

**N-H Bond Activation by Palladium(II) and Copper(I) Complexes Featuring a
Reactive Bidentate PN-Ligand**

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NMR and MS Spectra of New Ligands and Complexes

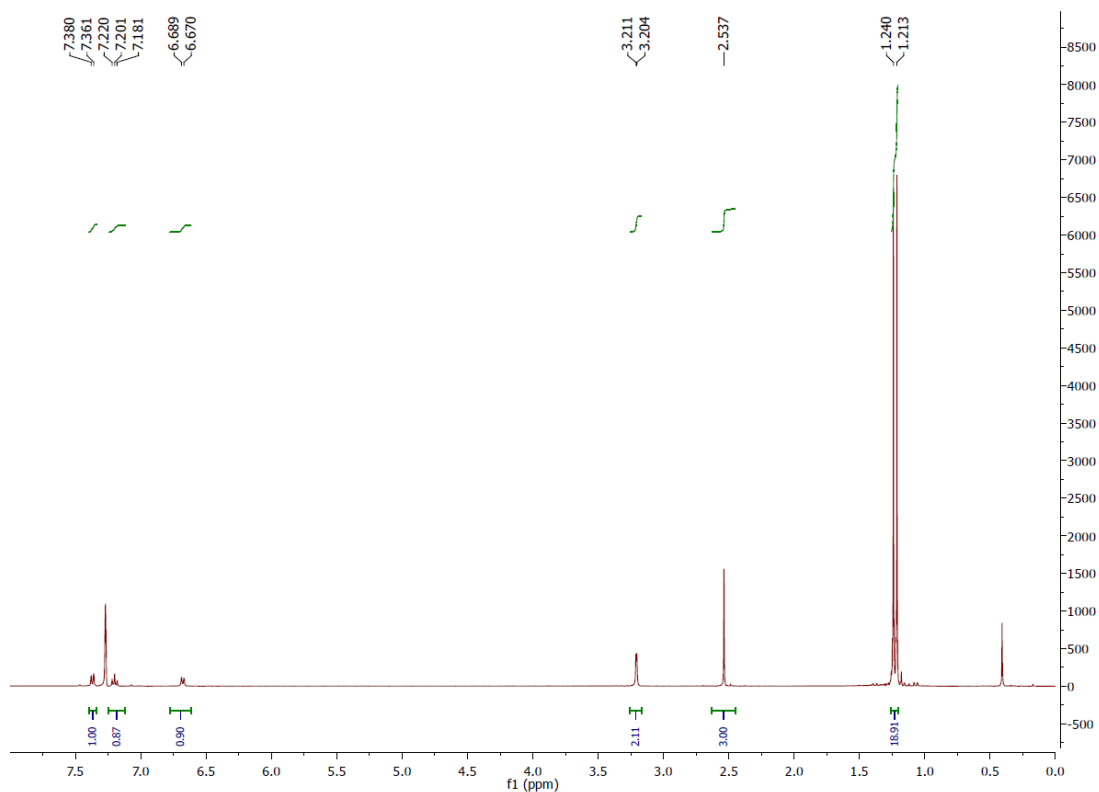


Fig. S1. ¹H NMR spectrum of ligand **L1H** (C₆D₆, 400 MHz, 298 K).

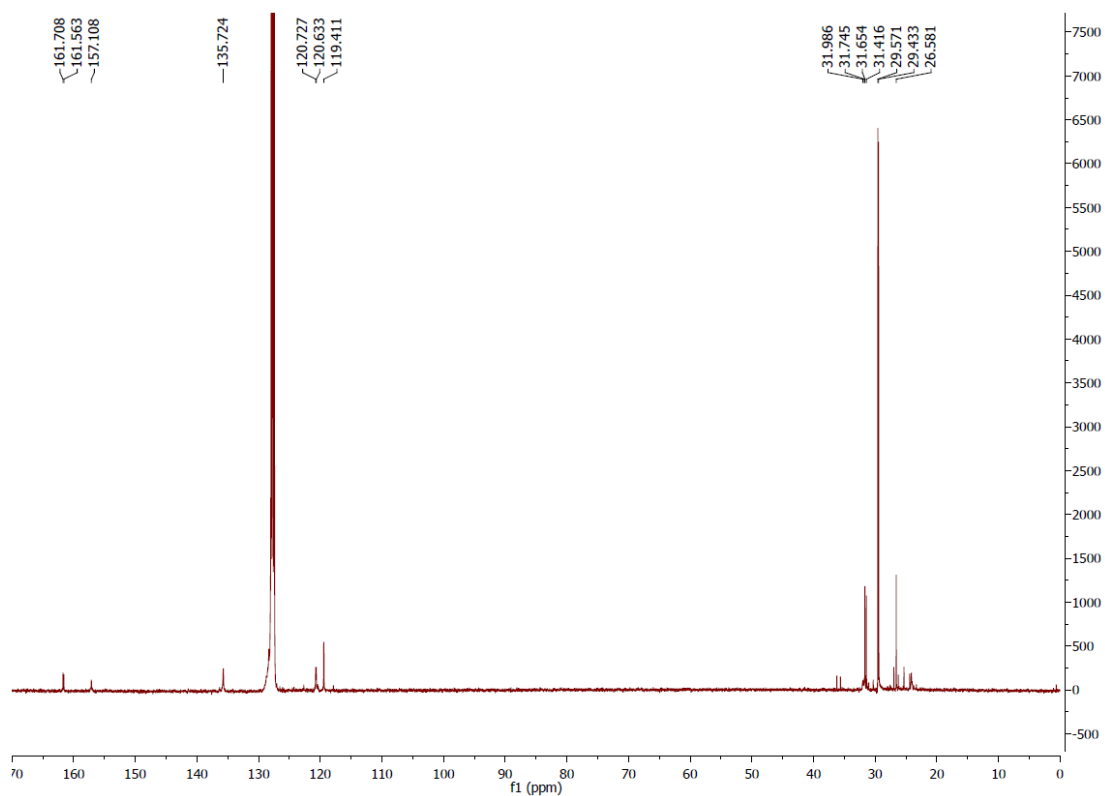


Fig. S2. ¹³C NMR spectrum of ligand **L1H** (C₆D₆, 100 MHz, 298 K).

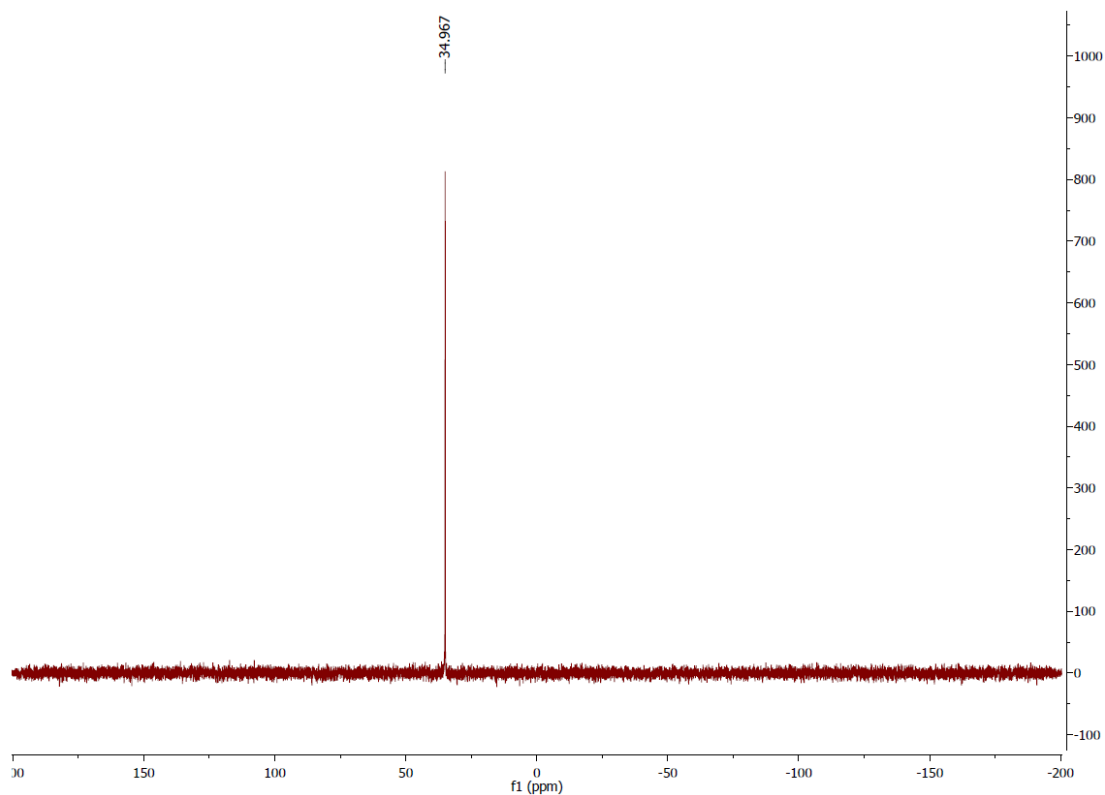


Fig. S3. ^{31}P NMR spectrum of ligand **L1H** (C_6D_6 , 162 MHz, 298 K).

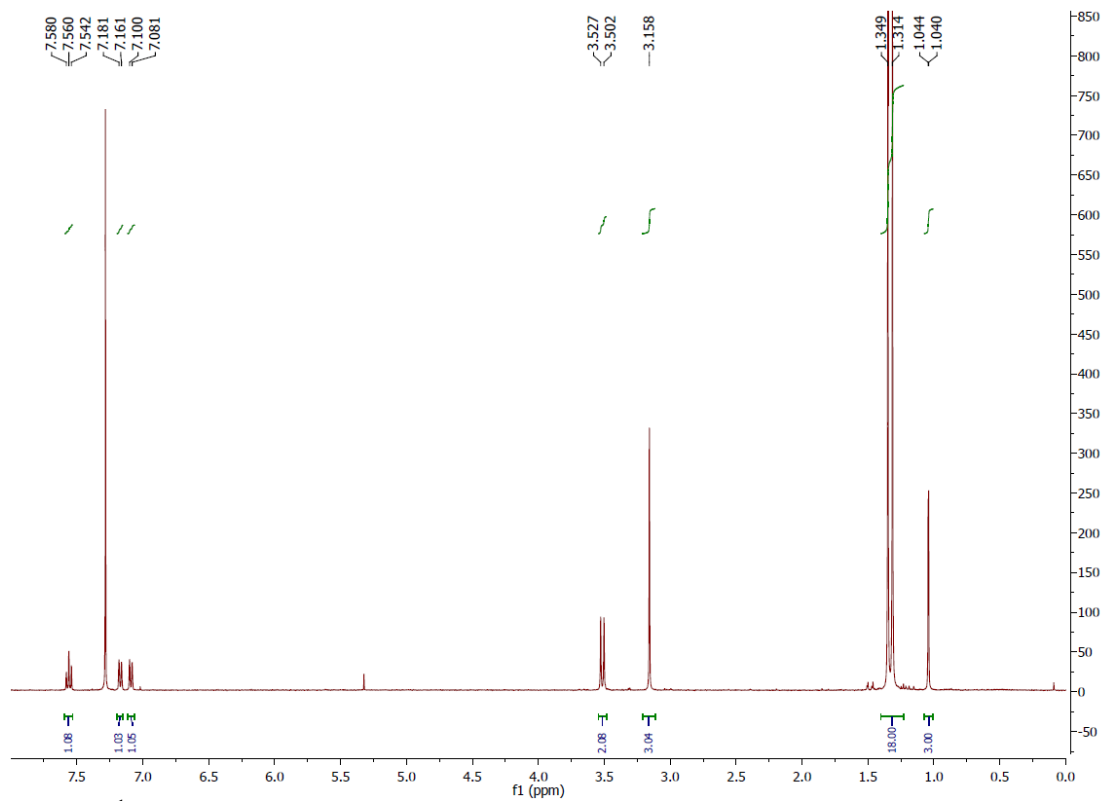


Fig. S4. ^1H NMR spectrum of complex **1** (CDCl_3 , 500 MHz, 298 K).

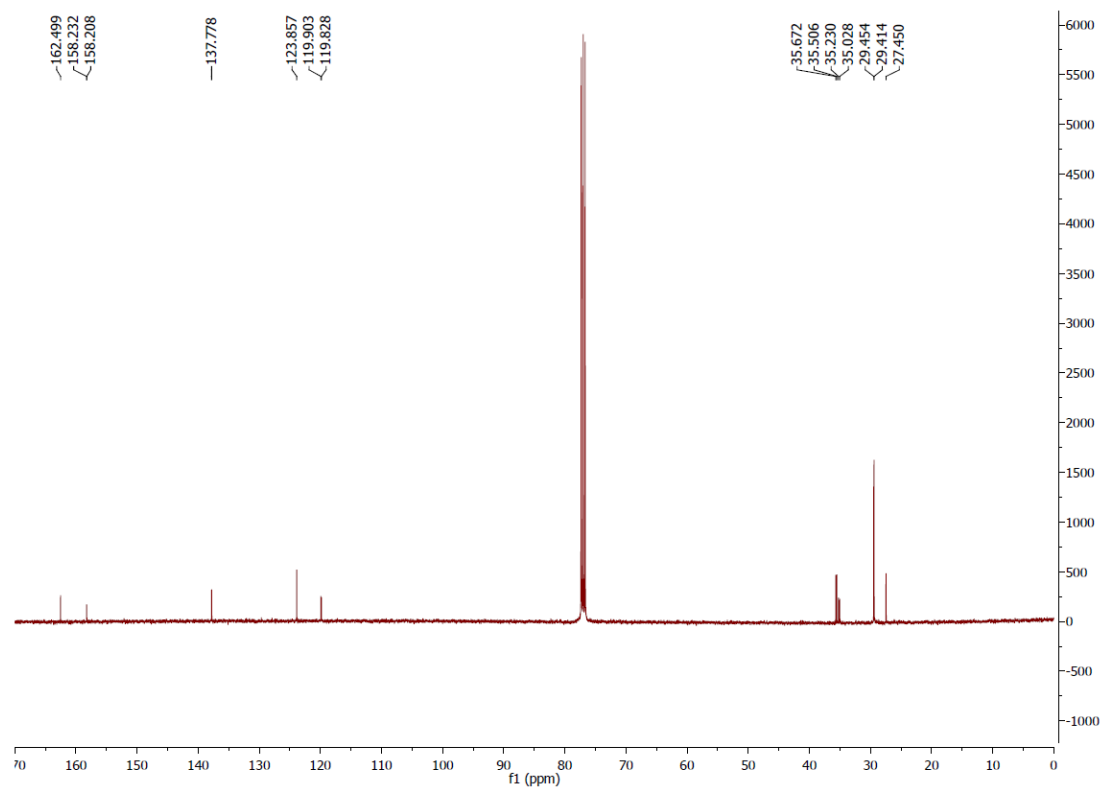


Fig. S5. ^{13}C NMR spectrum of complex **1** (CDCl_3 , 126 MHz, 298 K).

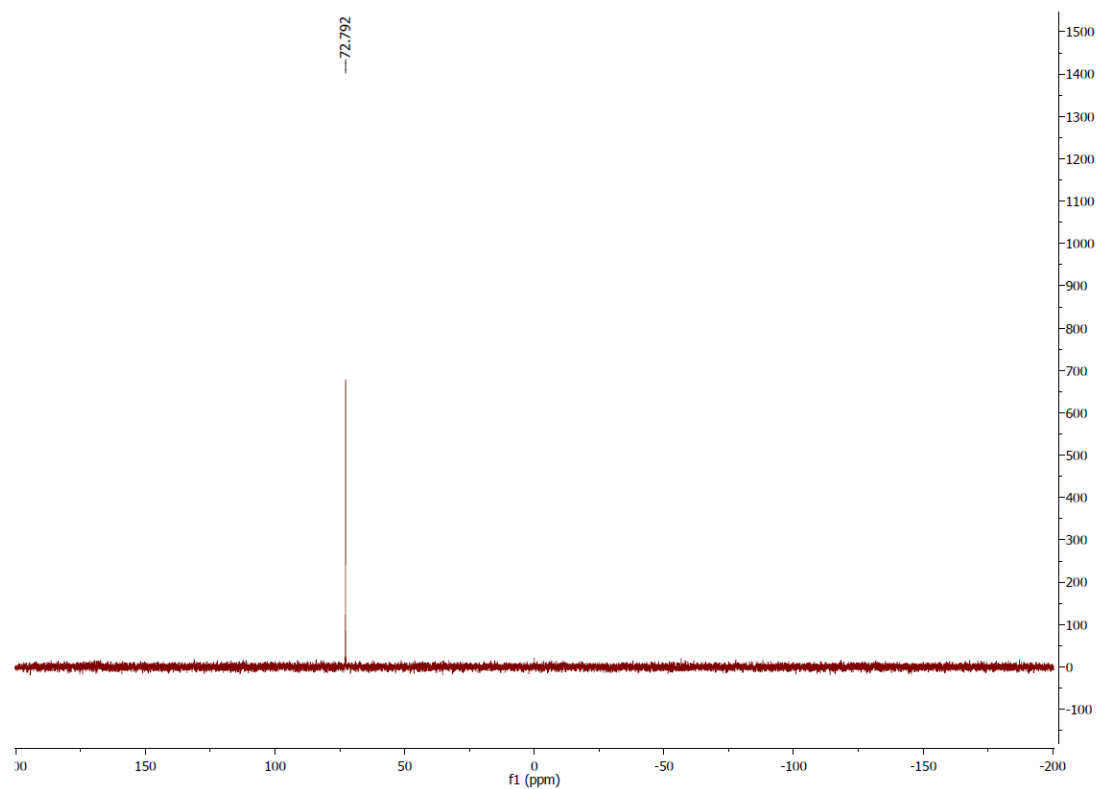


Fig. S6. ^{31}P NMR spectrum of complex **1** (CDCl_3 , 202 MHz, 298 K).

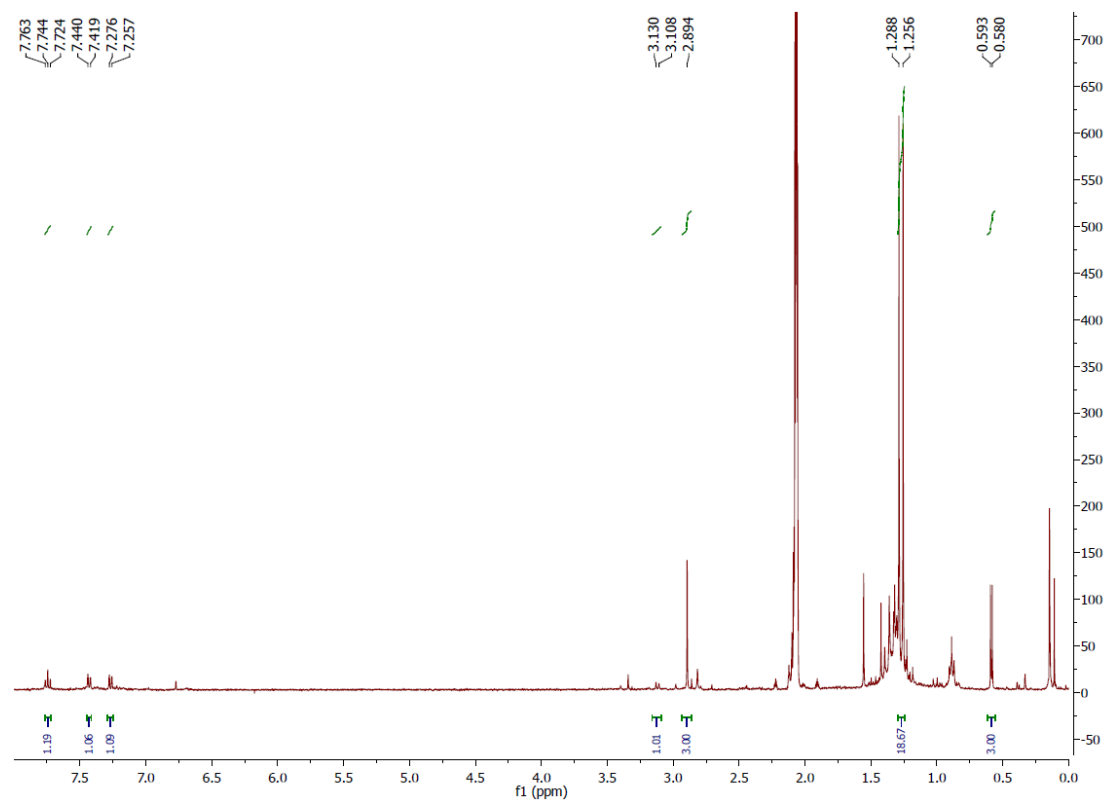


Fig. S7. ^1H NMR spectrum of complex **X** (acetone- d_6 , 400 MHz, 298 K).

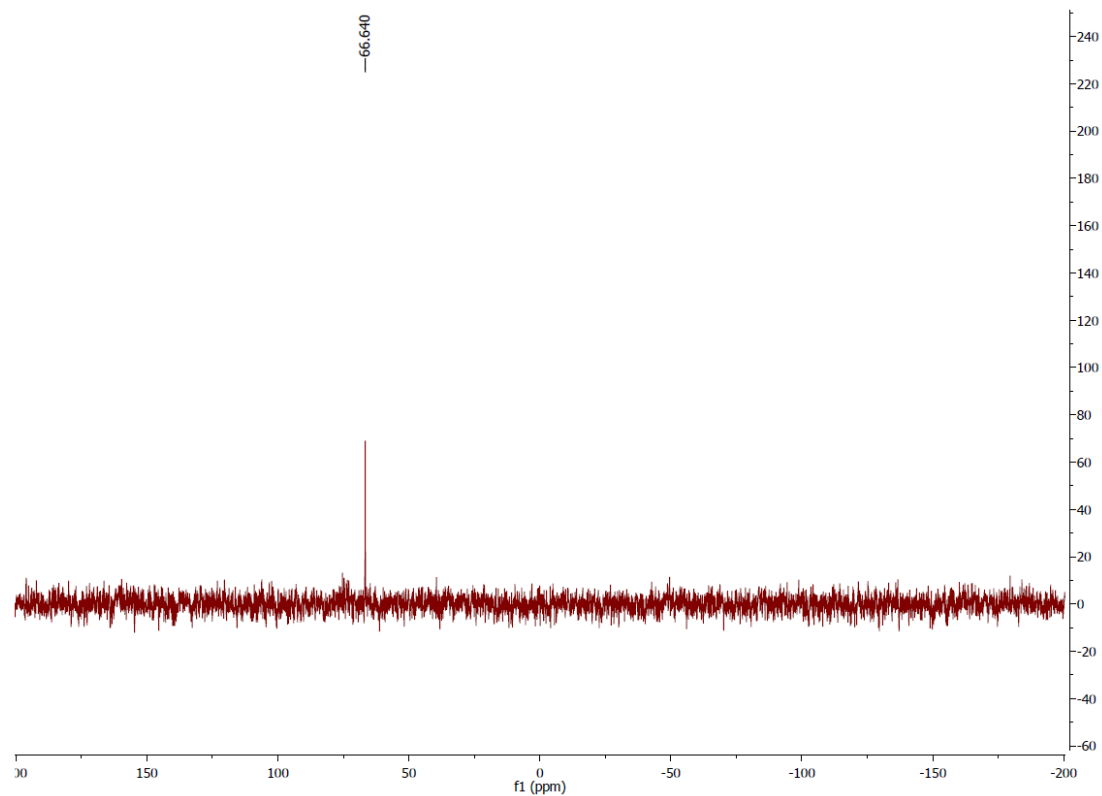


Fig. S8. ^{31}P NMR spectrum of complex **X** (acetone- d_6 , 162 MHz, 298 K).

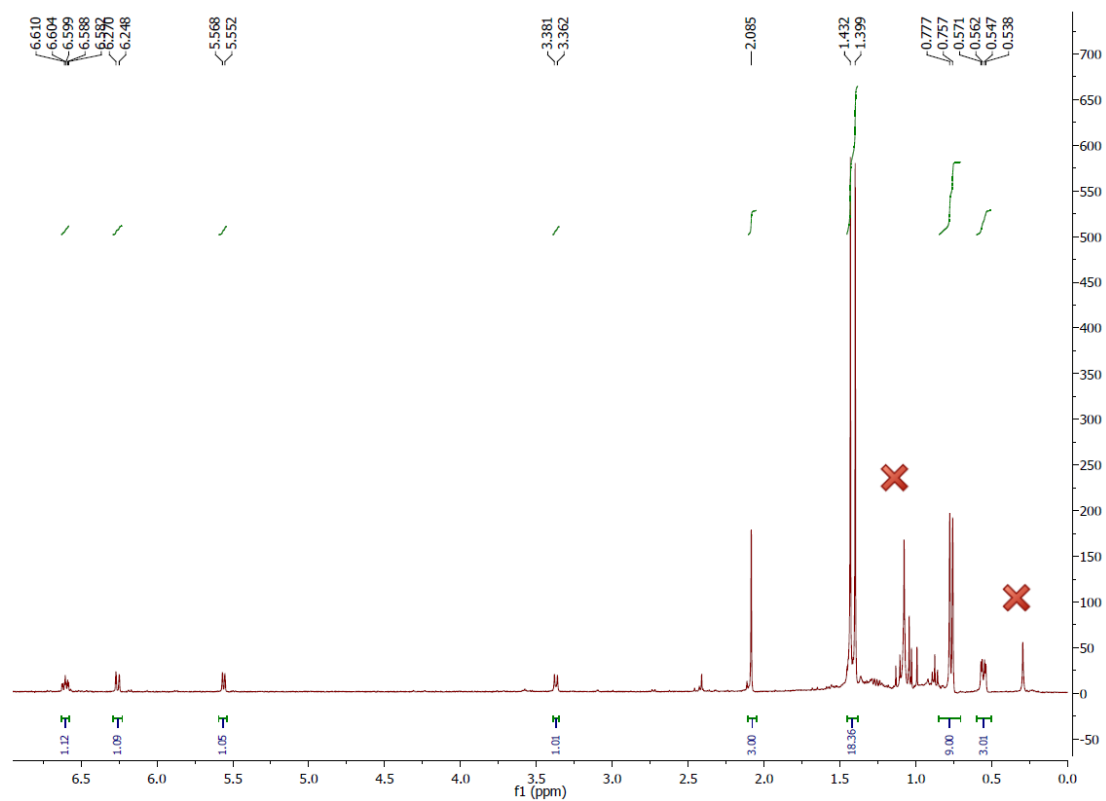


Fig. S9. ^1H NMR spectrum of complex **Y** (C_6D_6 , 400 MHz, 298 K). X at δ 1.06 is *tert*-butyl alcohol, at δ 0.30 grease.

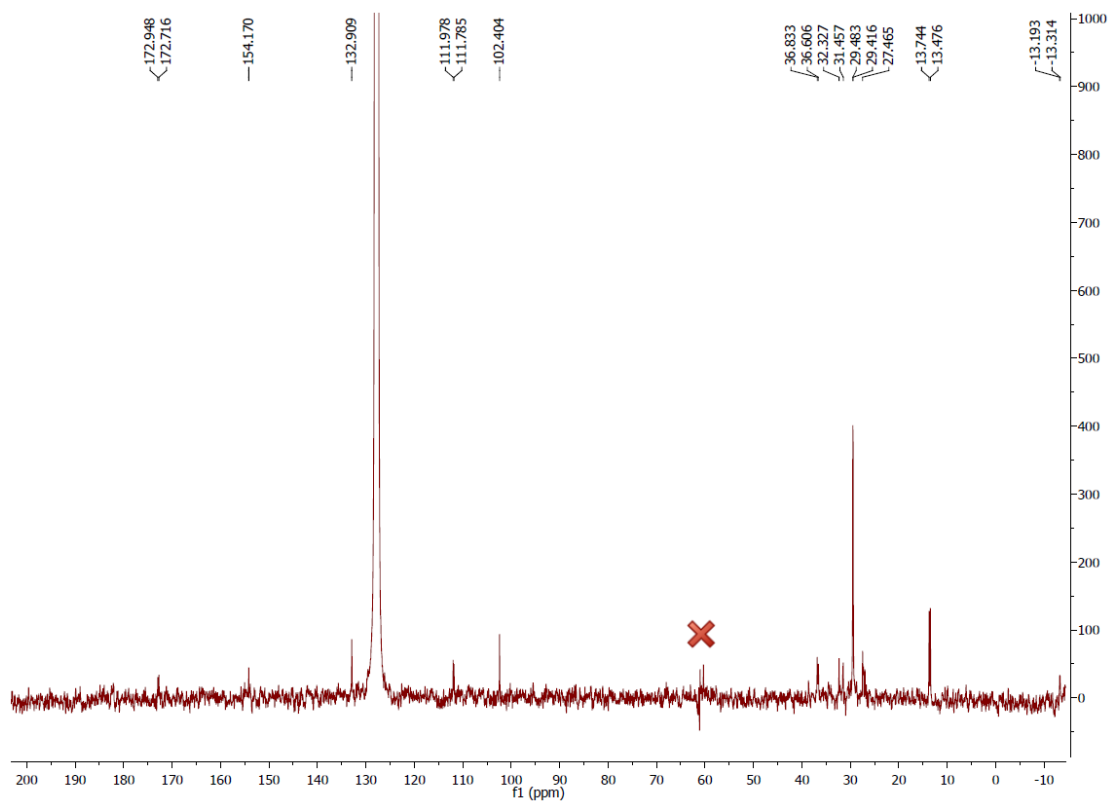


Fig. S10. ^{13}C NMR spectrum of complex **Y** (C_6D_6 , 100 MHz, 298 K). X at δ 60 is an artefact.

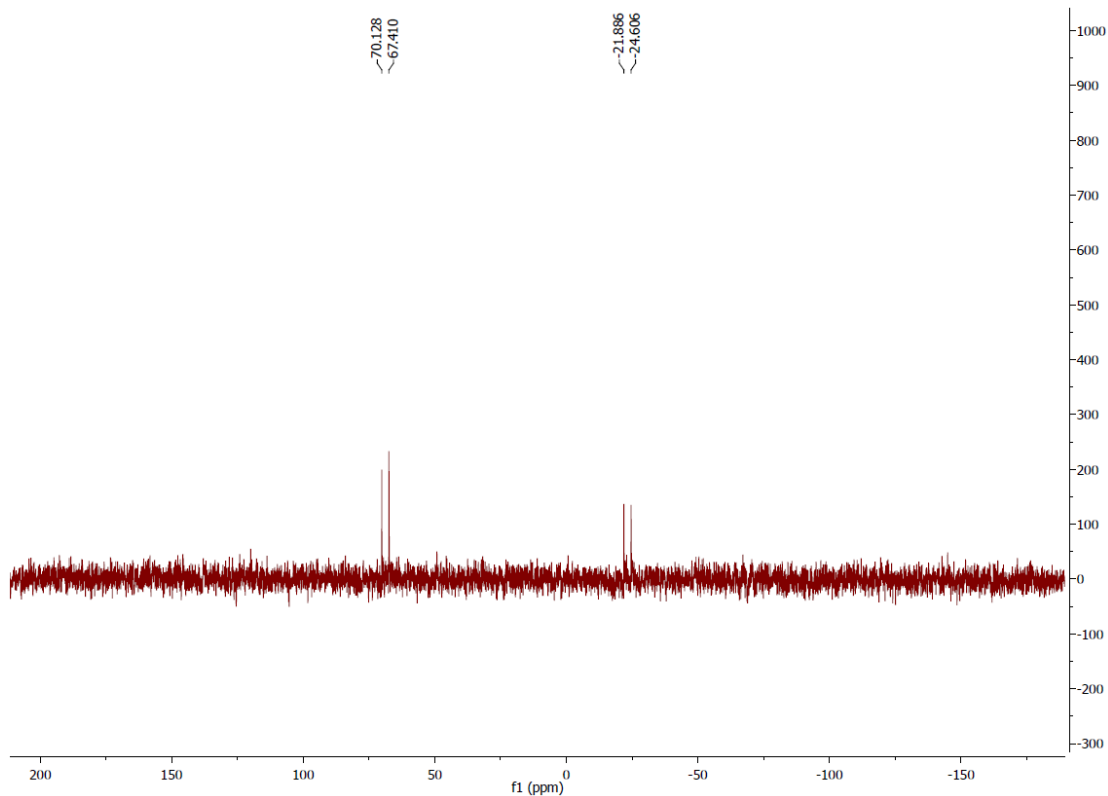


Fig. S11. ^{31}P NMR spectrum of complex **Y** (C_6D_6 , 162 MHz, 298 K).

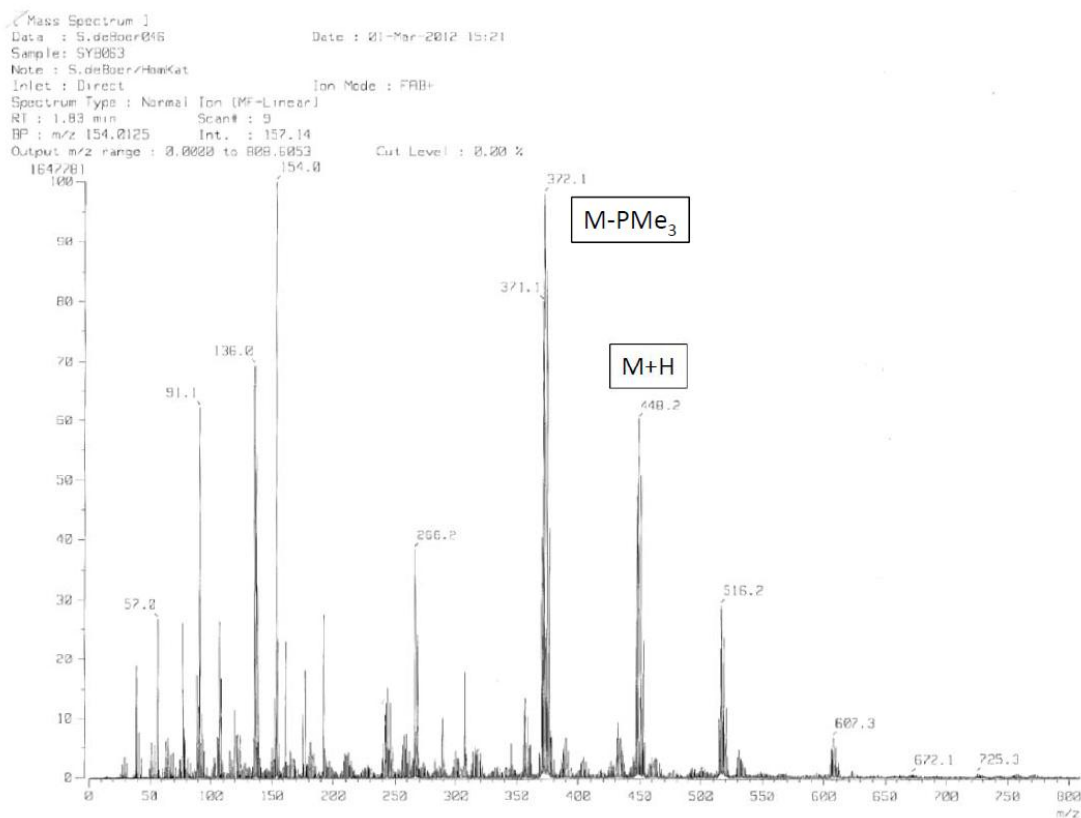


Fig. S12. Mass spectrum of complex **Y**.

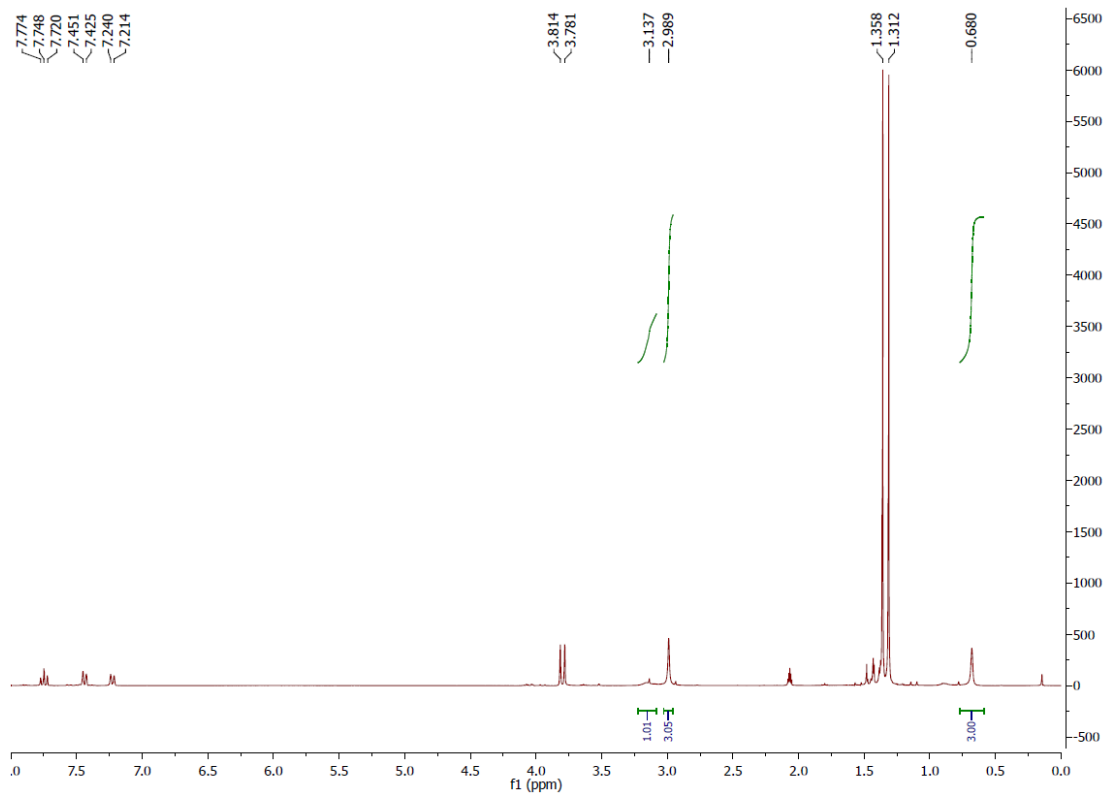


Fig. S13. ¹H NMR spectrum of complex **2** (acetone-*d*₆, 400 MHz, 298 K).

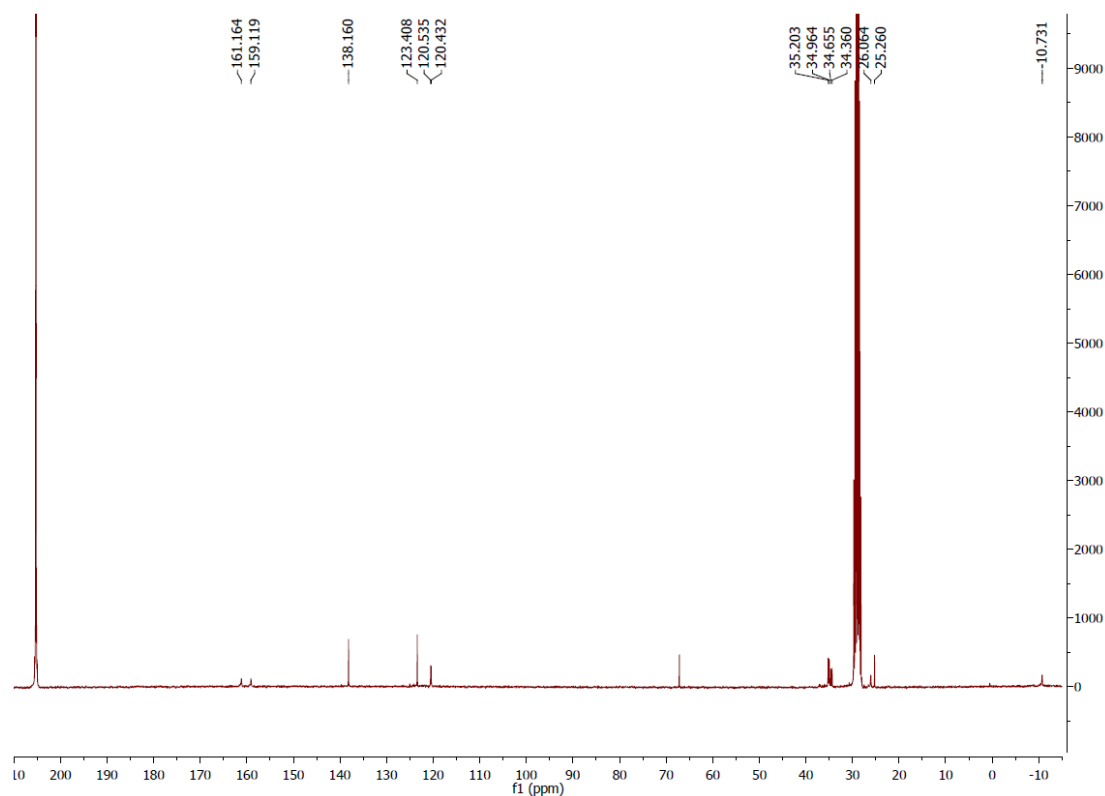


Fig. S14. ¹³C NMR spectrum of complex **2** (acetone-*d*₆, 100 MHz, 298 K).

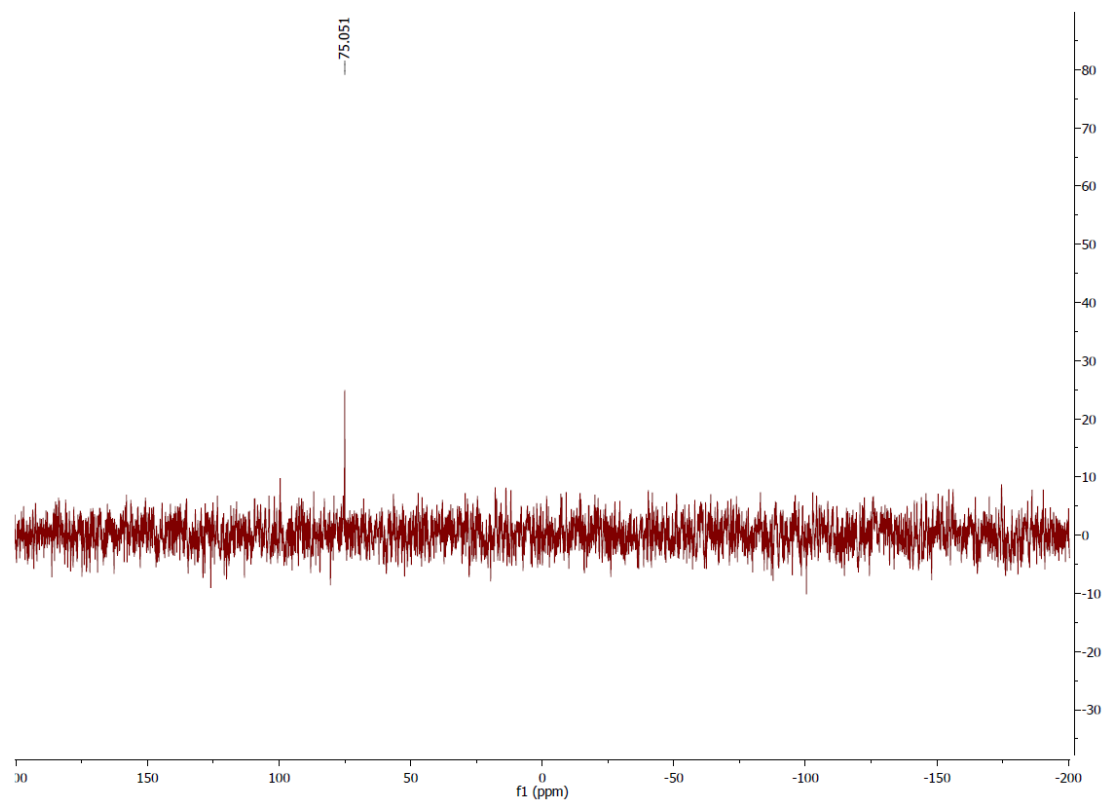


Fig. S15. ³¹P NMR spectrum of complex 2 (acetone-d₆, 162 MHz, 298 K).

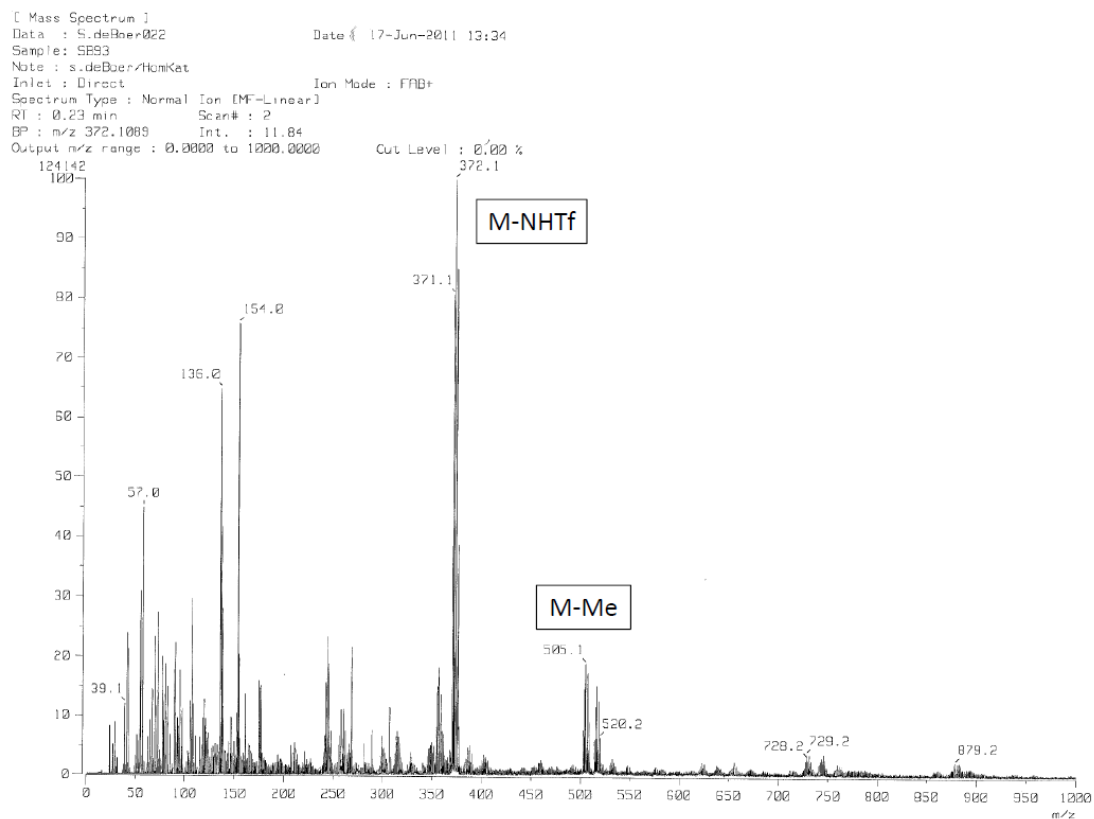


Fig. S16. Mass spectrum of complex 2.

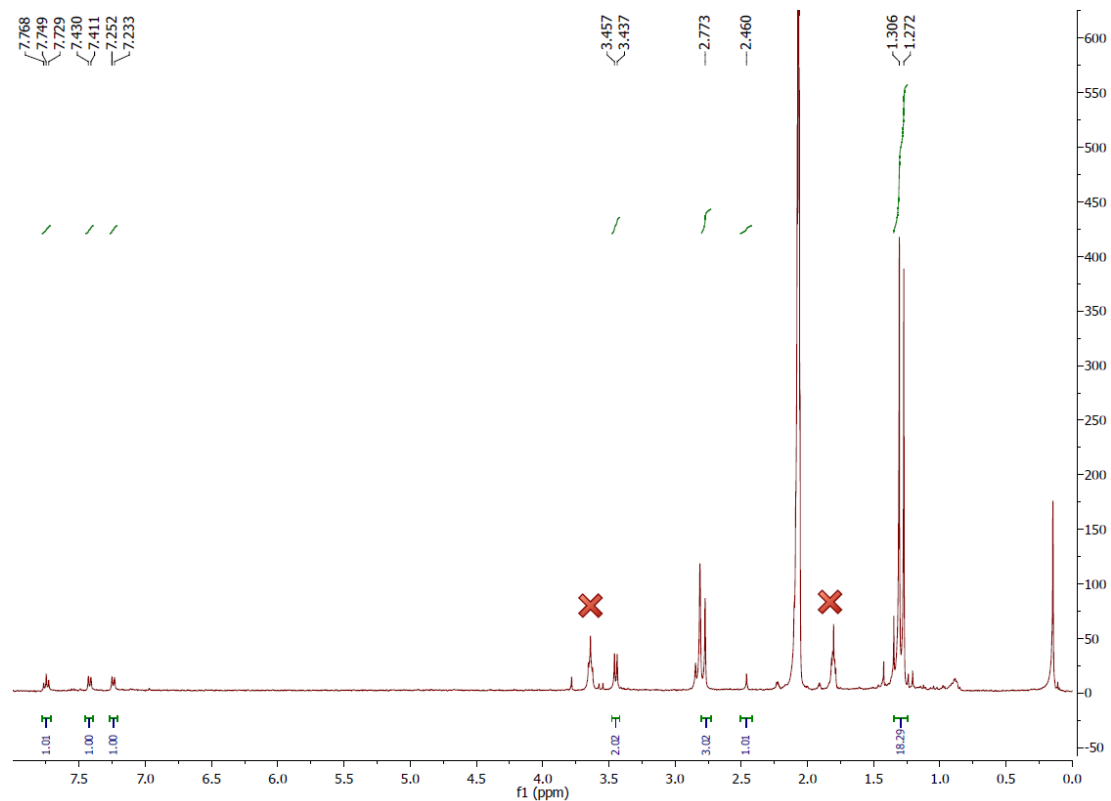


Fig. S17. ^1H NMR spectrum of complex **4** (acetone- d_6 , 400 MHz, 298 K). X at δ 3.63 and 1.81 is THF.

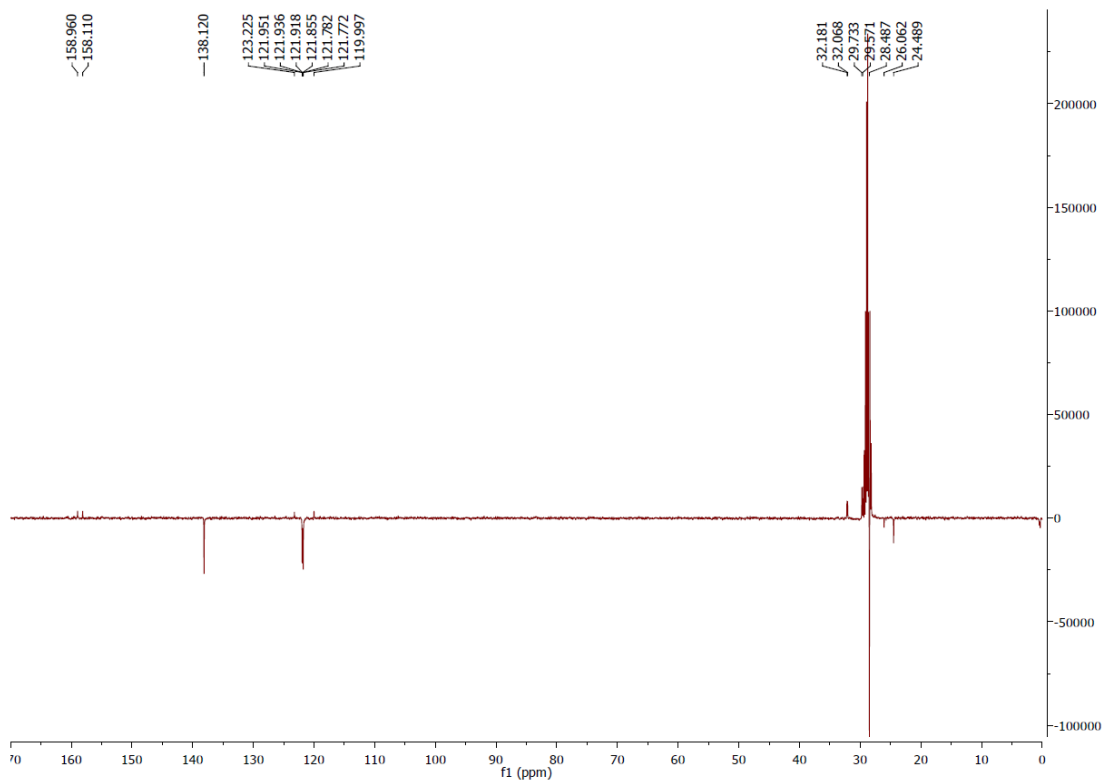


Fig. S18. ^{13}C (APT) NMR spectrum of complex **4** (acetone- d_6 , 100 MHz, 298 K).

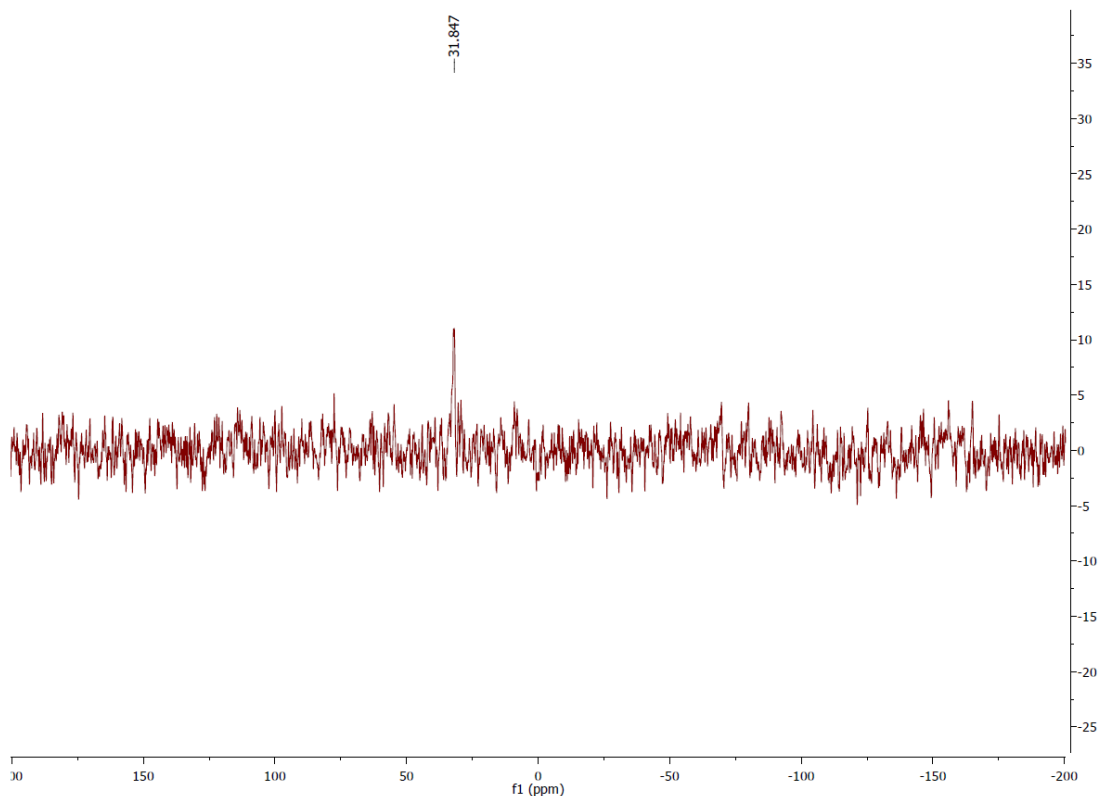


Fig. S19. ³¹P NMR spectrum of complex 4 (acetone-d₆, 162 MHz, 298 K).

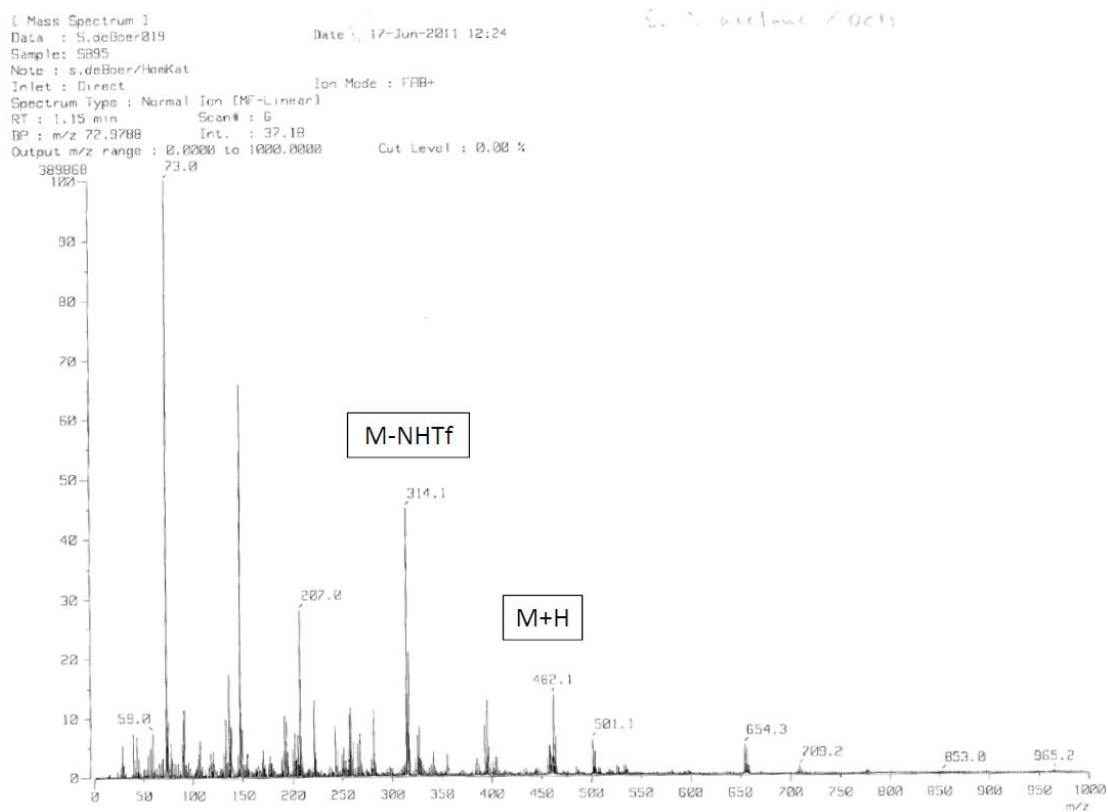


Fig. S20. Mass spectrum of complex 4.

