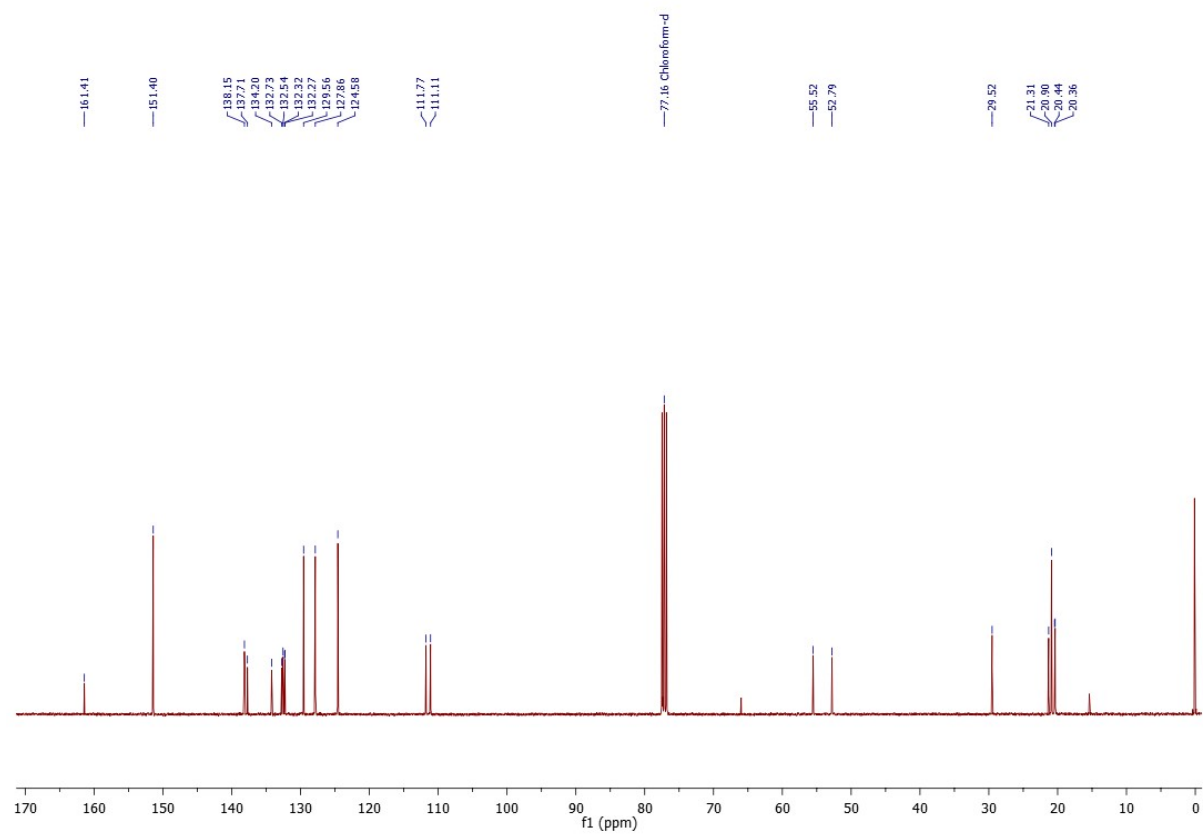


Figure S29. ^{13}C NMR spectrum (100 MHz, CDCl_3) of Pd-PEPPSI complex **3e**

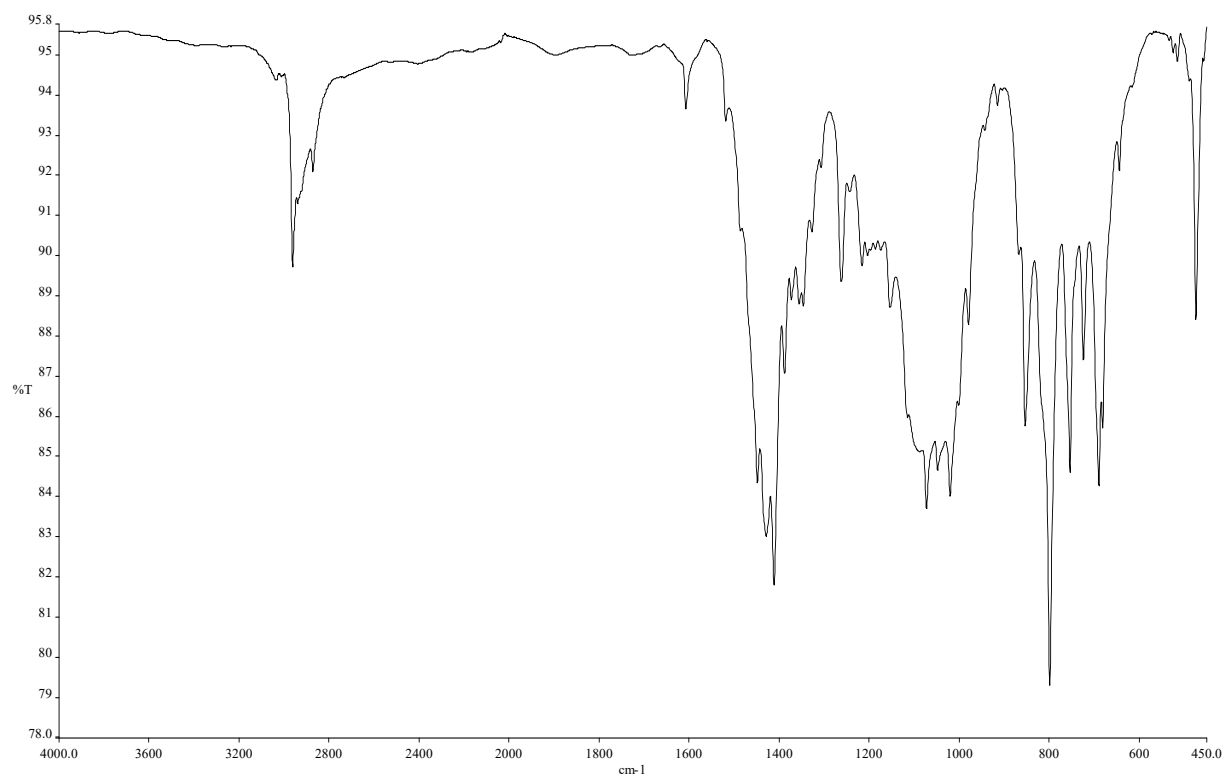


Figure S30. IR spectra on ATR unit of Pd-PEPPSI complex **3e**.

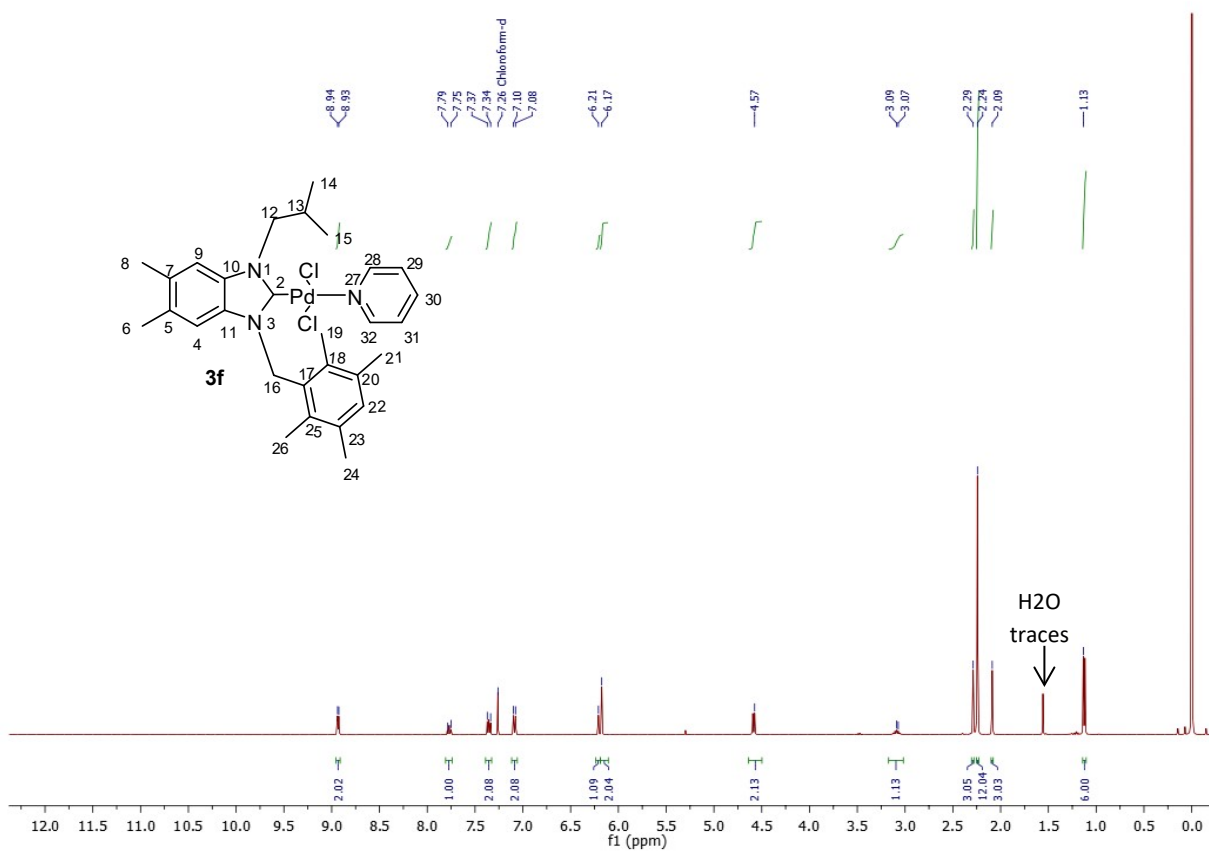


Figure S31. ^1H NMR spectrum (400 MHz, CDCl_3) of Pd-PEPPSI complex 3f.

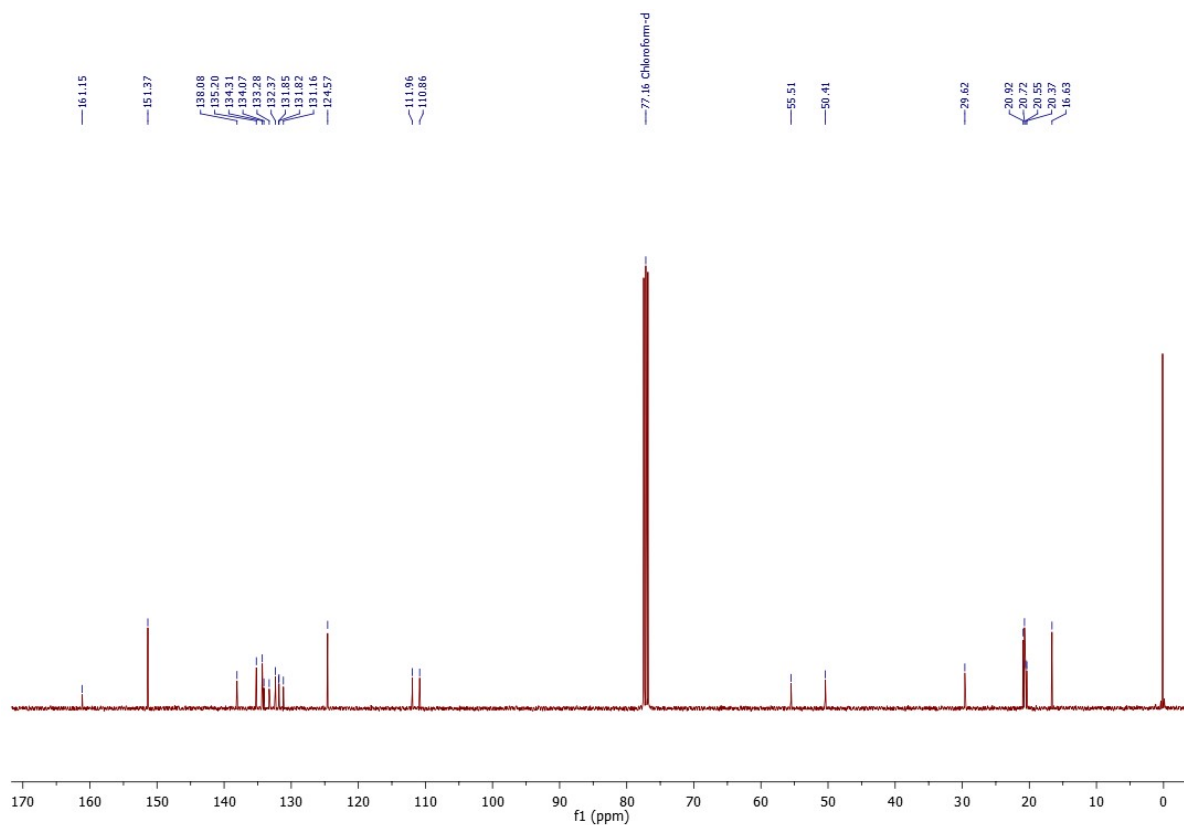


Figure S32. ^{13}C NMR spectrum (100 MHz, CDCl_3) of Pd-PEPPSI complex 3f

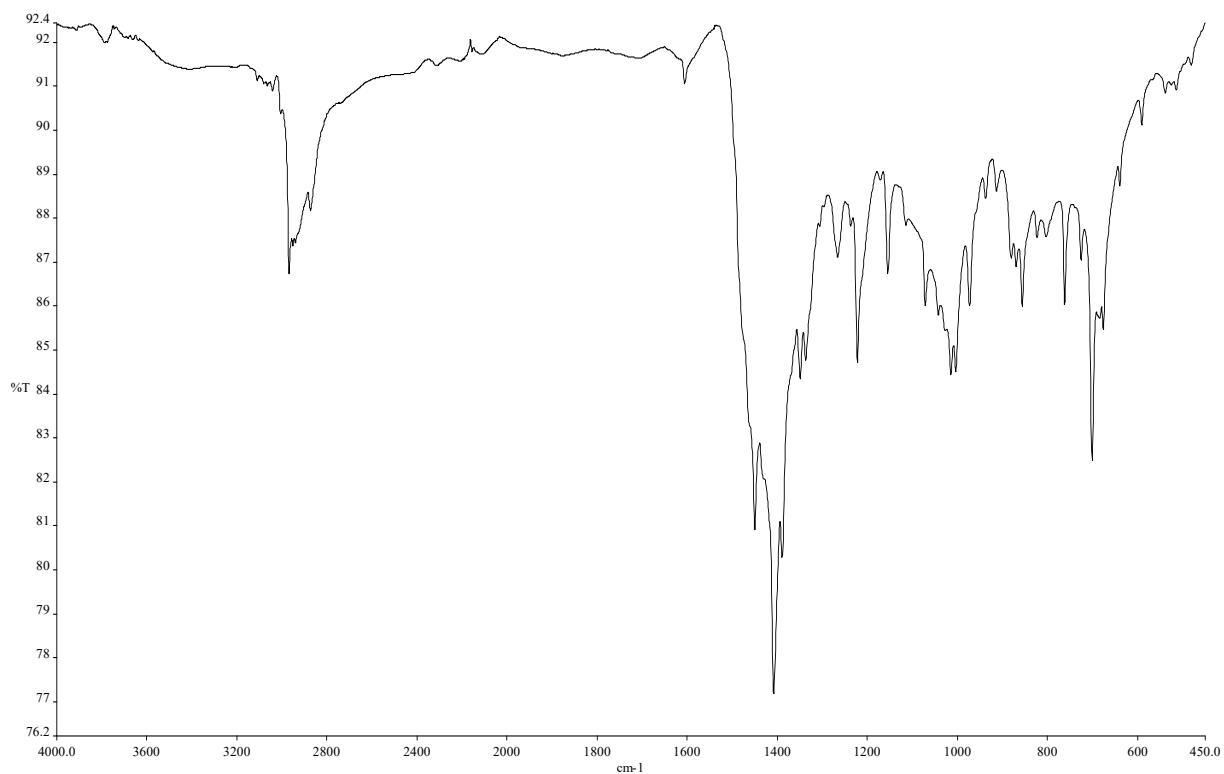


Figure S33. IR spectra on ATR unit of Pd-PEPPSI complex 3f.

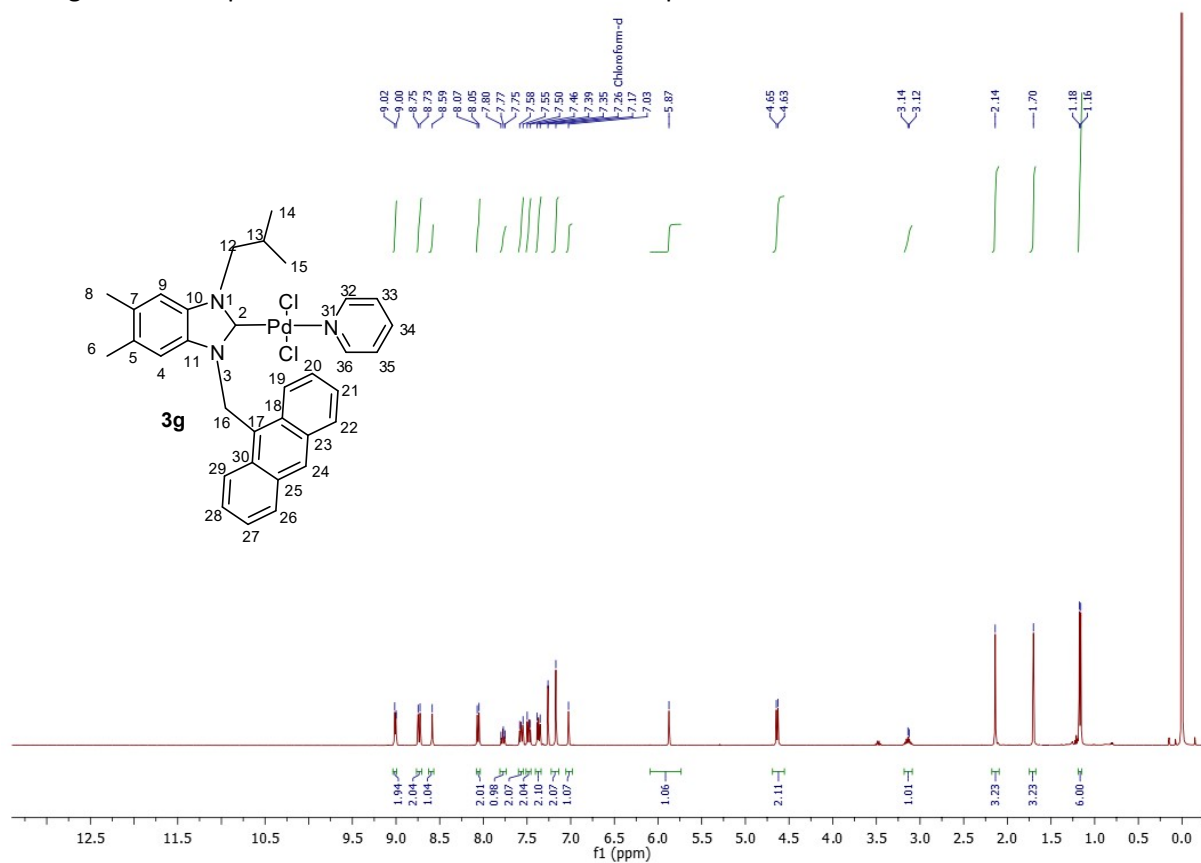


Figure S34. ¹³C NMR spectrum (400 MHz, CDCl₃) of Pd-PEPPSI complex 3g.

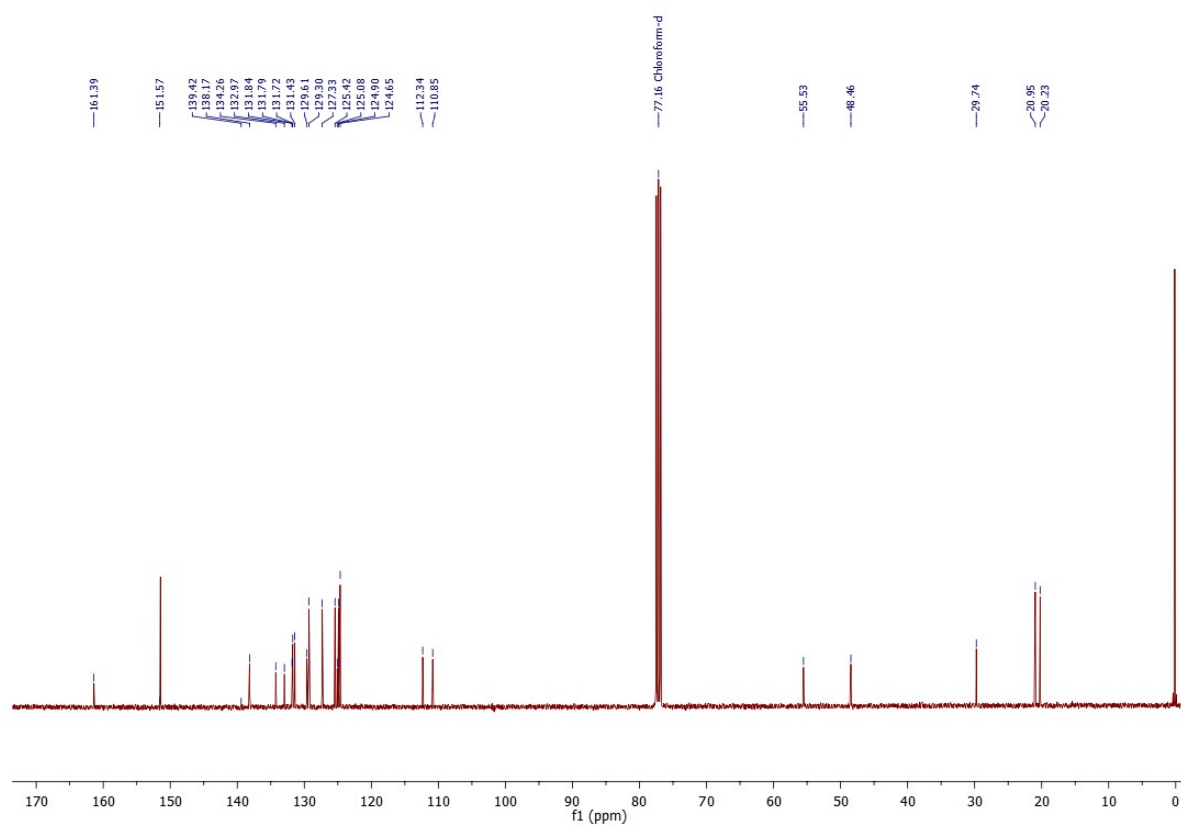


Figure S35. ^{13}C NMR spectrum (100 MHz, CDCl_3) of Pd-PEPPSI complex 3g.

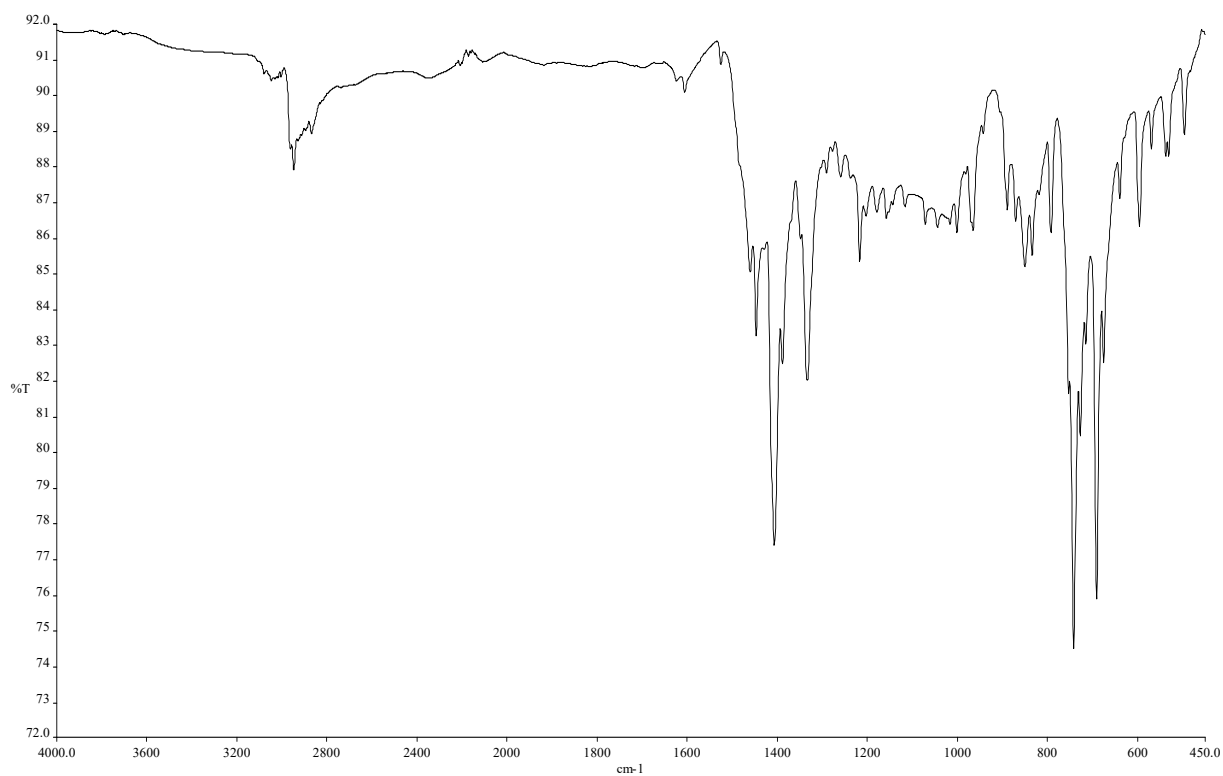


Figure S36. IR spectra on ATR unit of Pd-PEPPSI complex 3g.