

Supporting Information

belonging to the manuscript

Phosphine Functionalized Cp^C Ligands and their Metal Complexes

by

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Additional Spectra

$\text{Cp}^{\text{C}}\text{HBzPPH}_2$ (**2**):

Figure S1: ^1H NMR spectrum of **2**.

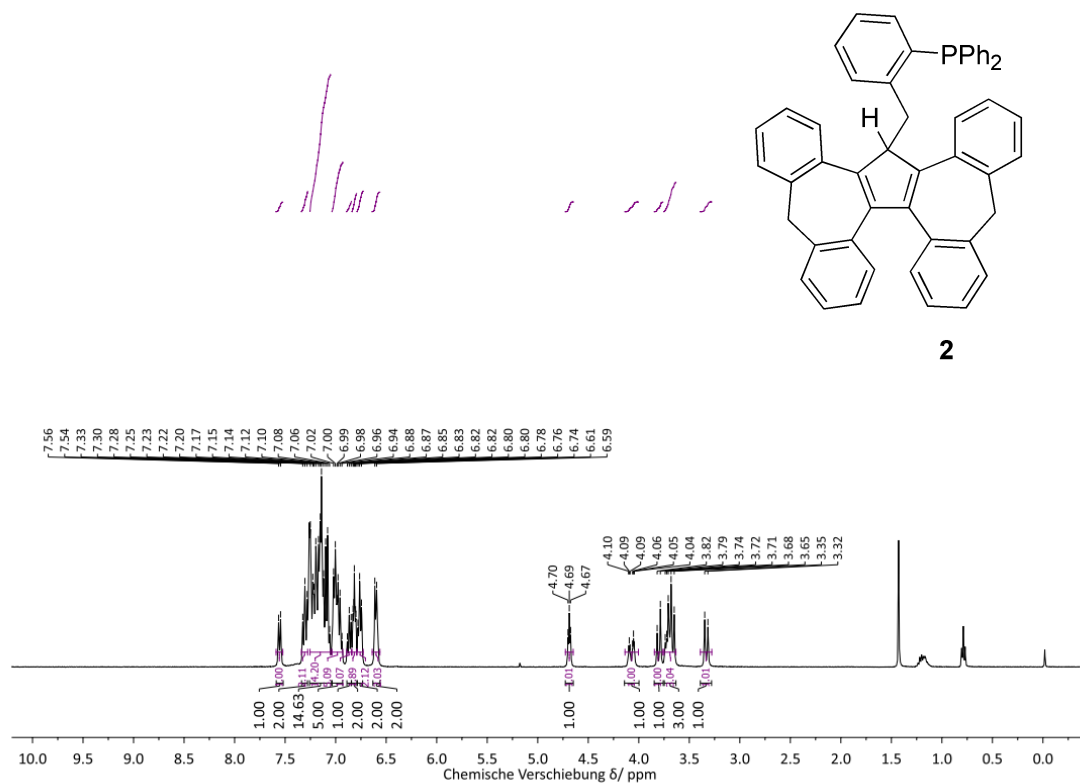


Figure S2: ^1H NMR spectrum of **2** (expanded).

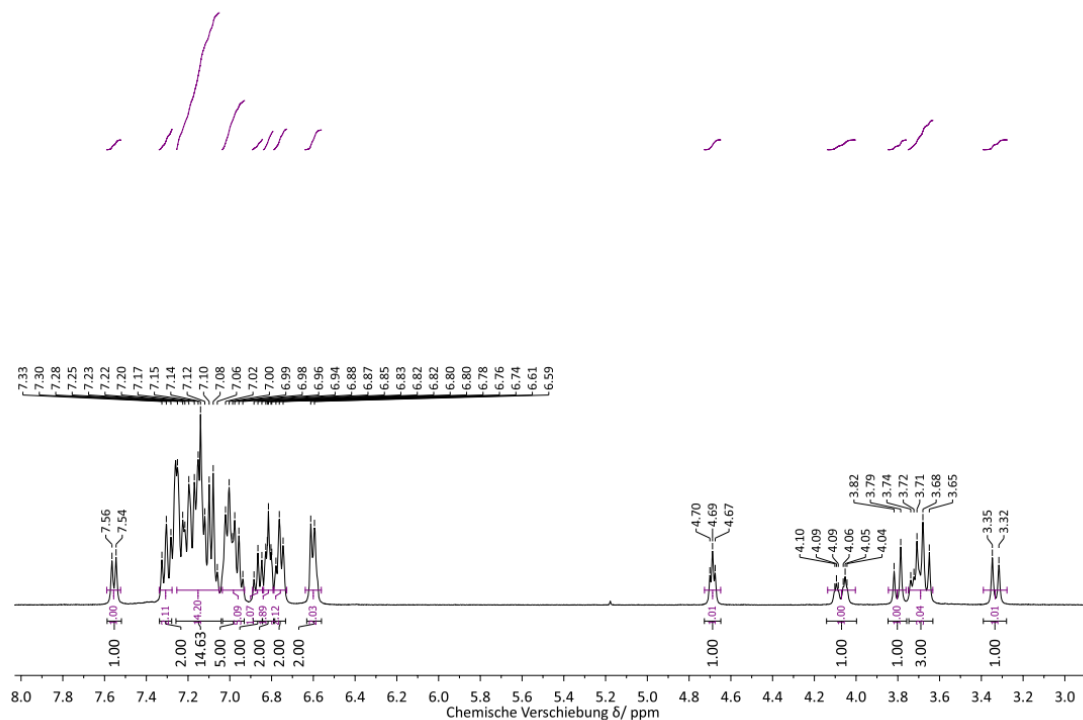


Figure S3: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2**.

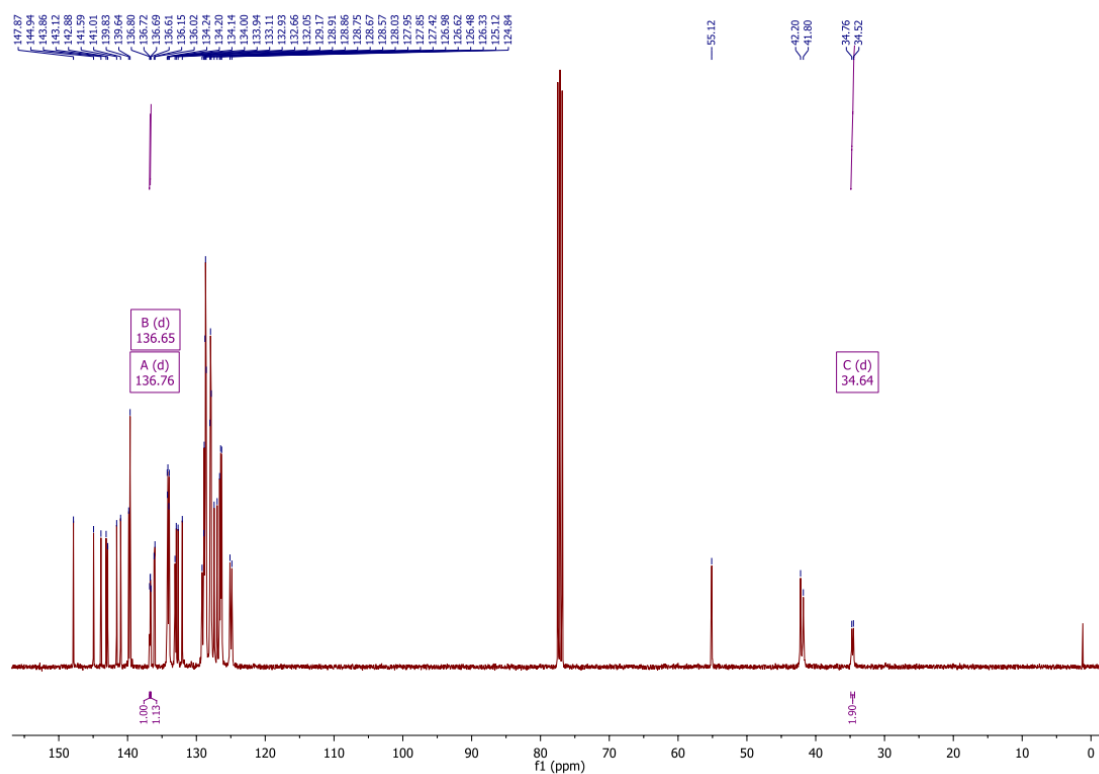


Figure S4: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** (expanded).

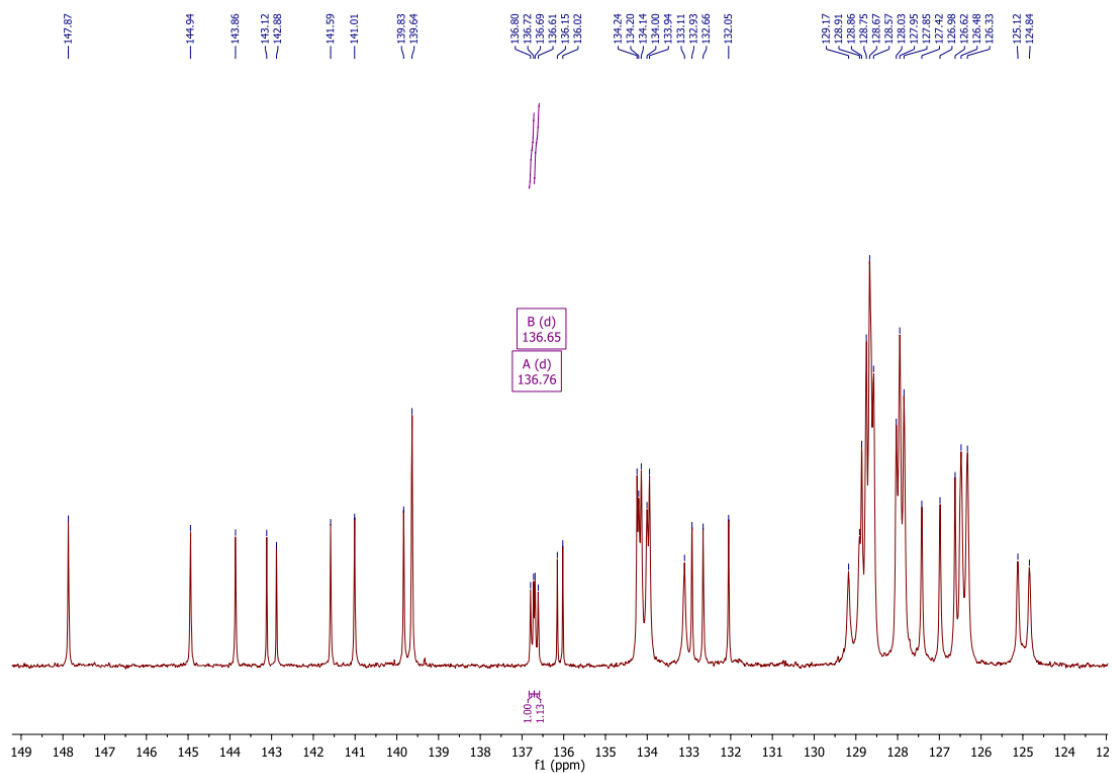


Figure S5: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **2**.

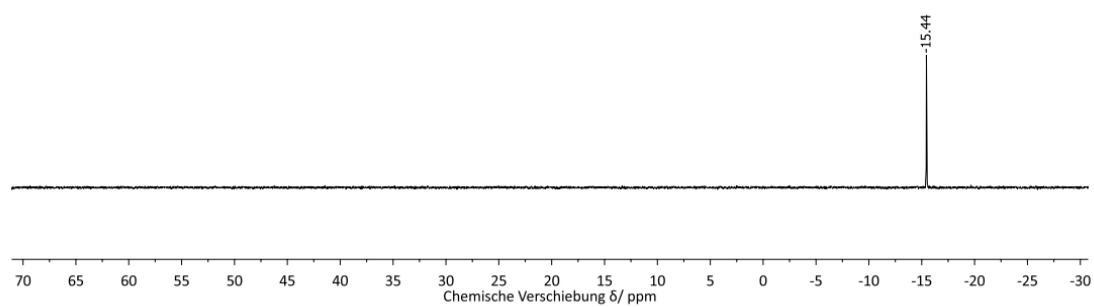


Figure S6: H,H-COSY NMR spectrum of **2**.

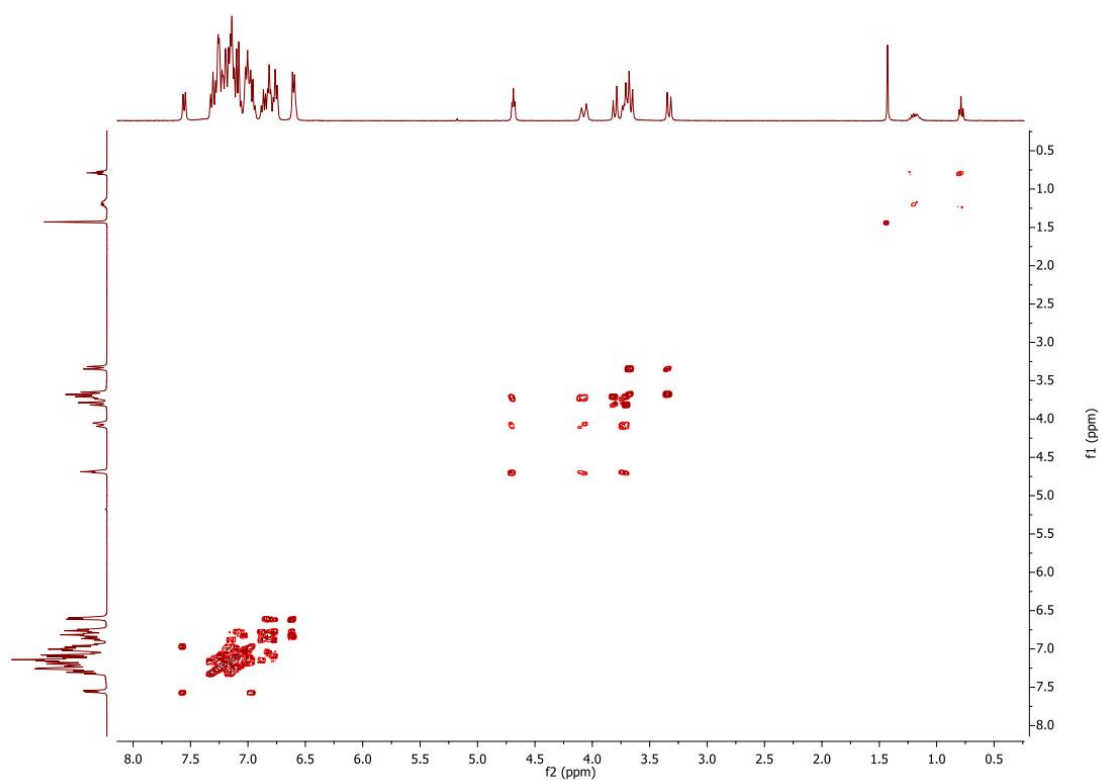


Figure S7: H,H-COSY NMR spectrum of **2** (expanded).

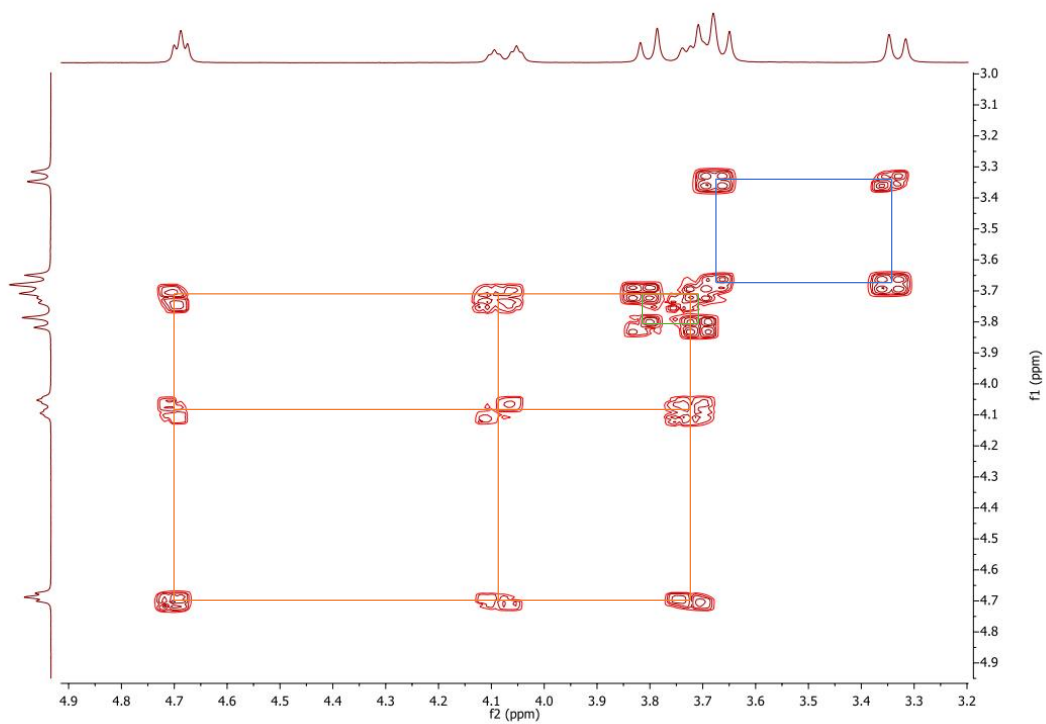


Figure S8: H,H-COSY NMR spectrum of **2** (expanded).

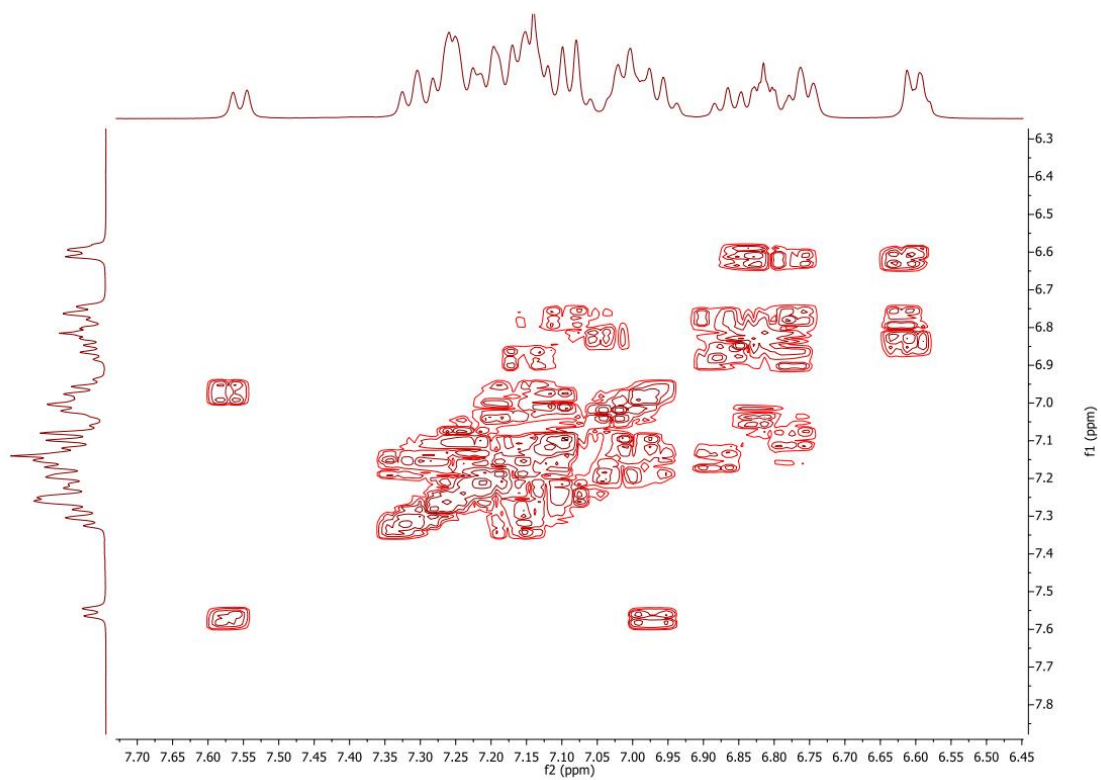


Figure S9: HMQC NMR spectrum of **2**.

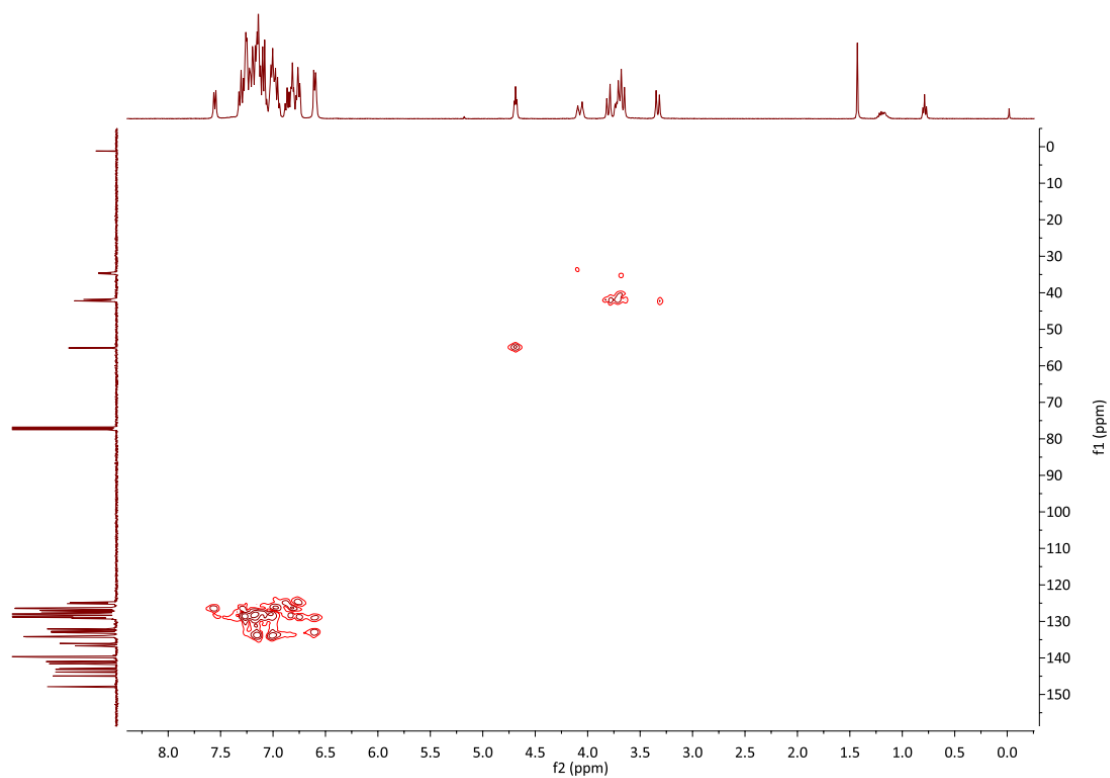
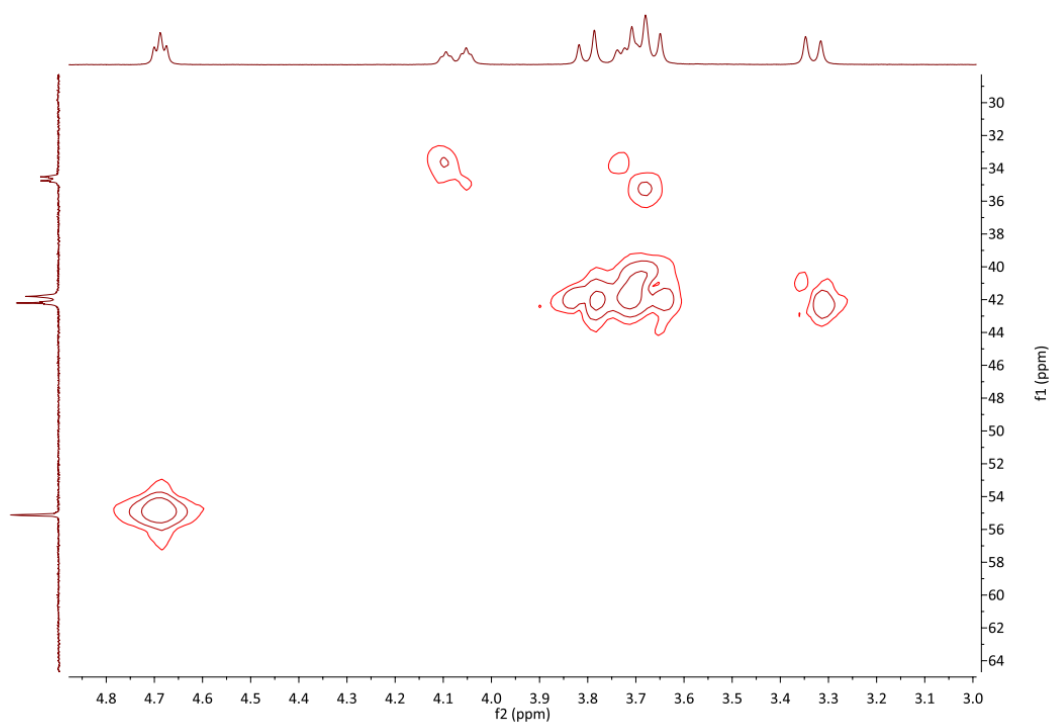


Figure S10: HMQC NMR spectrum of **2** (expanded).



$\text{Cp}^{\text{C}}(\text{BzPPh}_2)_2$ (**3**):

Figure S11: ^1H NMR spectrum of **3**.

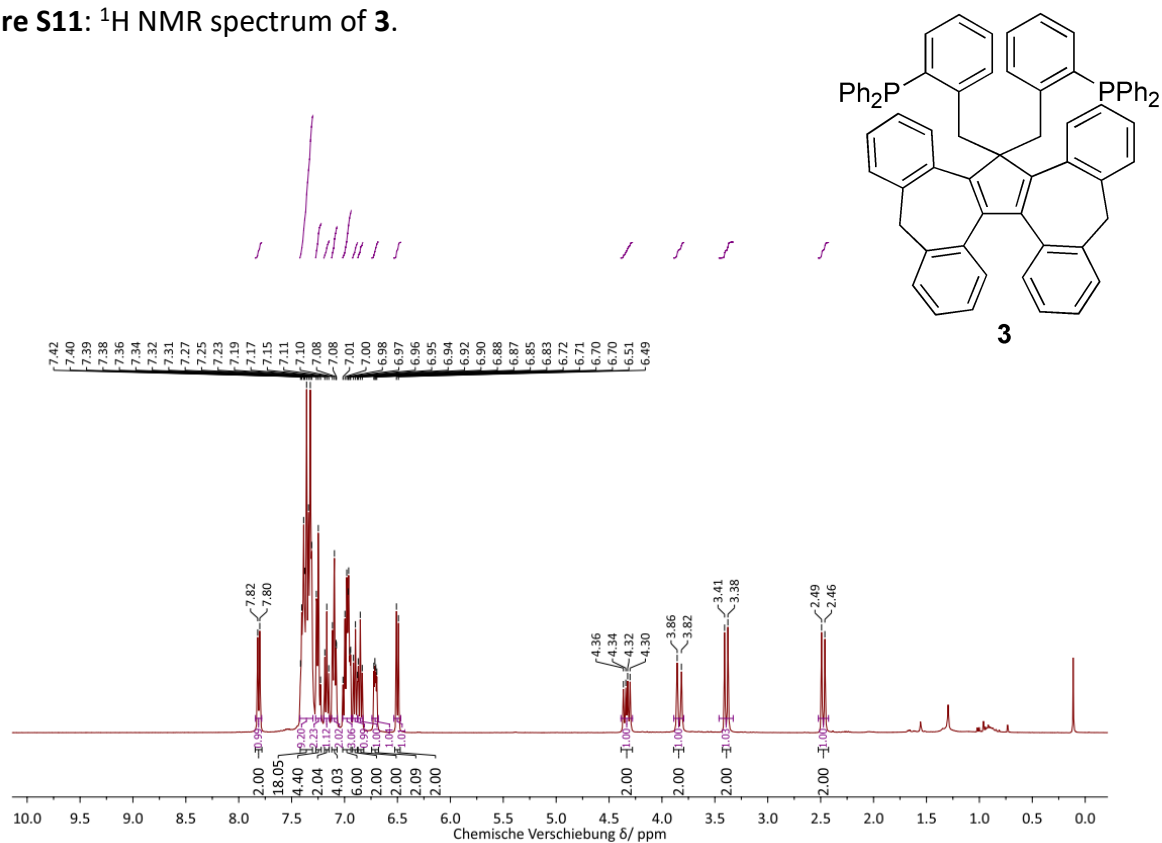


Figure S12: ^1H NMR spectrum of **3** (expanded).

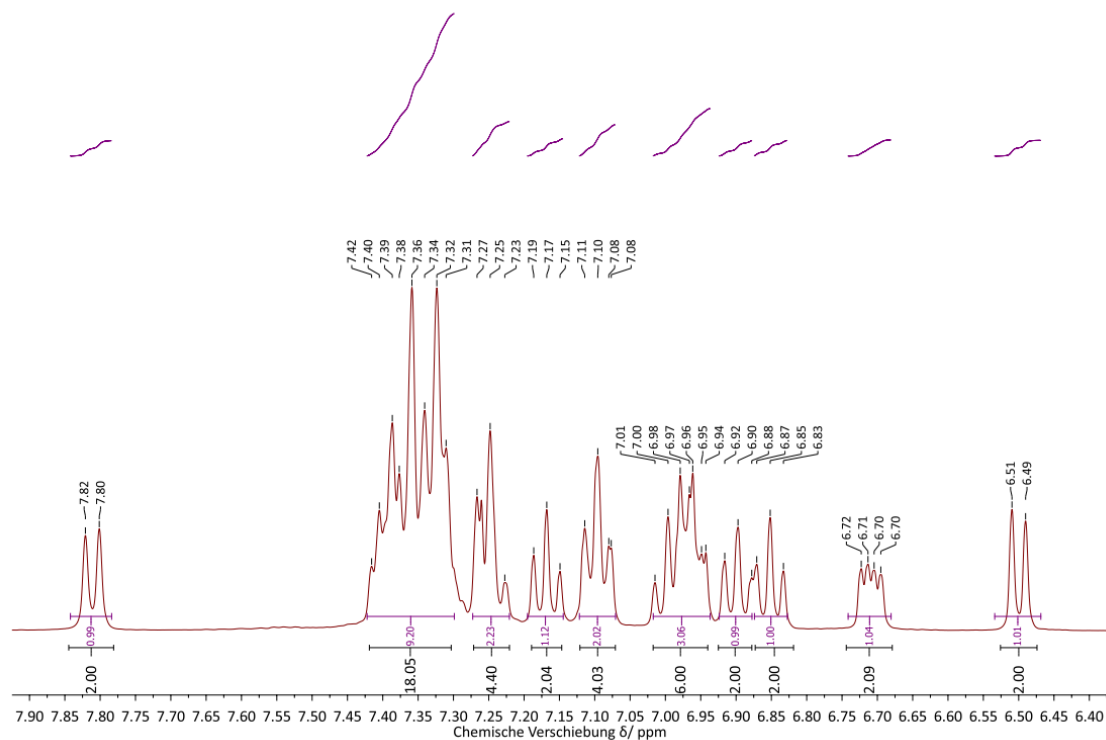


Figure S13: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3**.

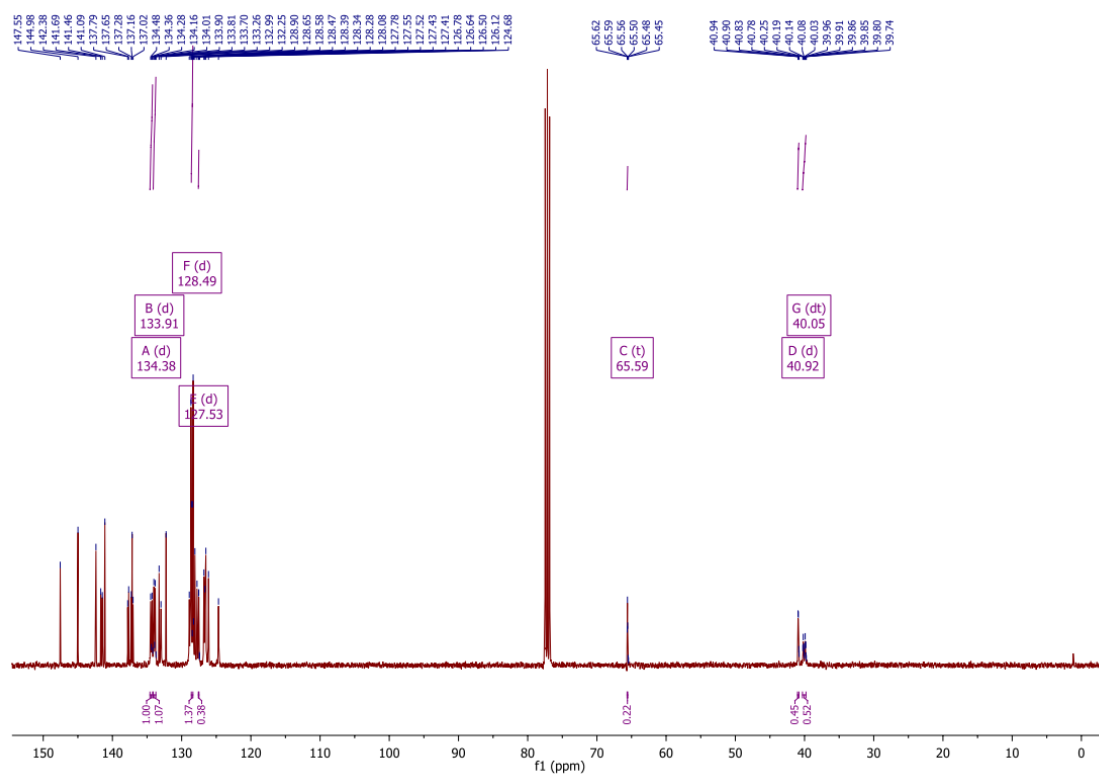


Figure S14: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** (expanded).

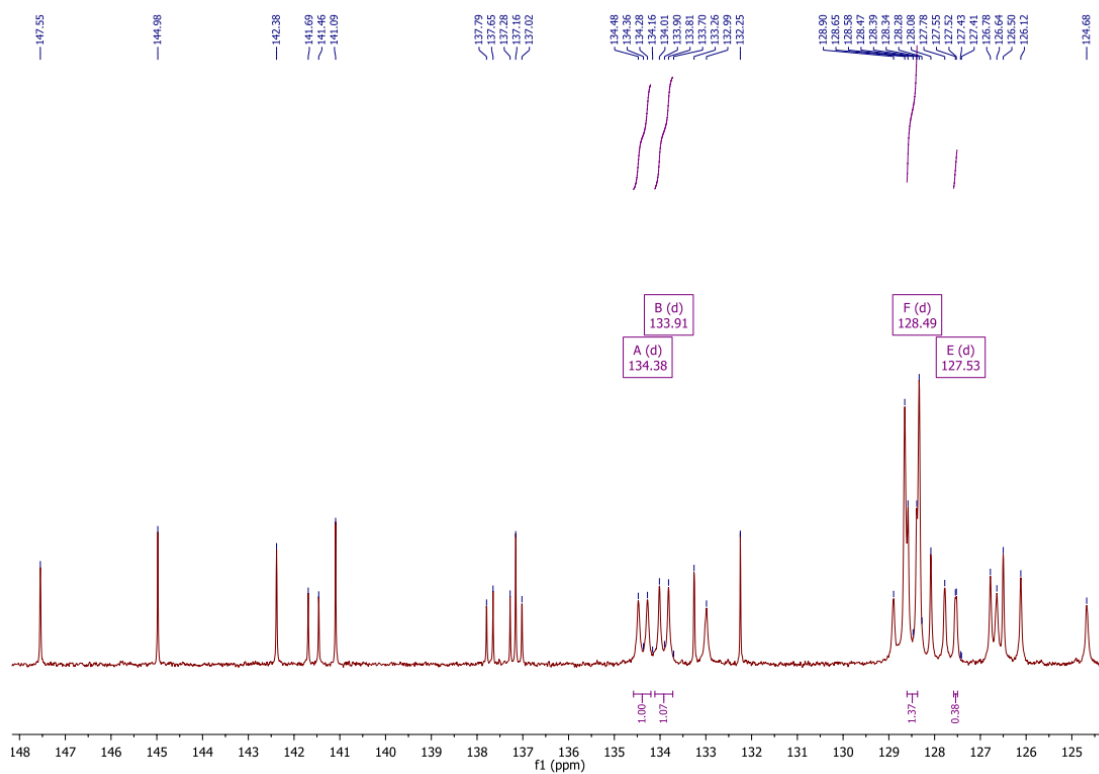


Figure S15: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **3**.

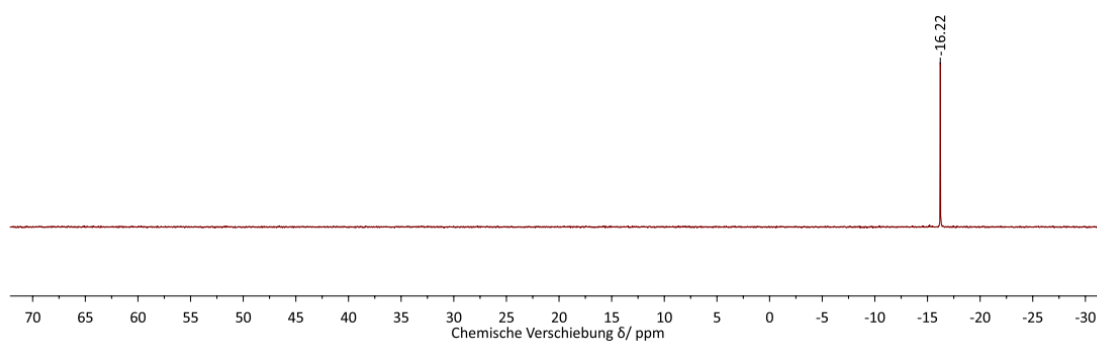


Figure S16: H,H-COSY NMR spectrum of **3**.

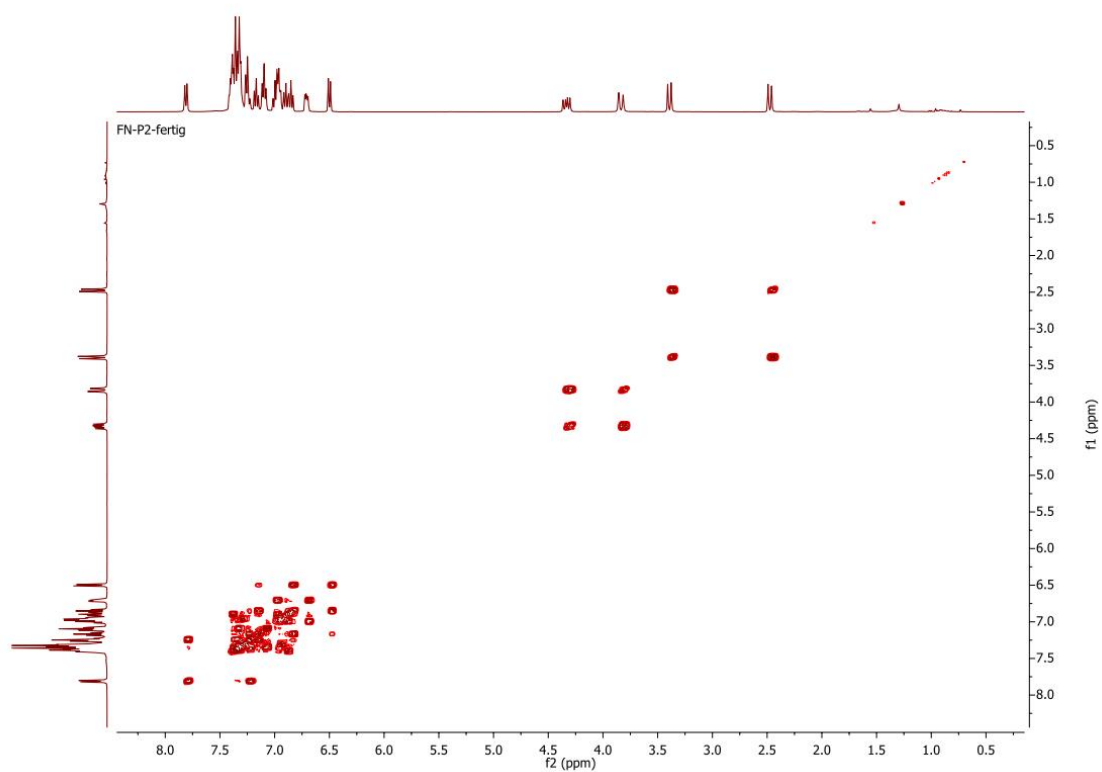


Figure S17: H,H-COSY NMR spectrum of **3** (expanded).

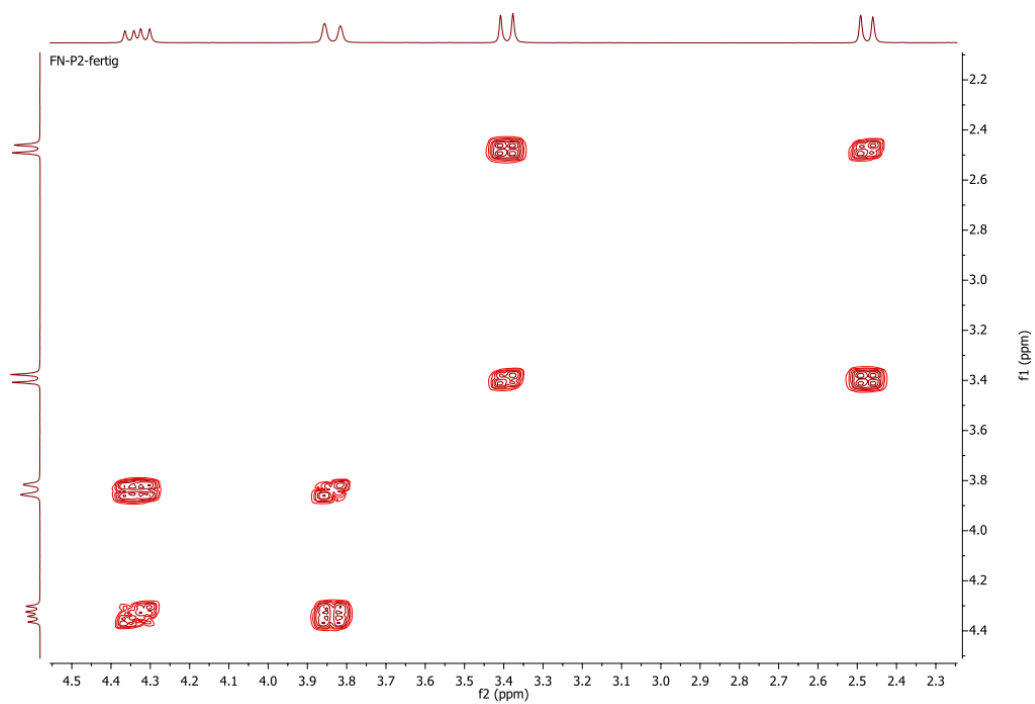


Figure S18: H,H-COSY NMR spectrum of **3** (expanded).

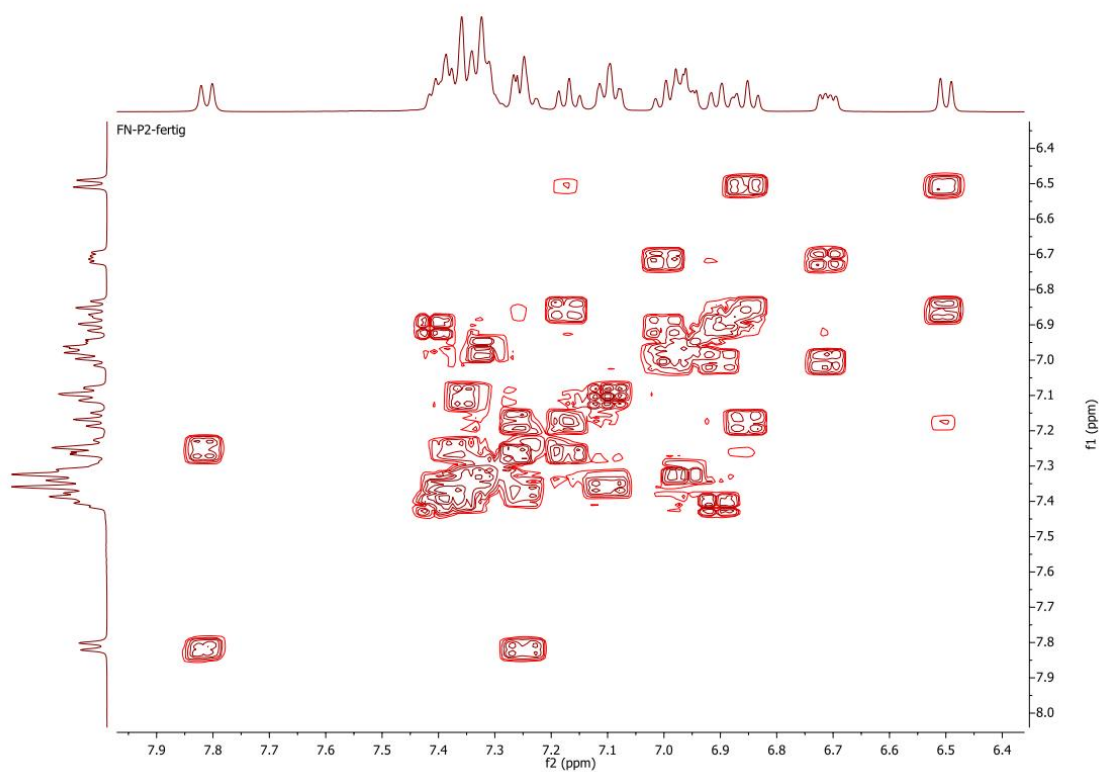


Figure S19: HMQC NMR spectrum of **3**.

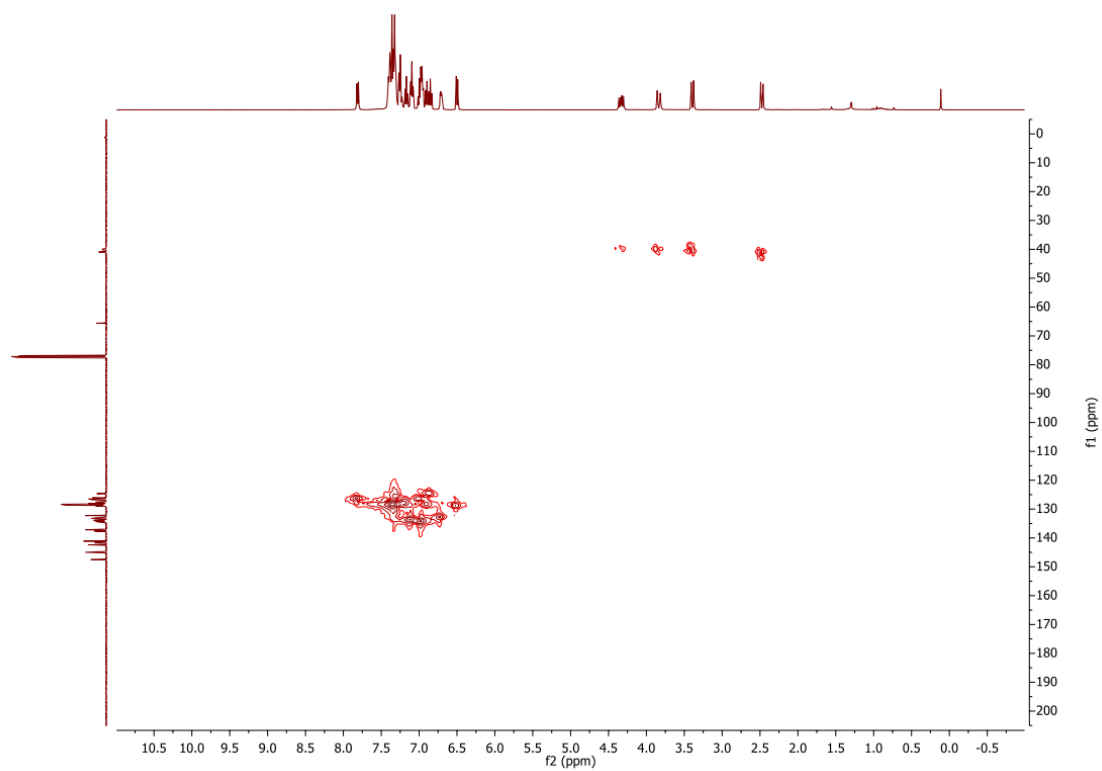


Figure S20: HMQC NMR spectrum of **3** (expanded).

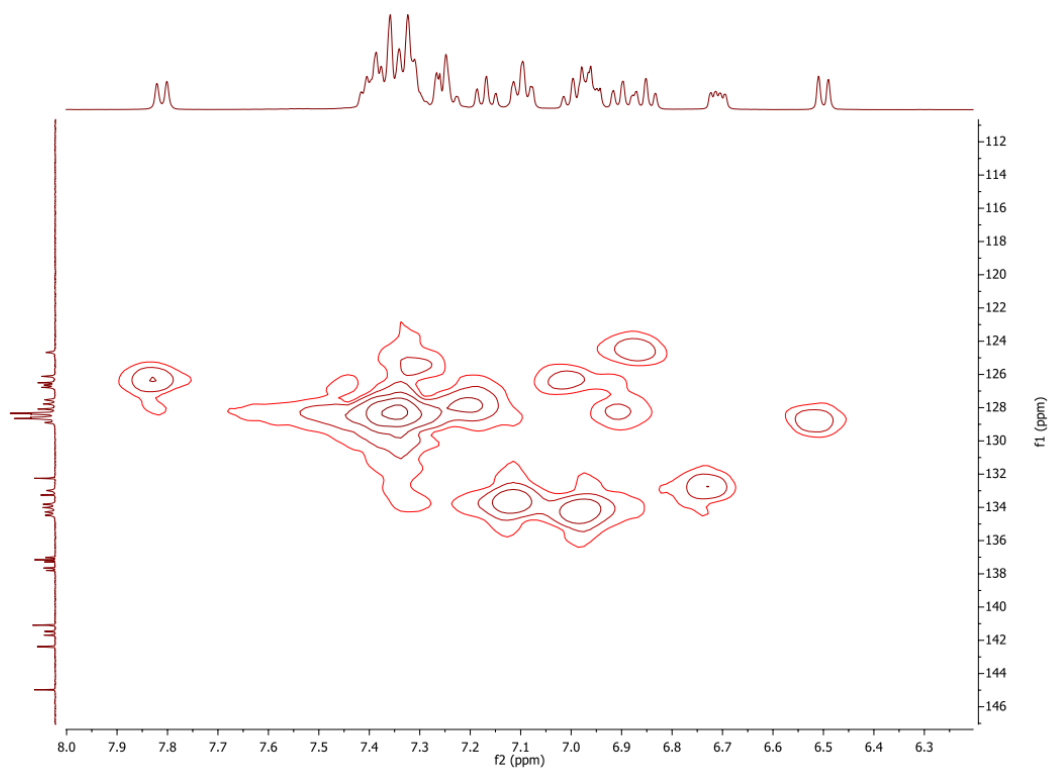


Figure S21: ^1H NMR spectrum of **4**.

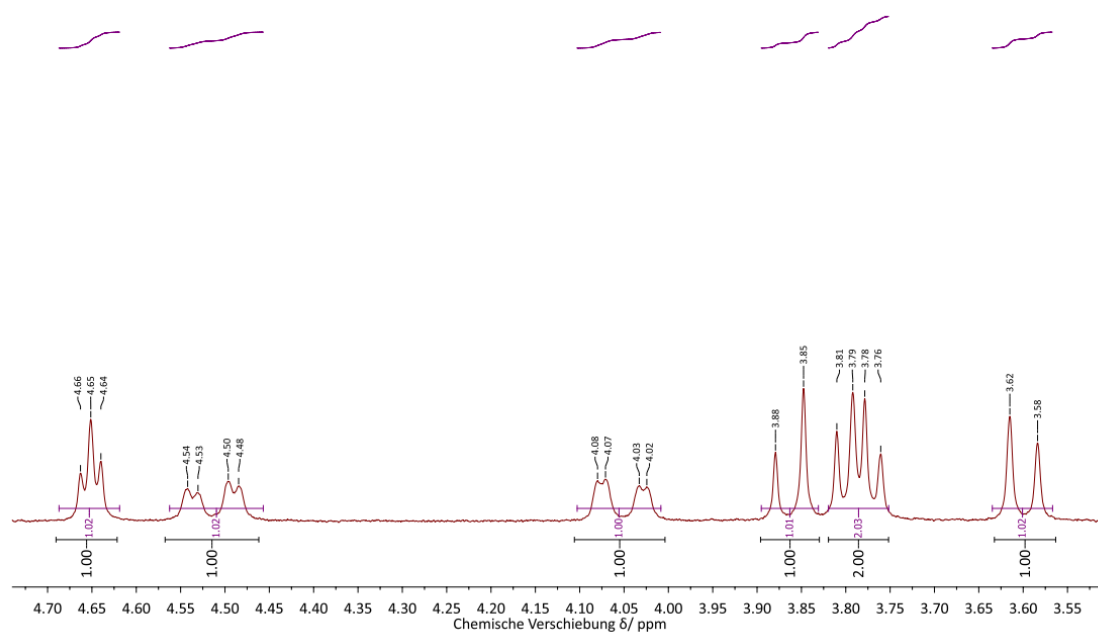


Figure S23: ^1H NMR spectrum of **4** (expanded).

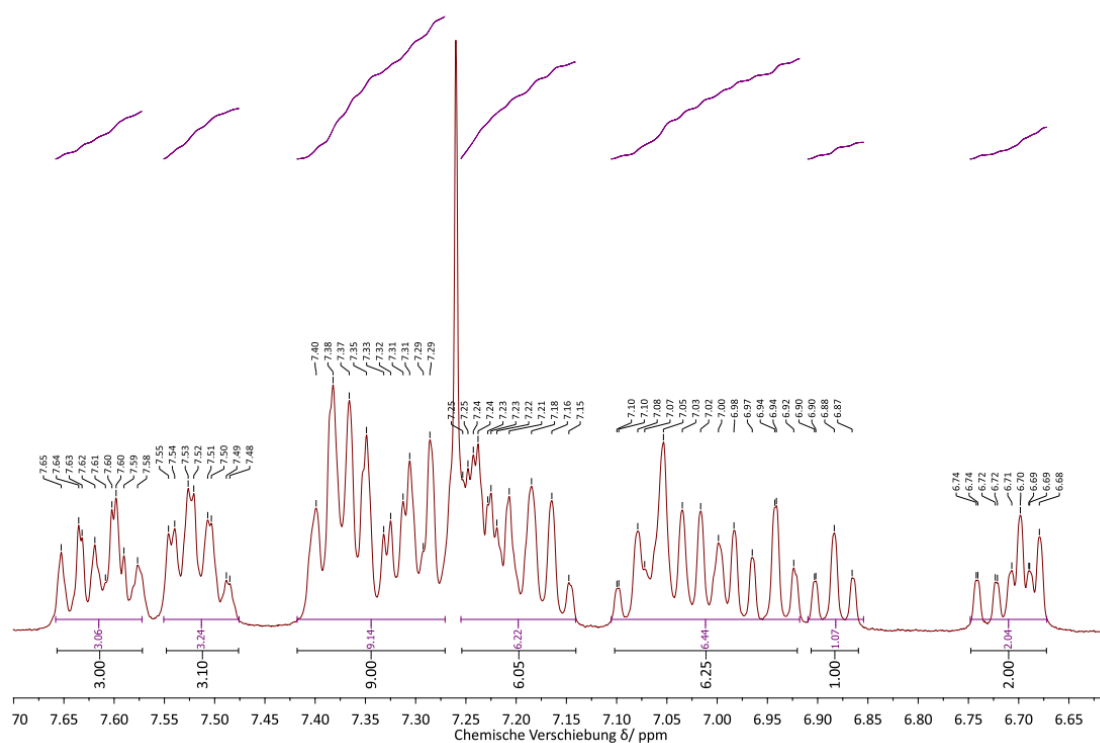


Figure S24: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4**.

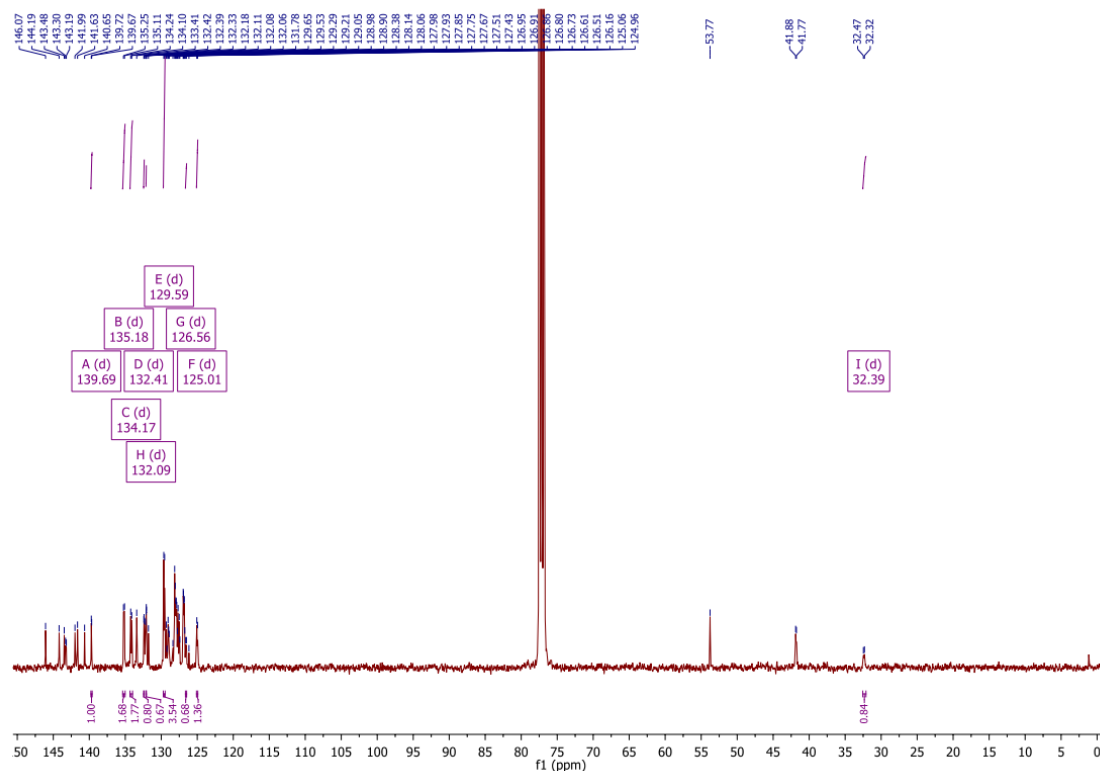


Figure S25: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4** (expanded).

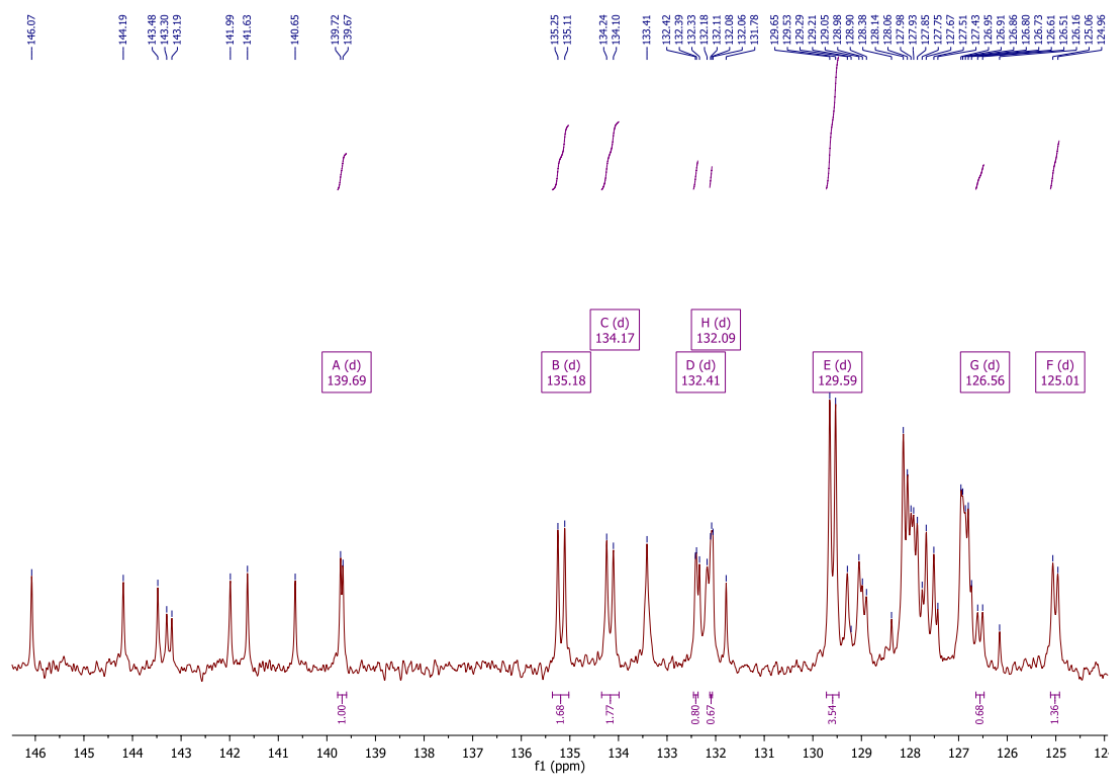


Figure S26: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **4**.

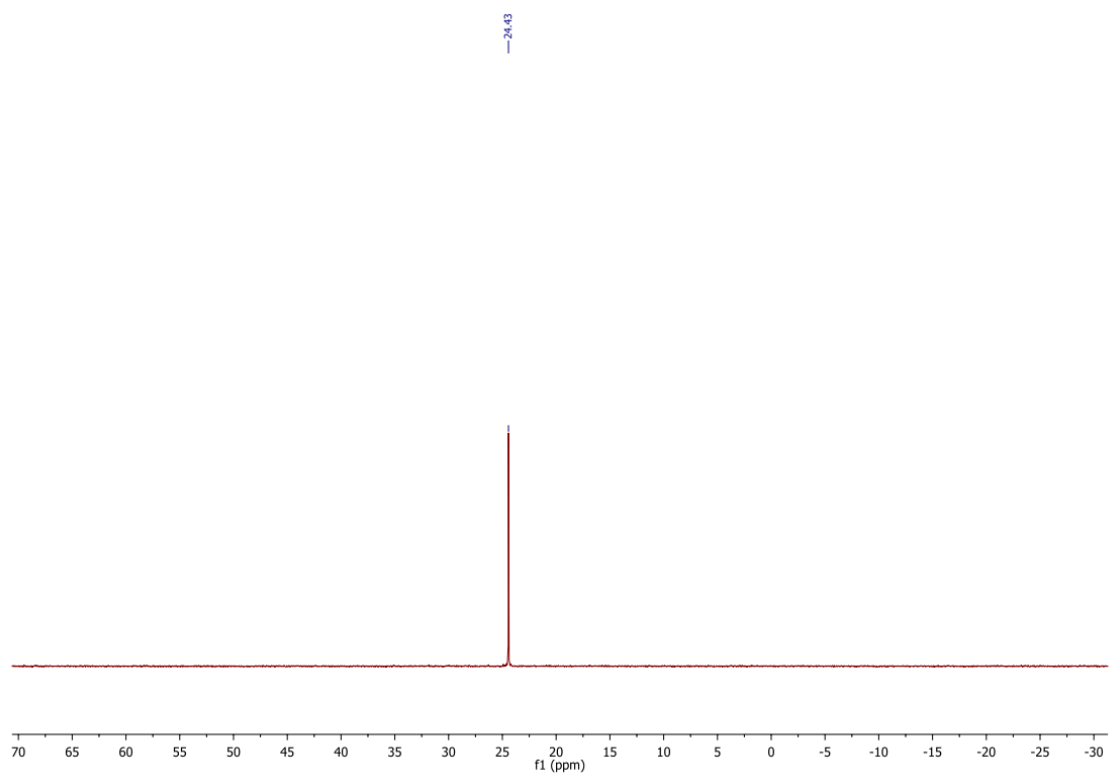


Figure S27: H,H-COSY NMR spectrum of **4**.

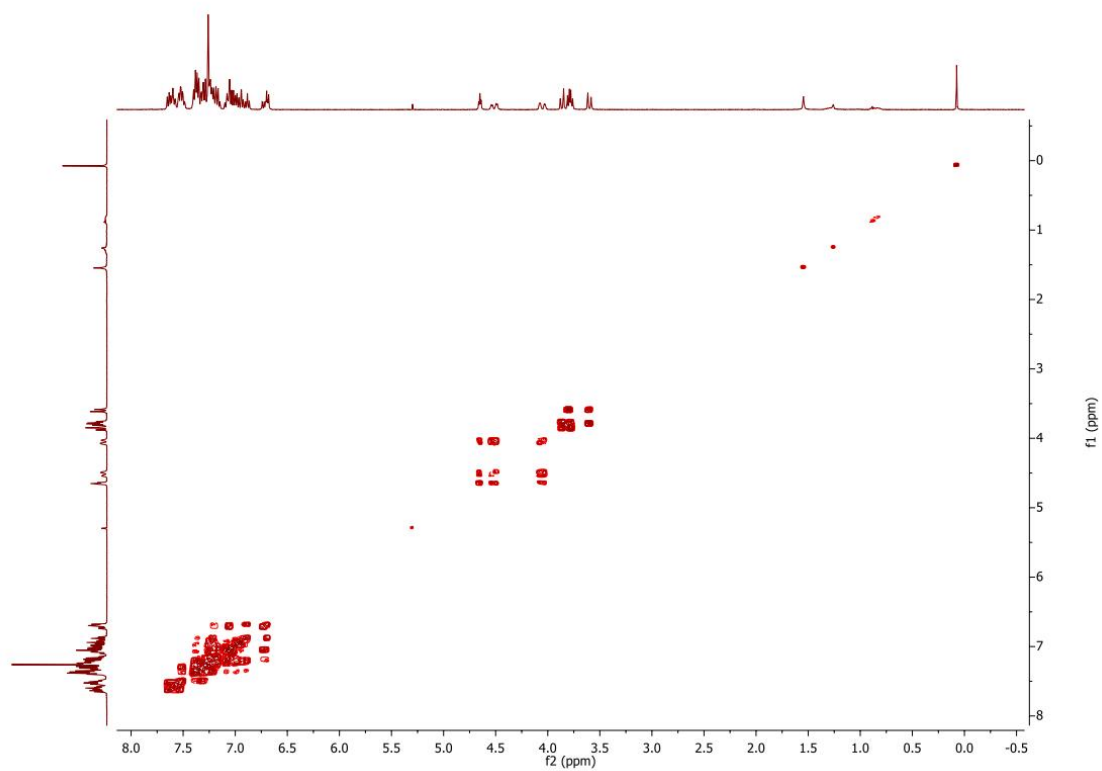


Figure S28: H,H-COSY NMR spectrum of **4** (expanded).

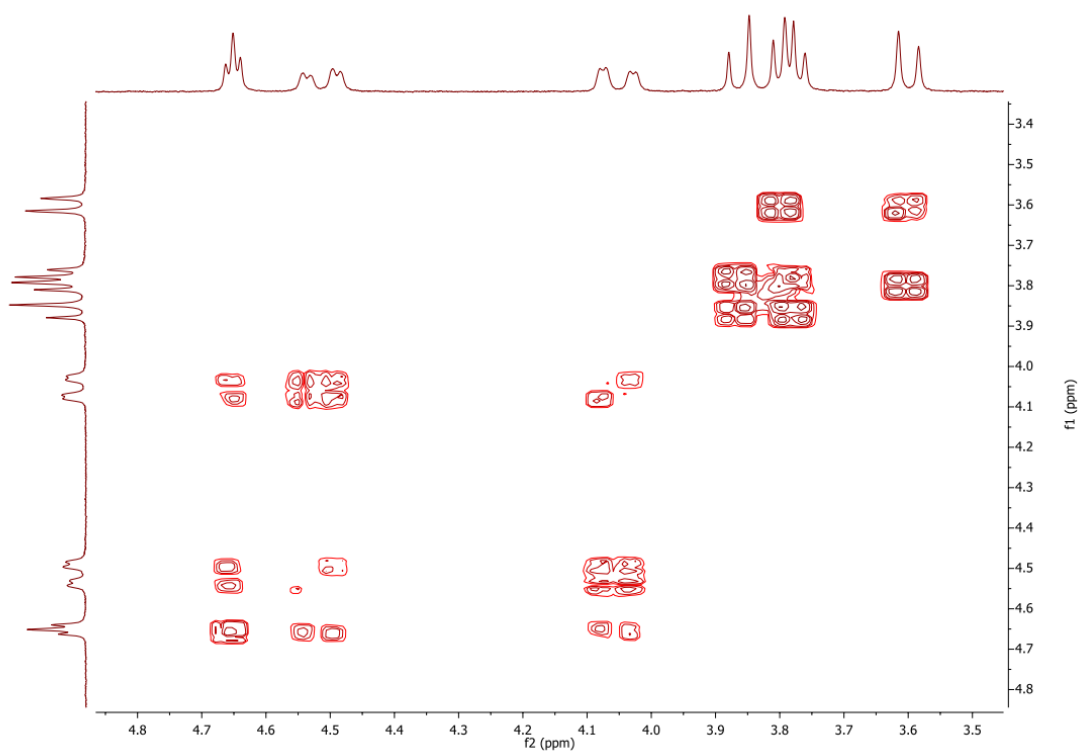


Figure S29: H,H-COSY NMR spectrum of **4** (expanded).

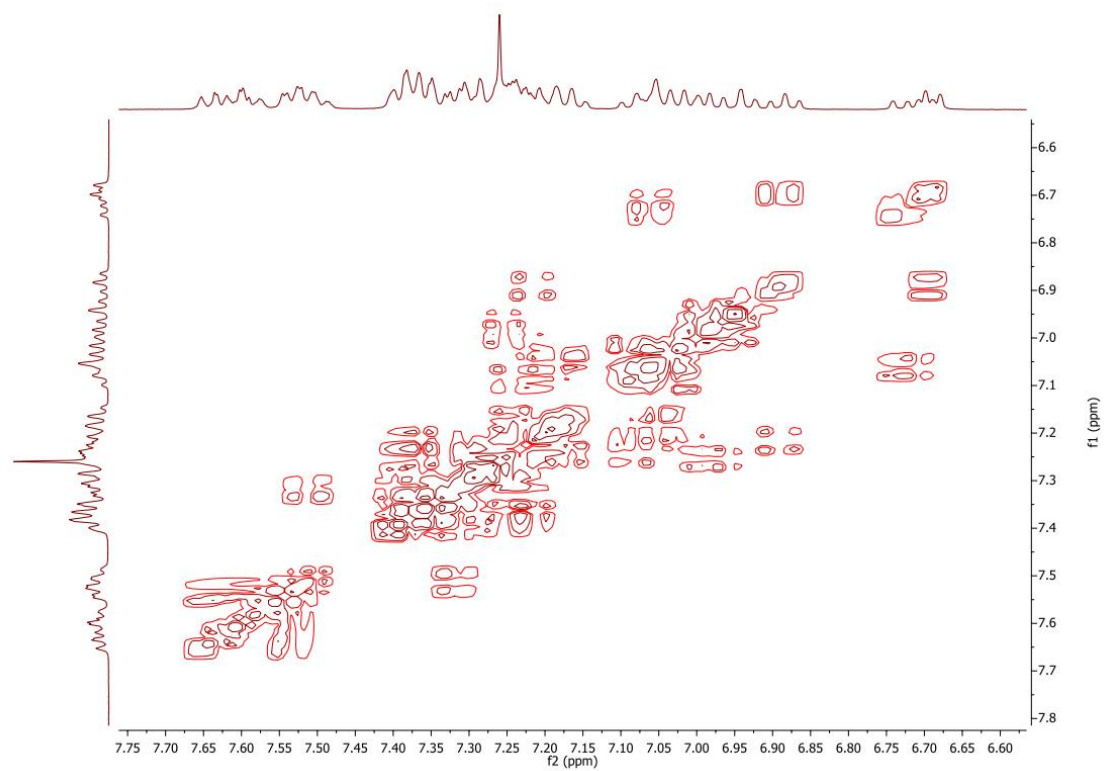


Figure S30: HMQC NMR spectrum of **4**.

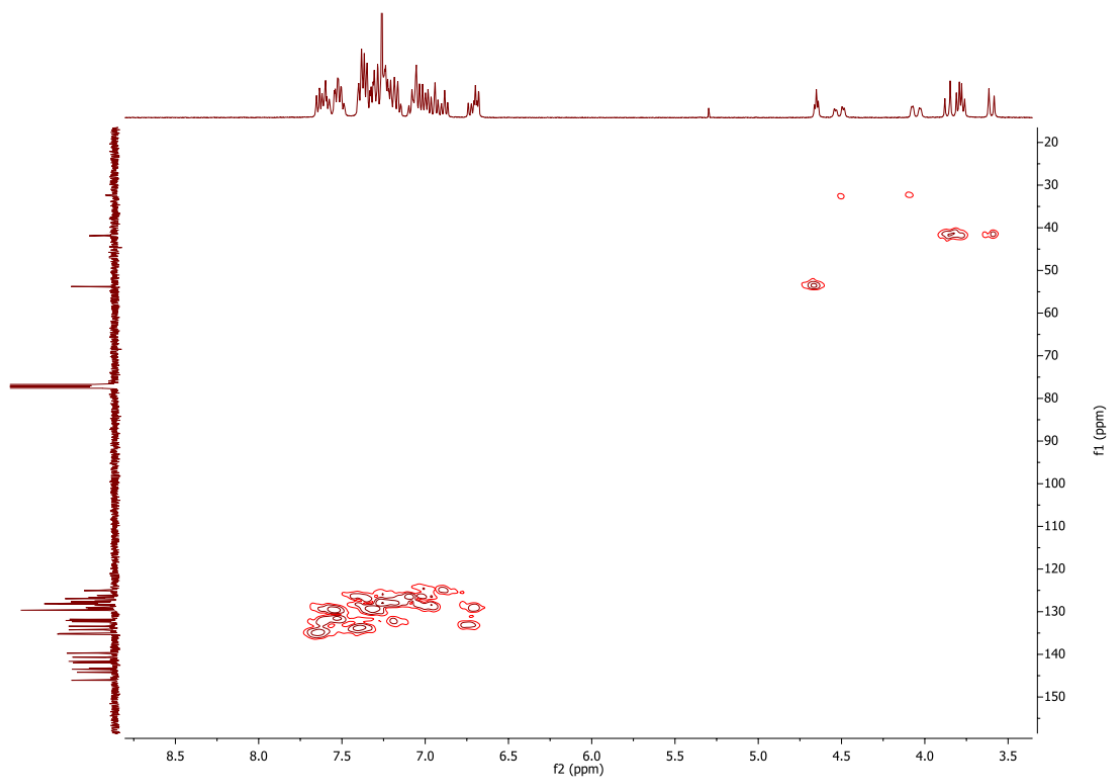
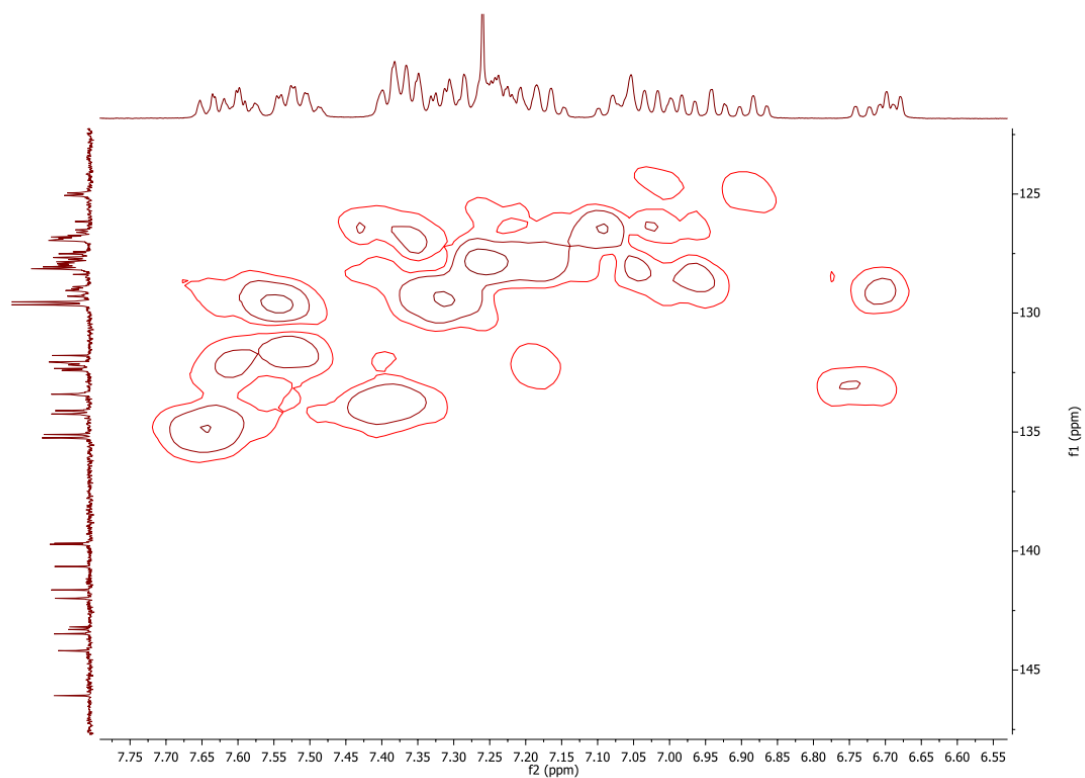


Figure S31: HMQC NMR spectrum of **4** (expanded).



[[η^5 -Cp^CHBzPPh₂]⁺Tl⁻ (5**):**

Figure S32: ¹H NMR spectrum of **5**.

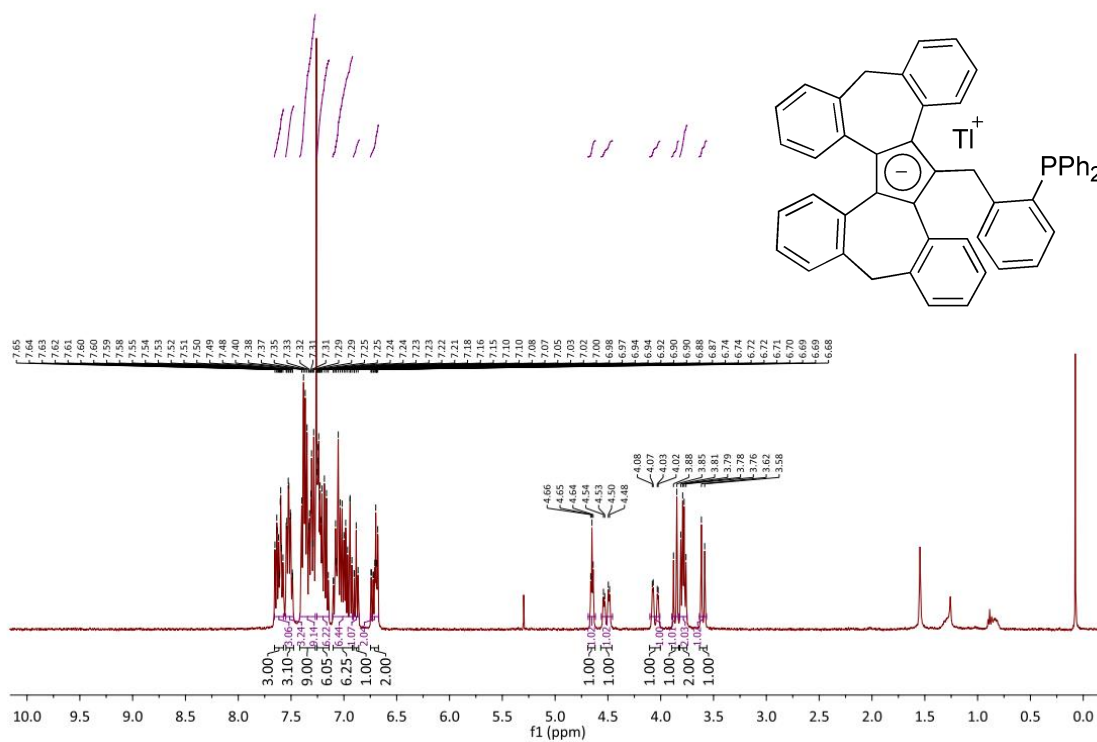


Figure S33: ^1H NMR spectrum of **5** (expanded).

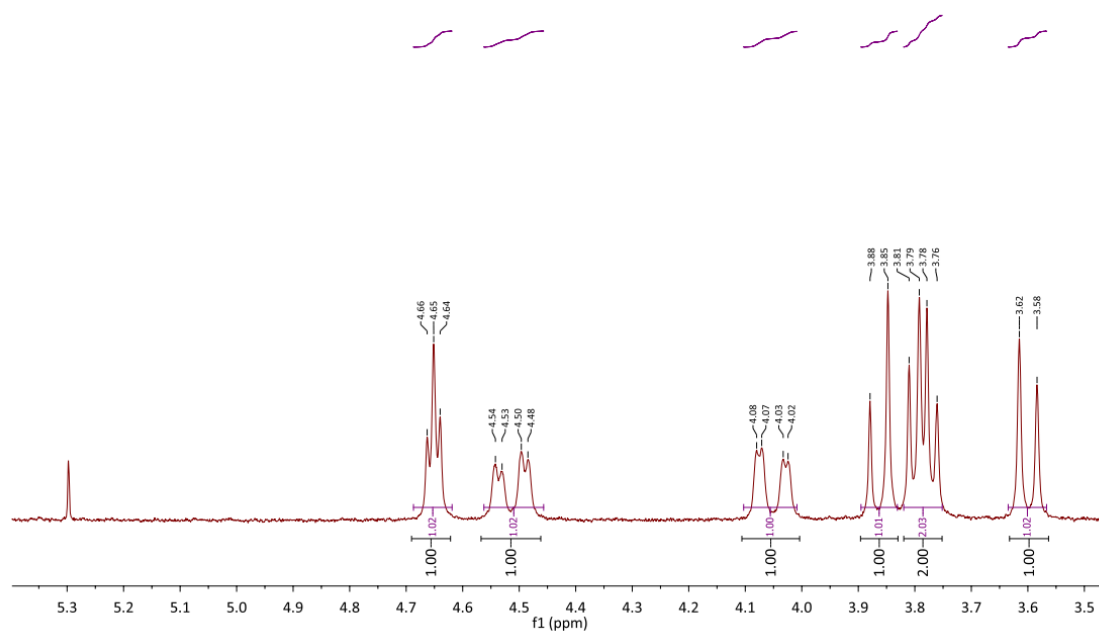


Figure S34: ^1H NMR spectrum of **5** (expanded).

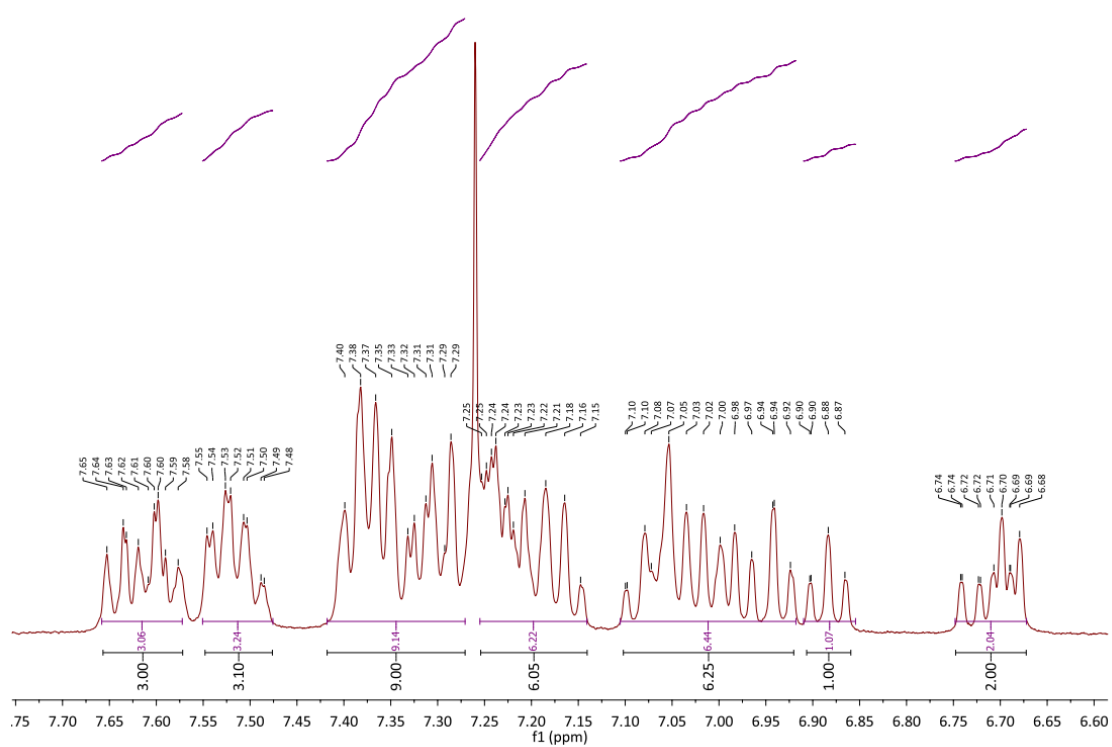


Figure S35: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5**.

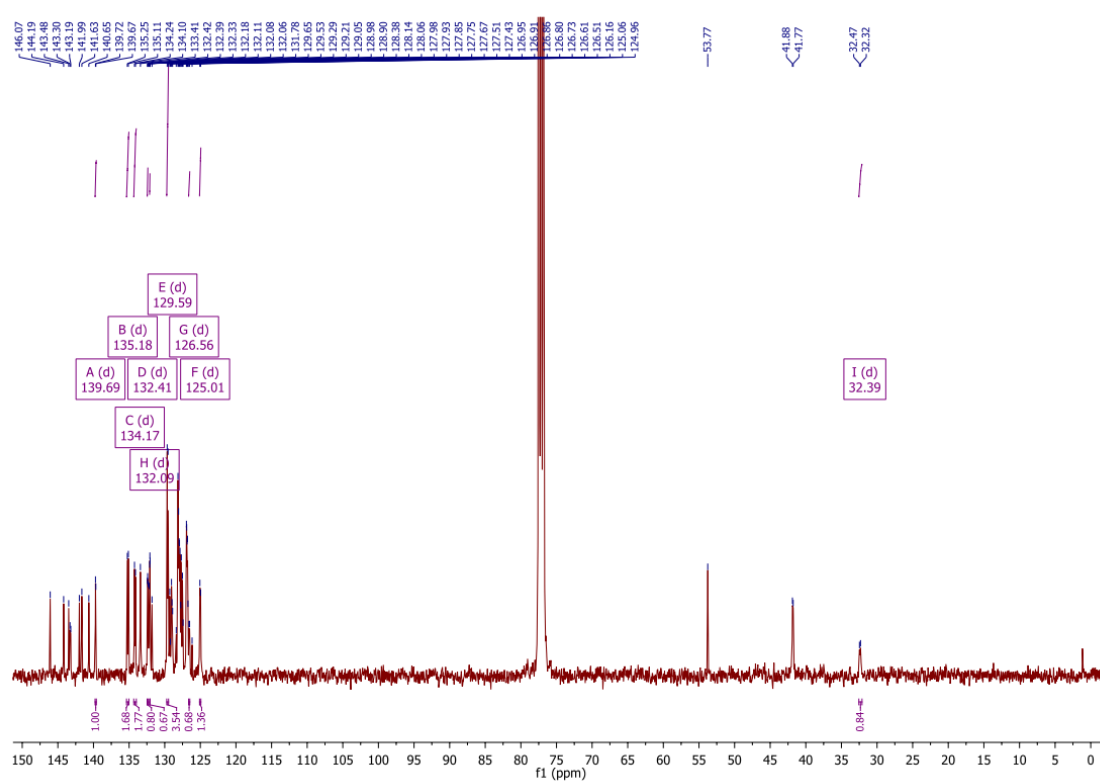


Figure S36: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **5** (expanded).

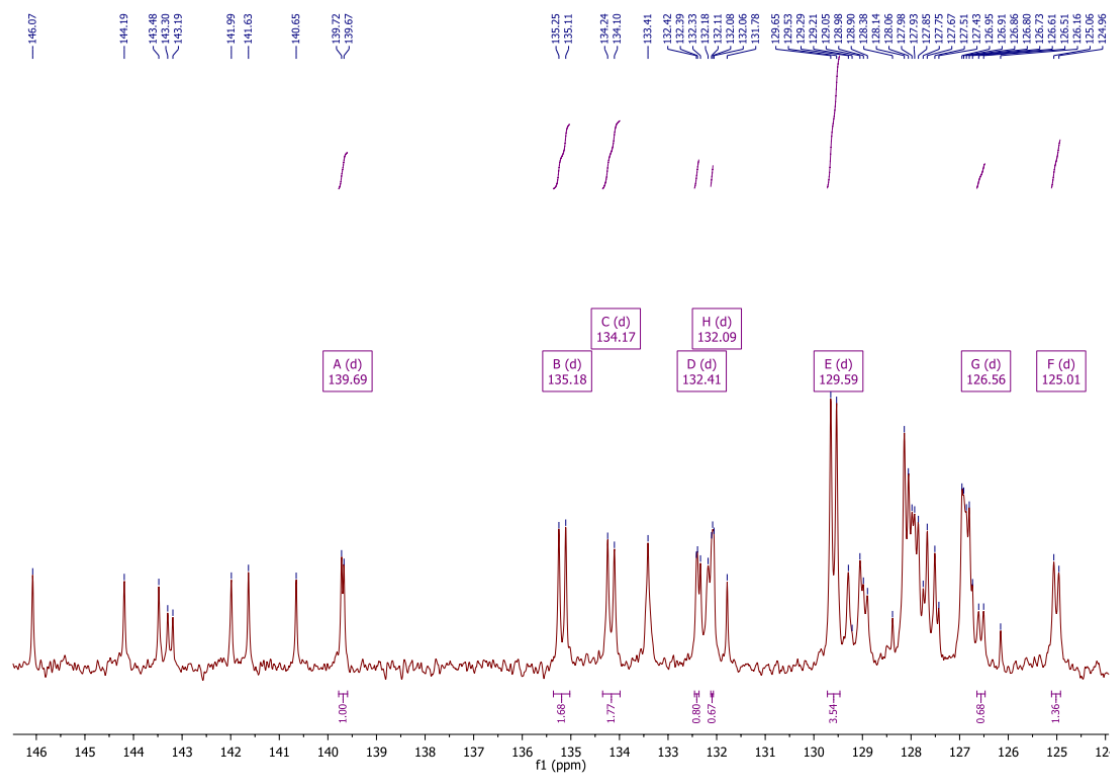


Figure S37: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **5**.

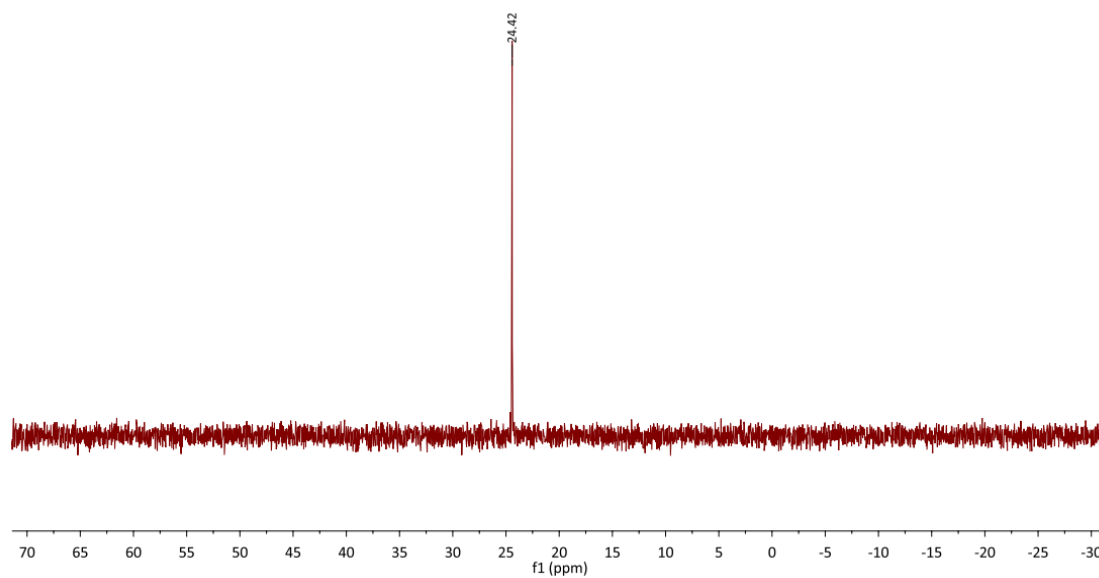


Figure S38: H,H-COSY NMR spectrum of **5**.

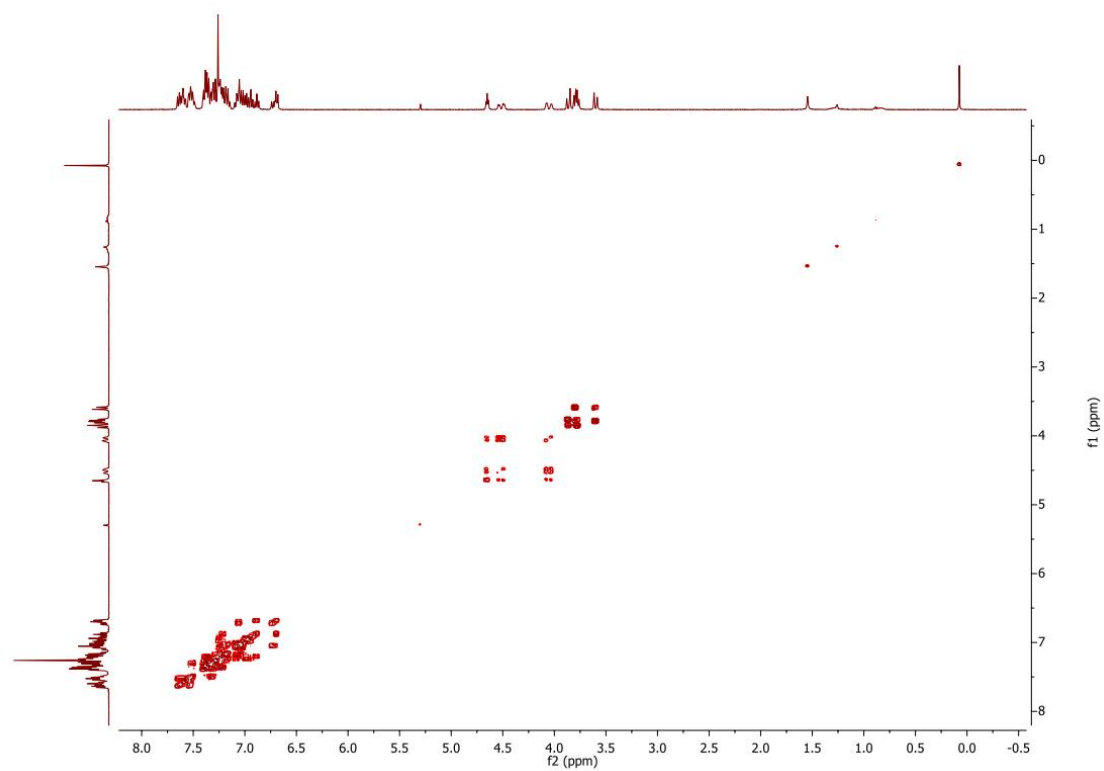


Figure S39: H,H-COSY NMR spectrum of **5** (expanded).

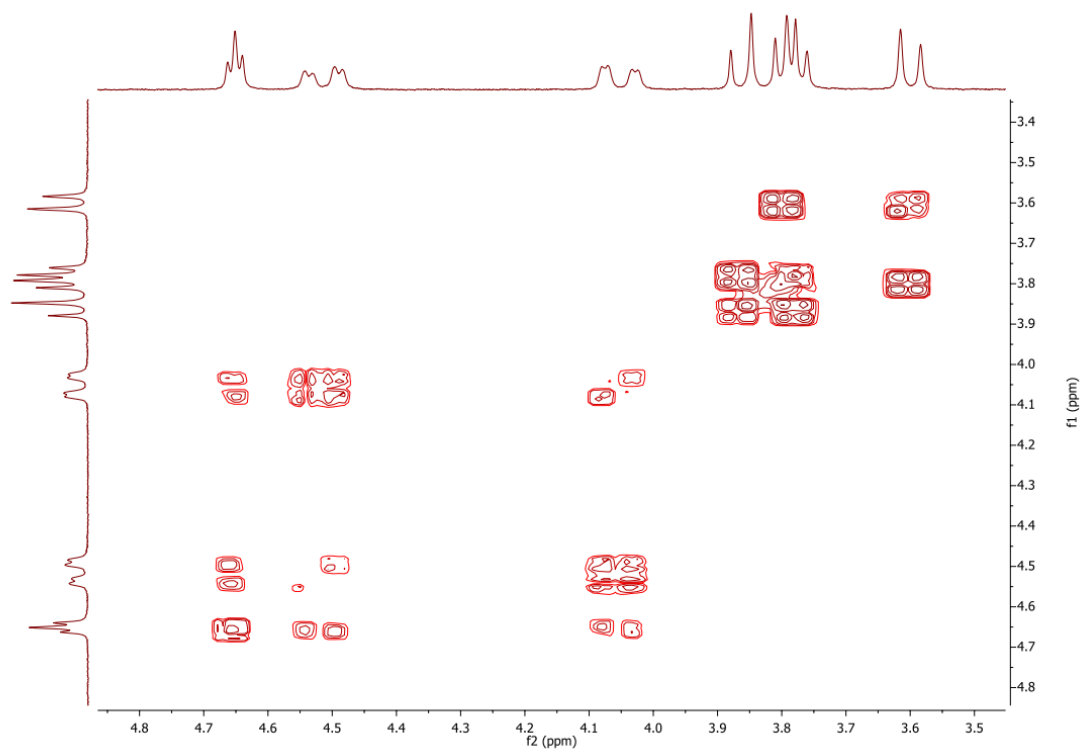


Figure S40: H,H-COSY NMR spectrum of **5** (expanded).

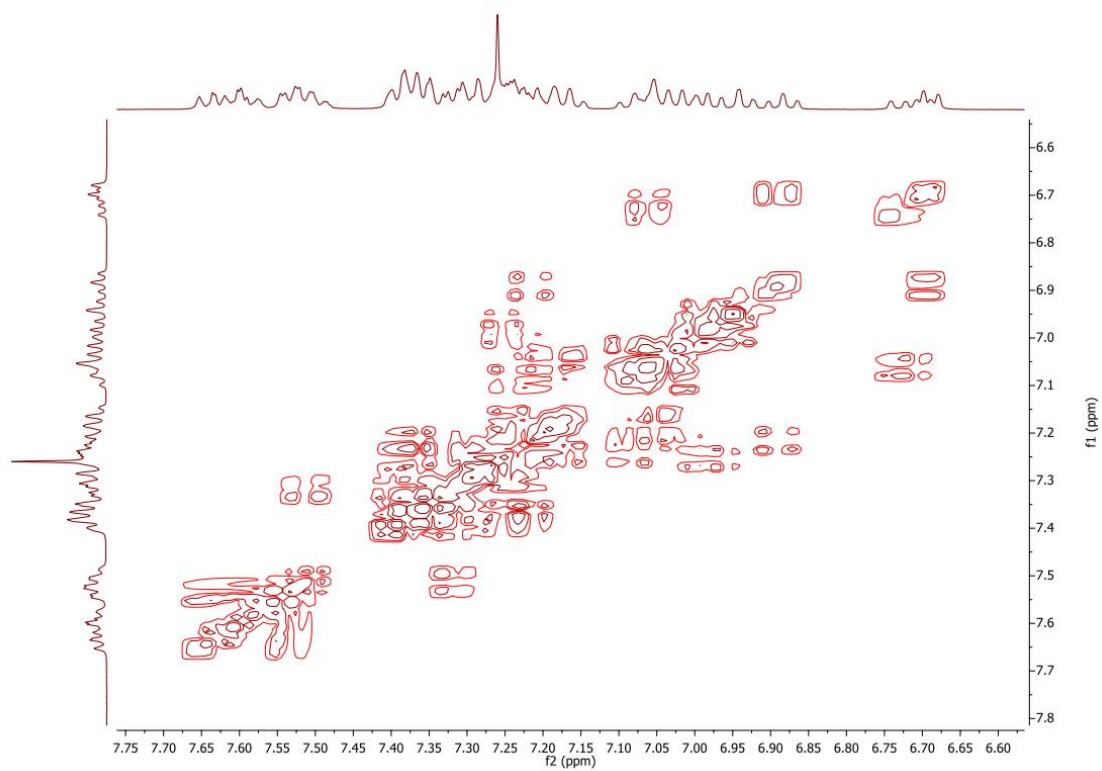


Figure S41: HMQC NMR spectrum of **5**.

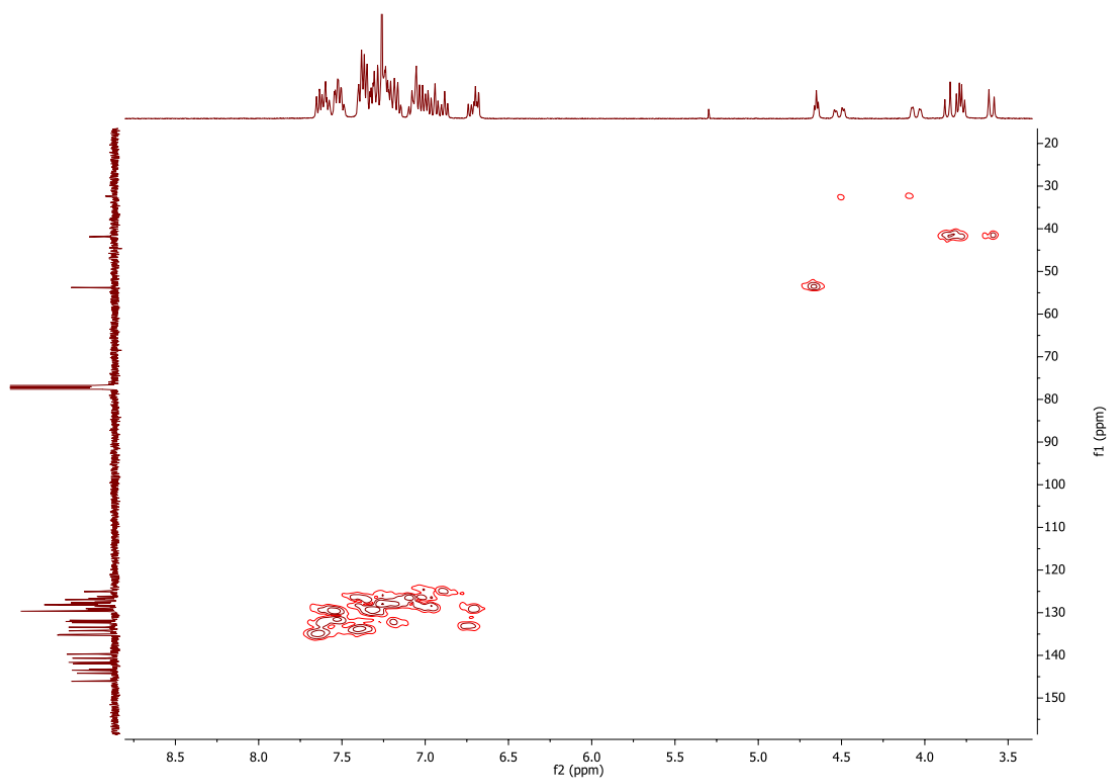
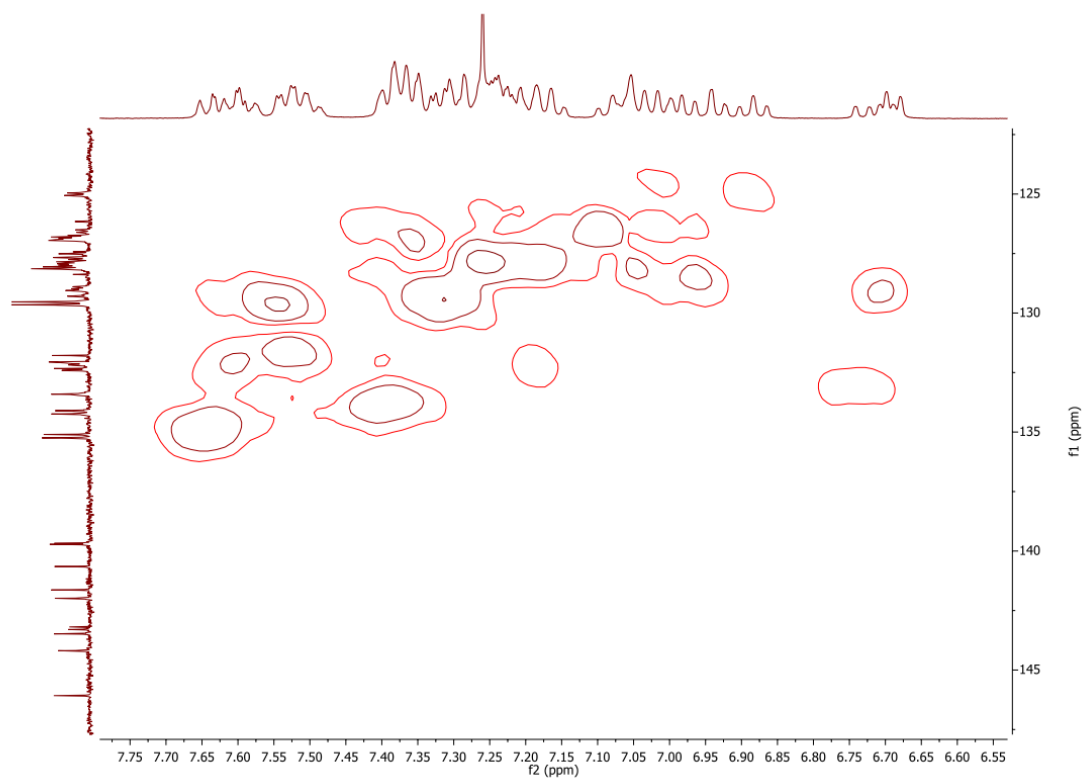


Figure S42: HMQC NMR spectrum of **5** (expanded).



$[(\eta^5\text{-Cp}^t\text{BzPPh}_2)\text{Ru}(\text{NCMe})_2]\text{PF}_6$ (6):

Figure S43: ^1H NMR spectrum of **6**.

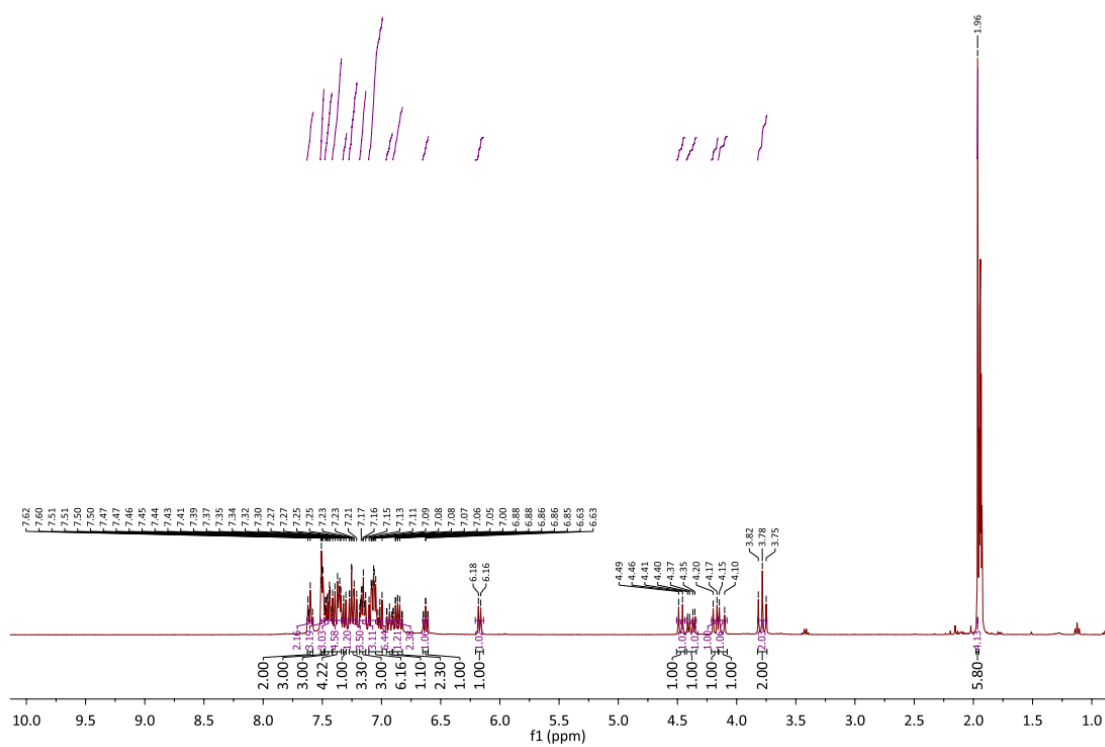


Figure S44: ^1H NMR spectrum of **6** (expanded).

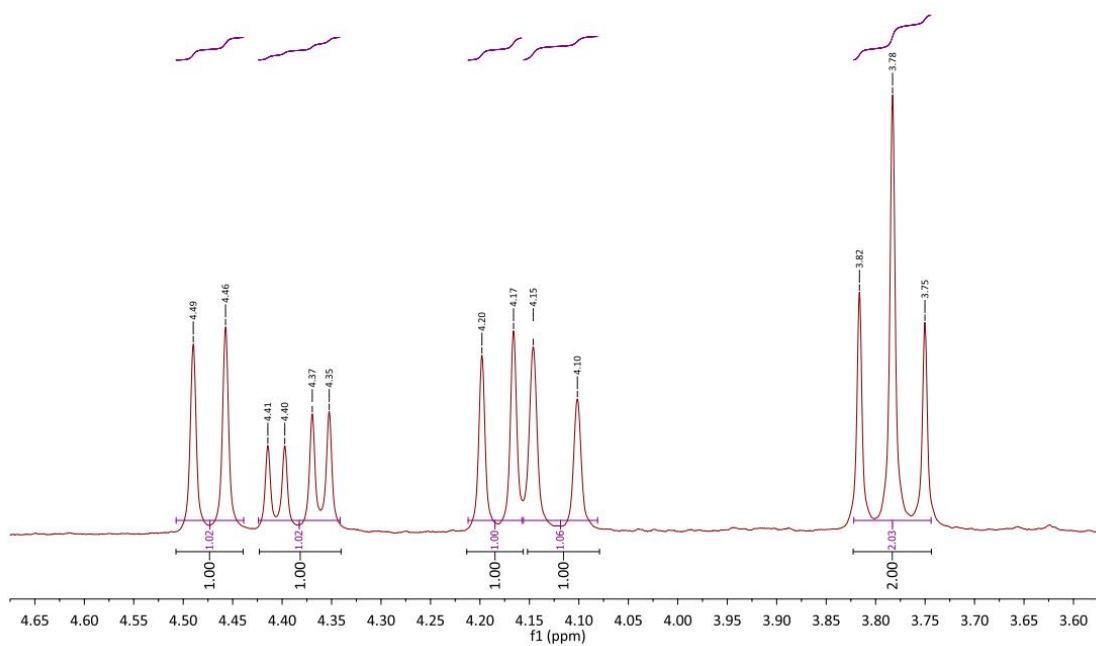


Figure S45: ^1H NMR spectrum of **6** (expanded).

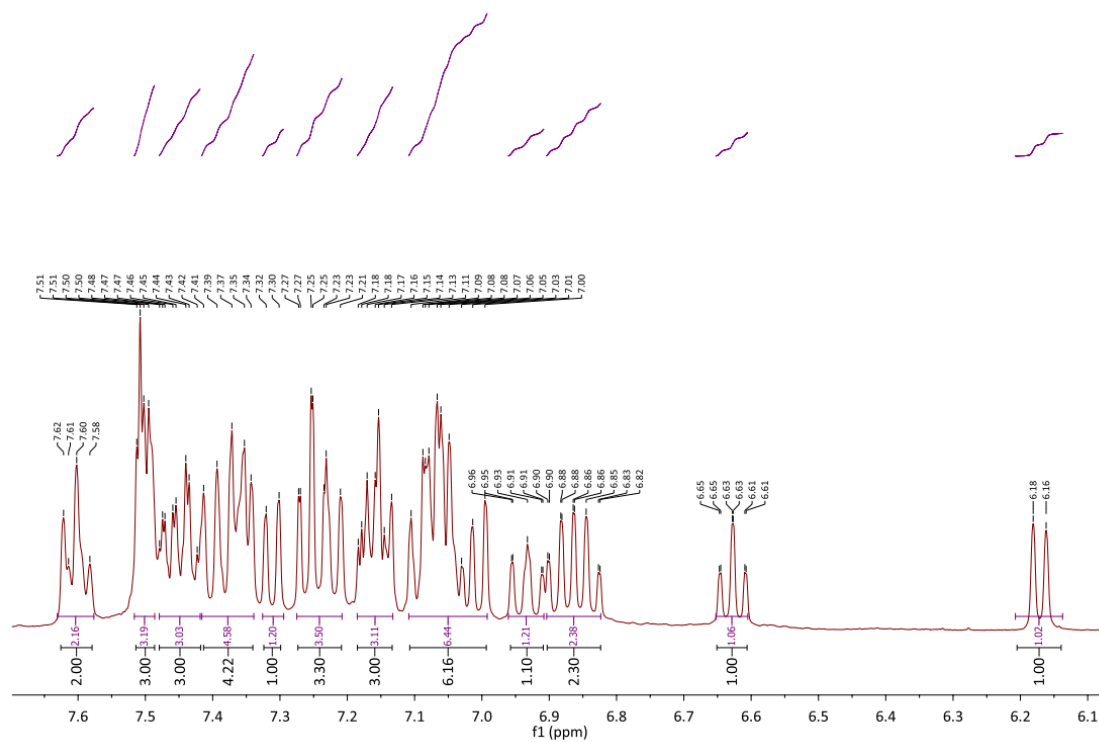


Figure S46: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6**.

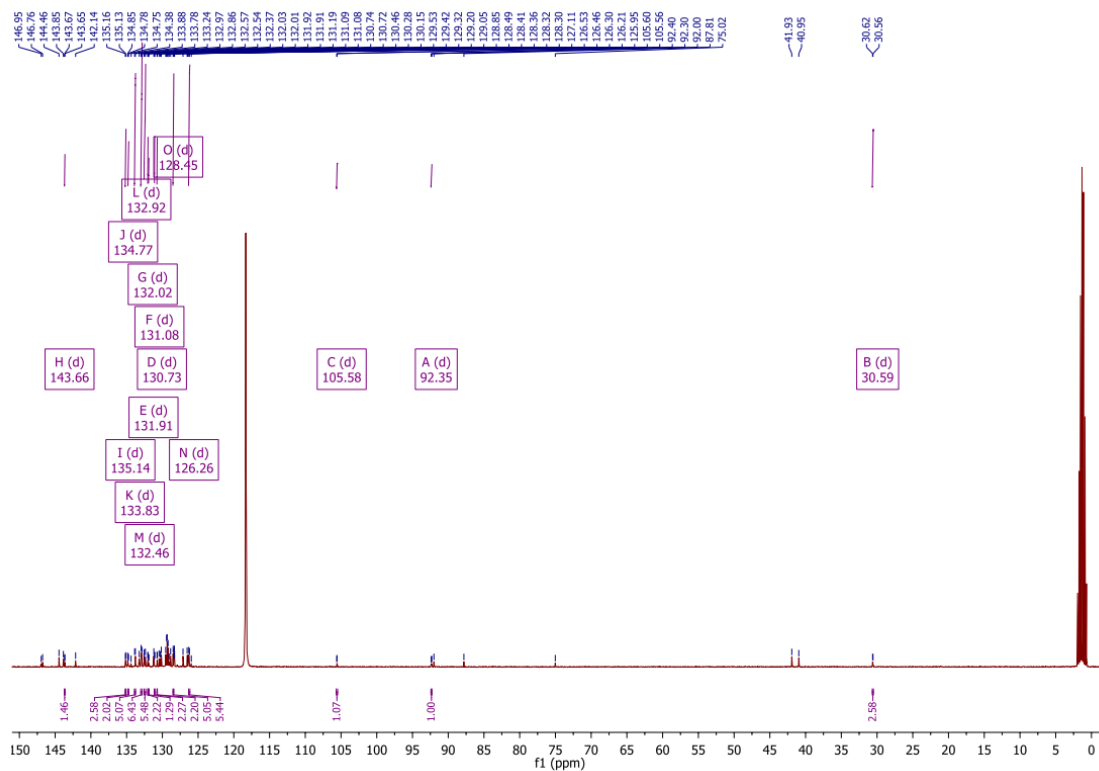


Figure S47: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6** (expanded).

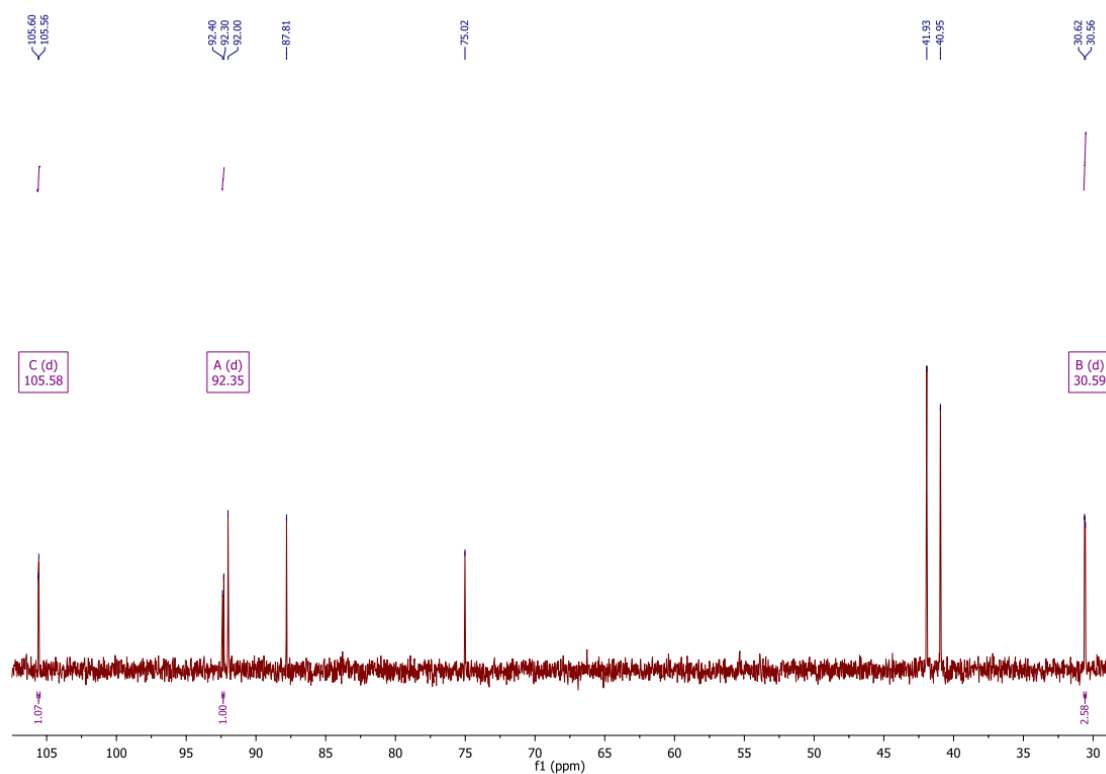


Figure S48: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6** (expanded).

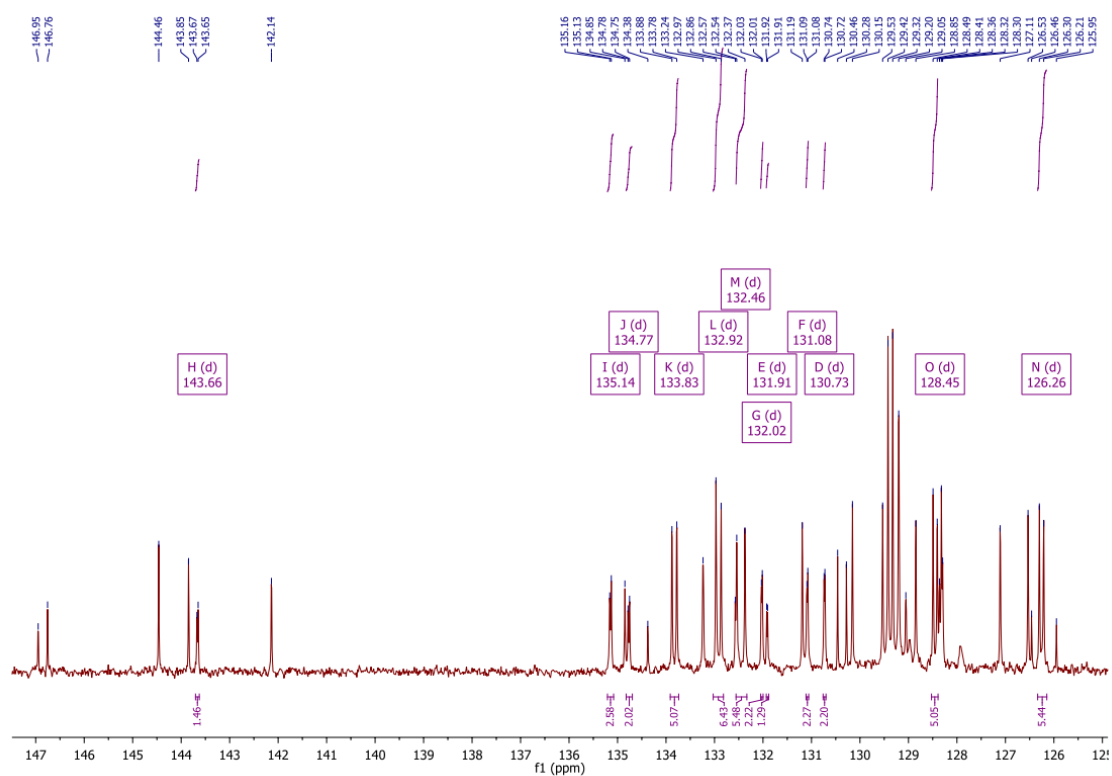


Figure S49: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **6**.

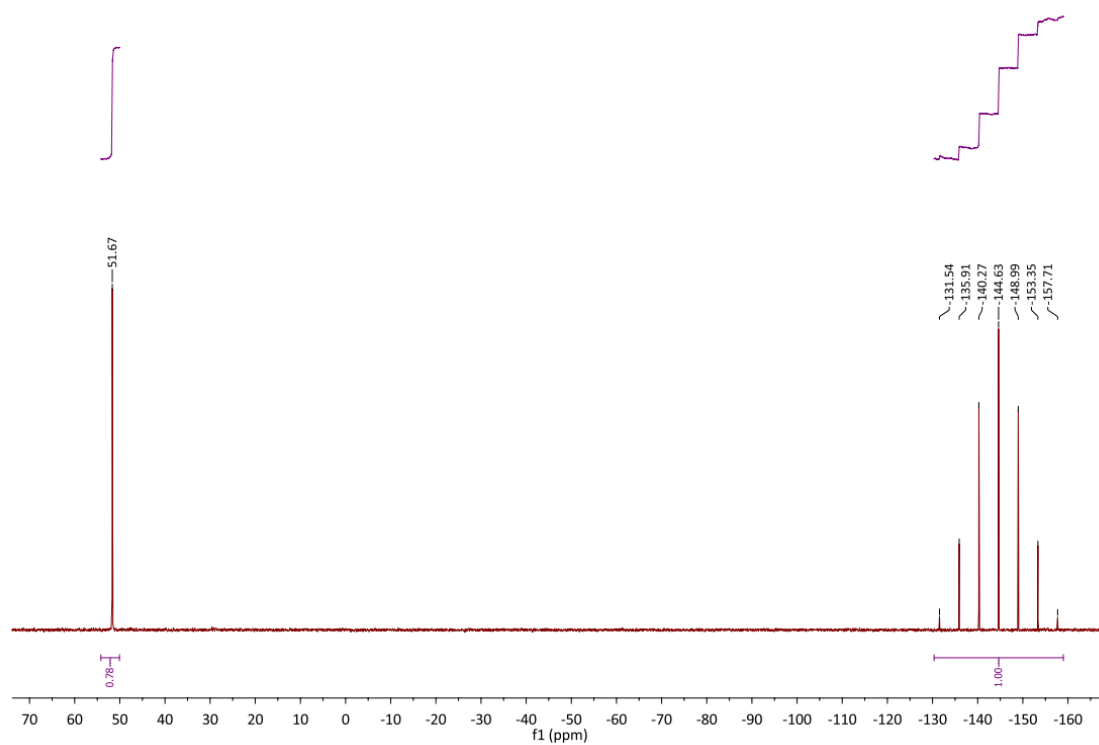


Figure S50: $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **6**.

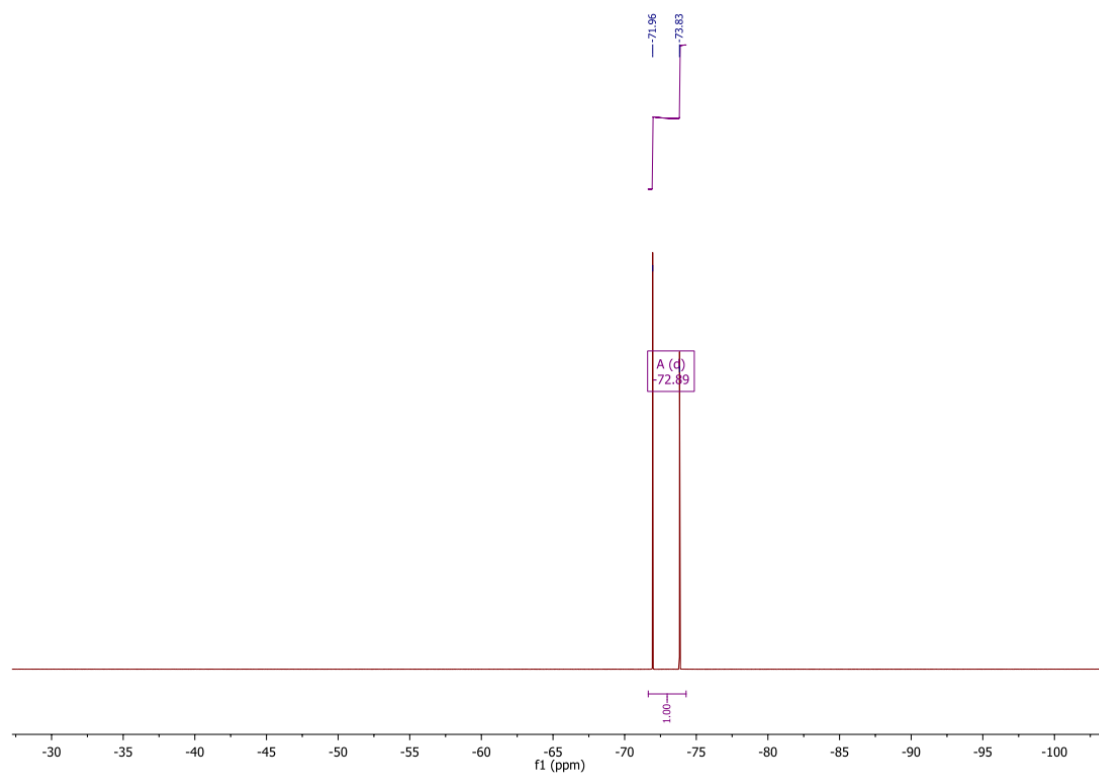


Figure S51: H,H-COSY NMR spectrum of **6**.

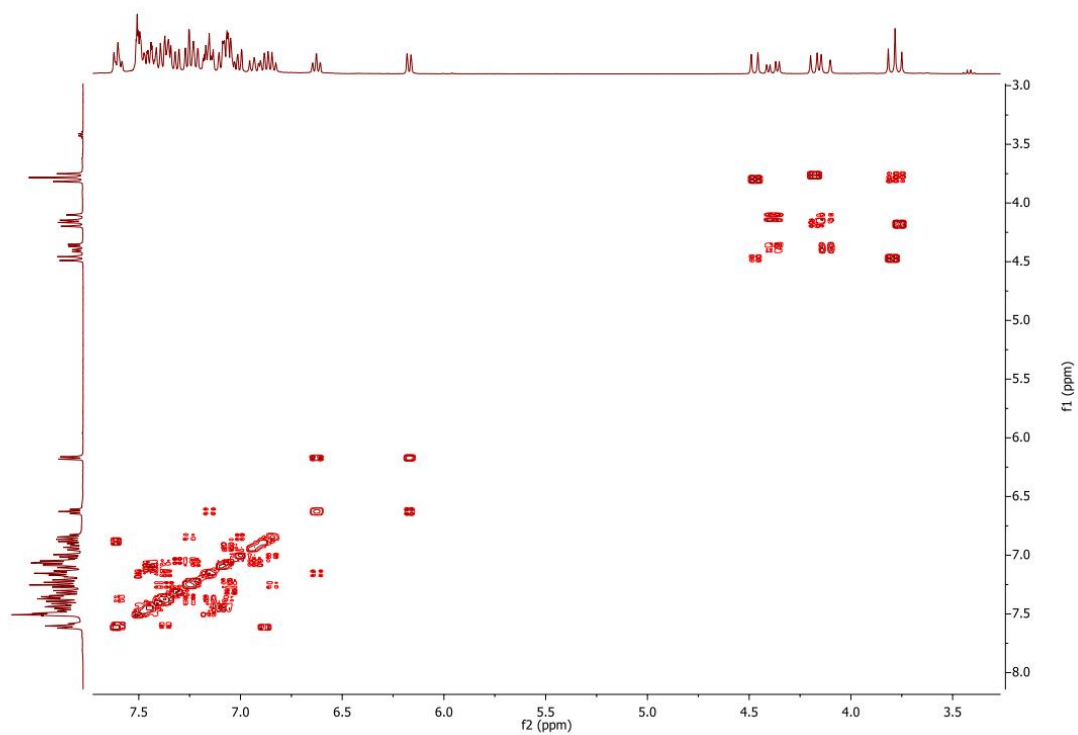


Figure S52: H,H-COSY NMR spectrum of **6** (expanded).

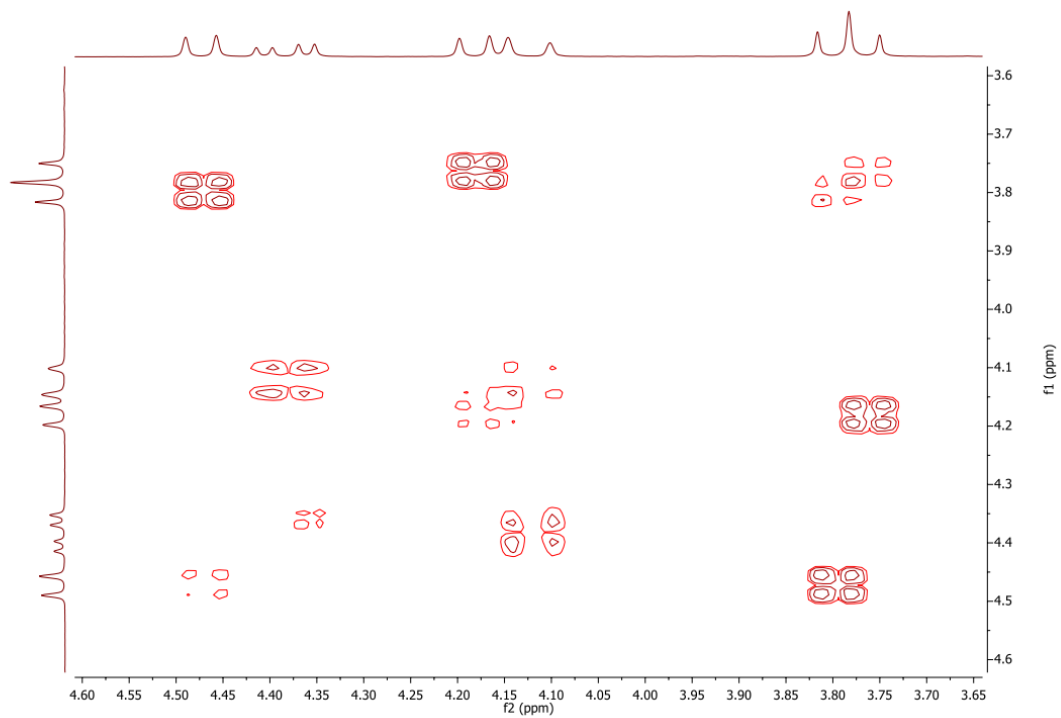


Figure S53: H,H-COSY NMR spectrum of **5** (expanded).

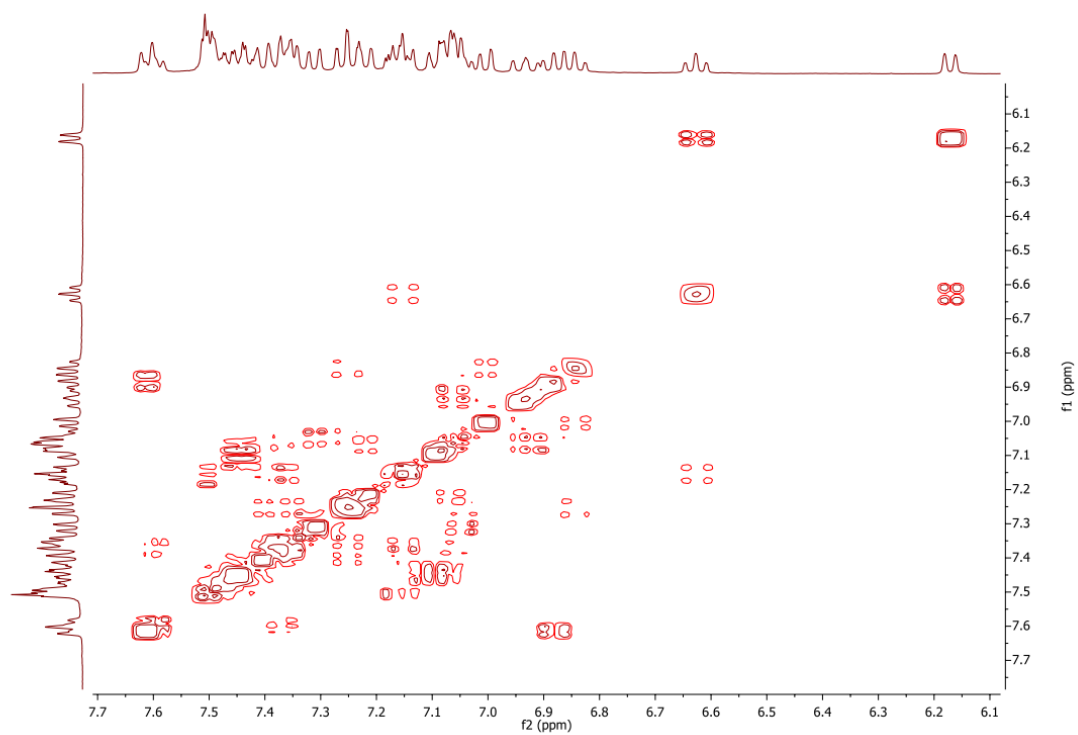


Figure S54: HMQC NMR spectrum of **6**.

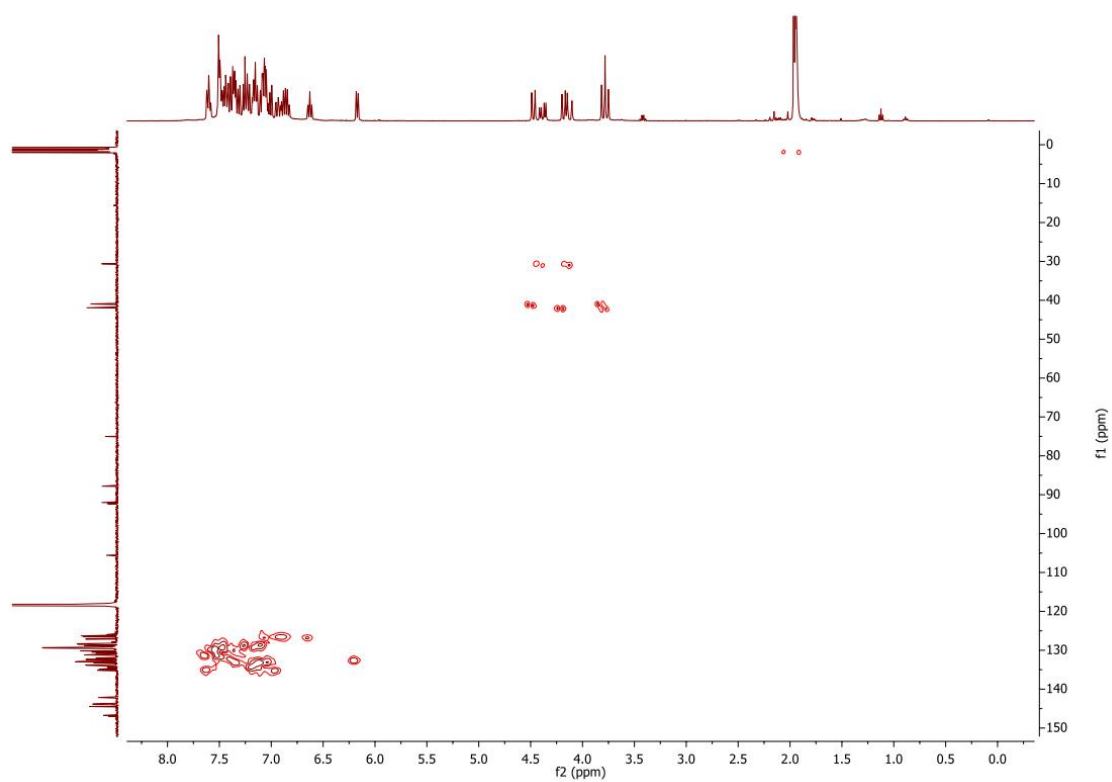
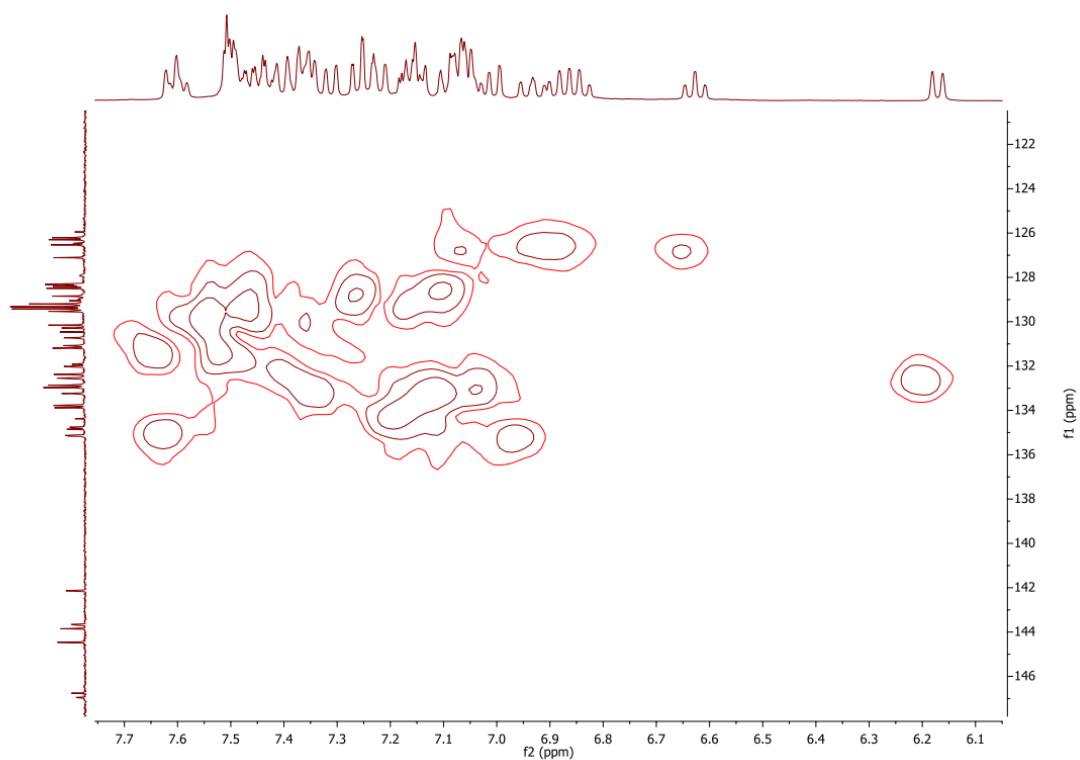


Figure S55: HMQC NMR spectrum of **6** (expanded).



$[\text{Cp}^{\text{C}}(\text{BzPPh}_2(\text{AuCl})_2)]$ (**7**):

Figure S56: ^1H NMR spectrum of **7**.

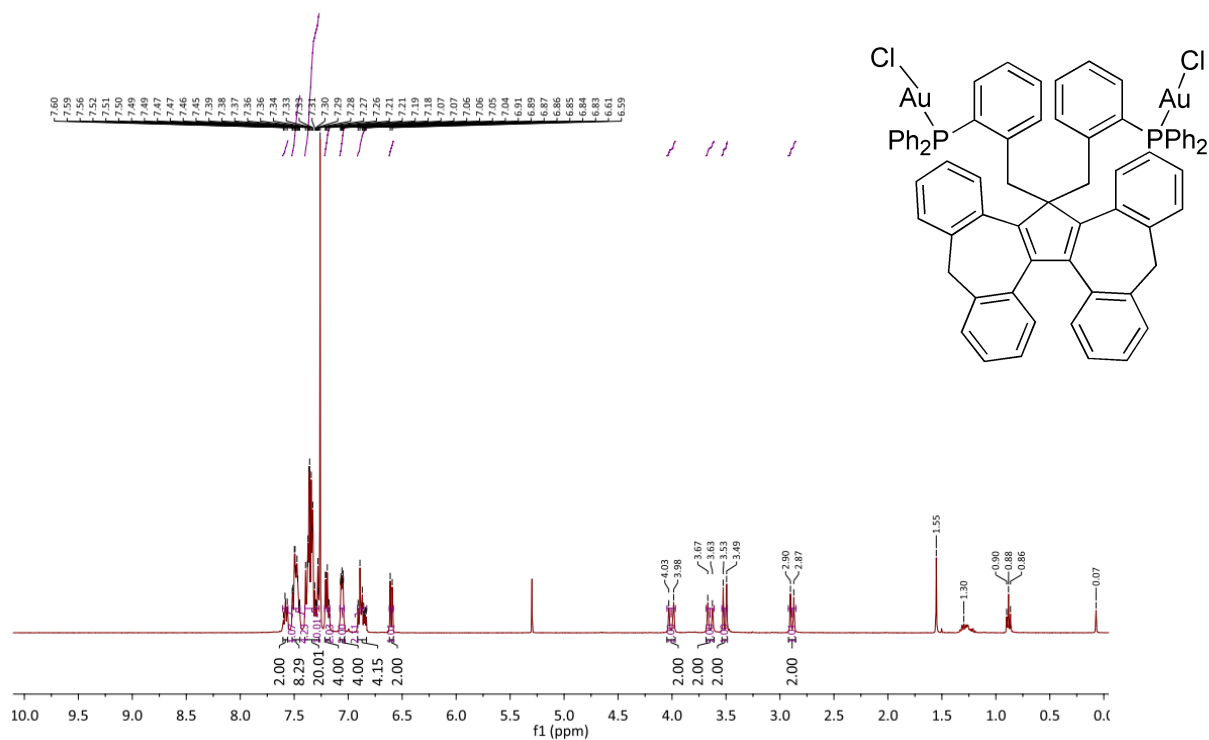


Figure S57: ^1H NMR spectrum of **7** (expanded).

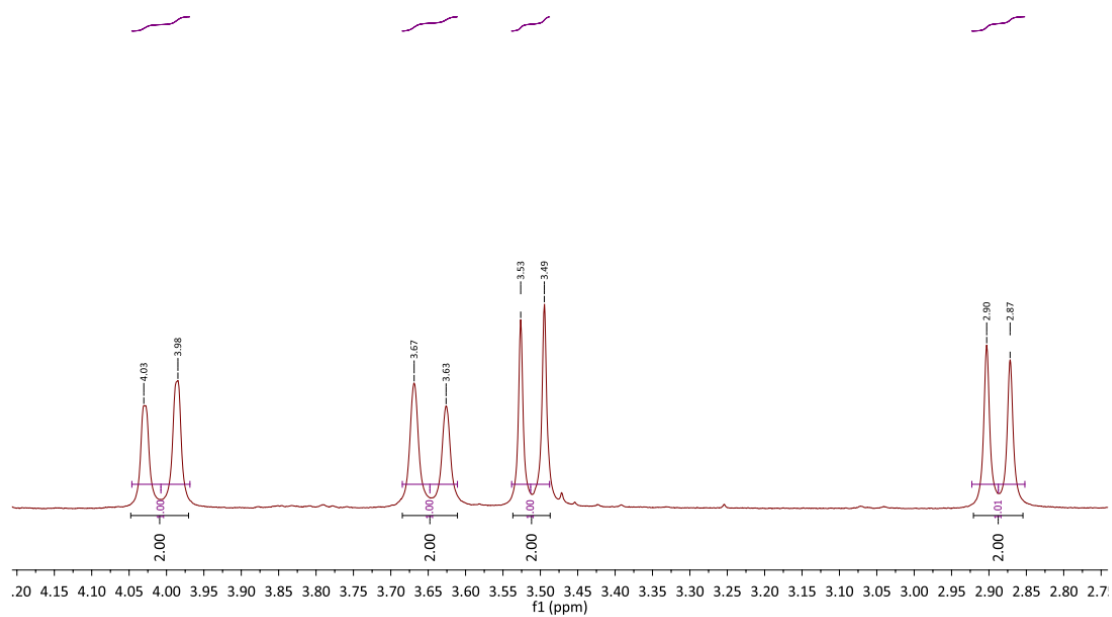


Figure S58: ^1H NMR spectrum of **7** (expanded).

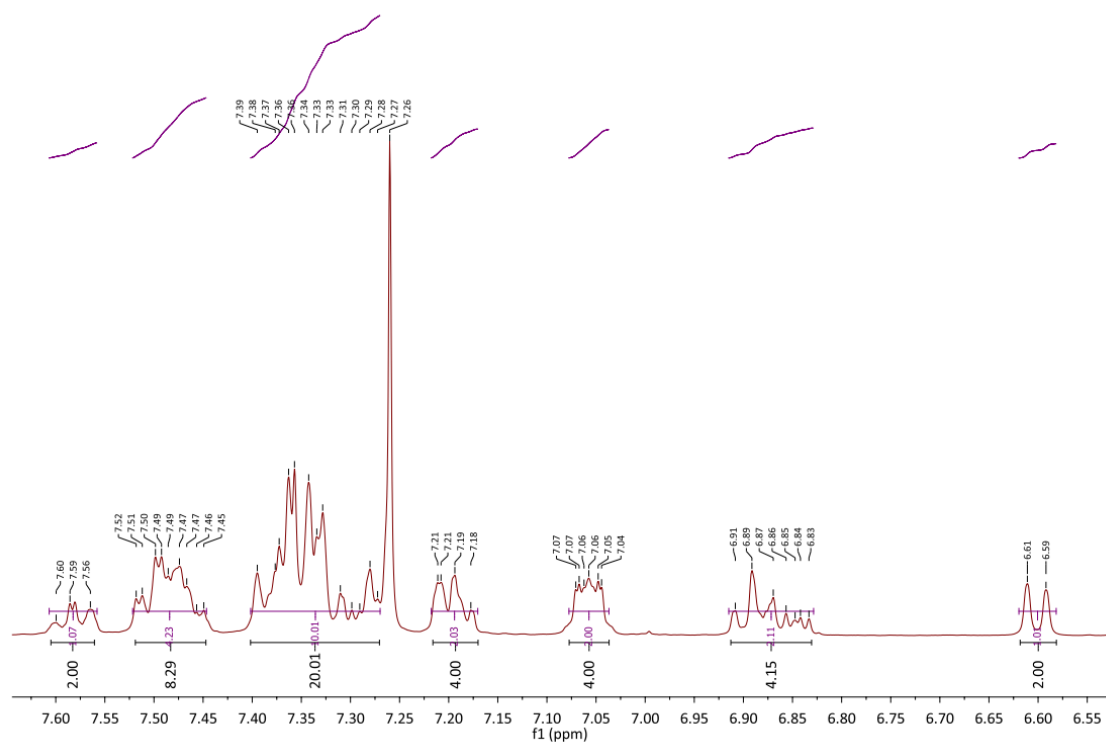
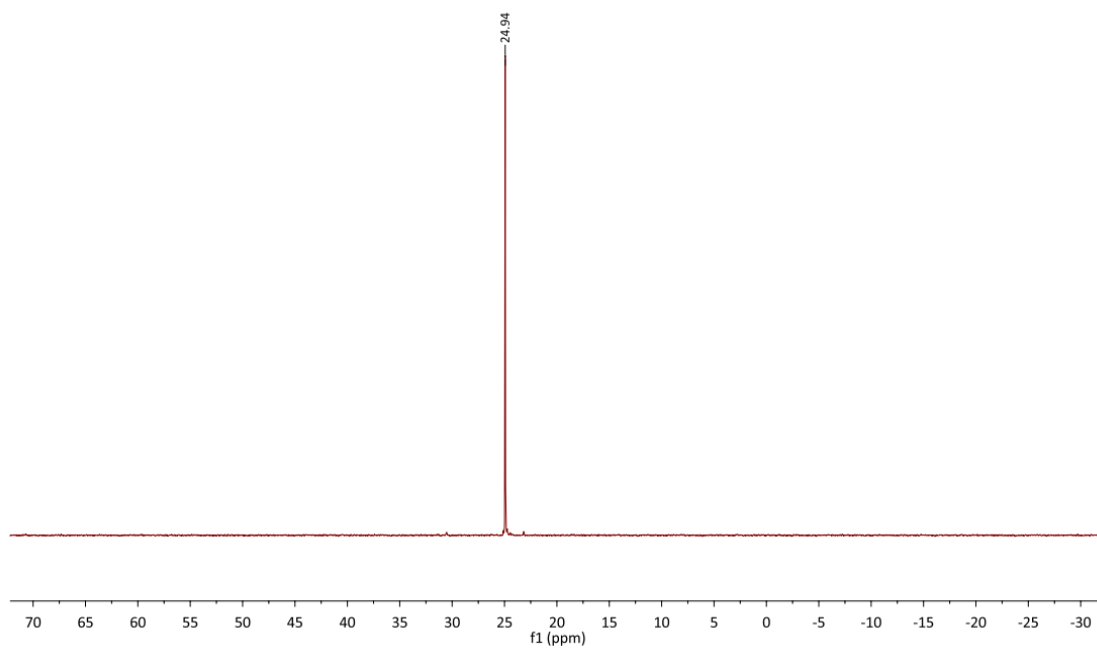


Figure S59: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **7**.



$[\text{Cp}^{\text{C}}(\text{BzPPh}_2)_2(\text{PdCl}(\mu^2\text{-Cl}))_2]$ (**8**):

Figure S60: ^1H NMR spectrum of **8**.

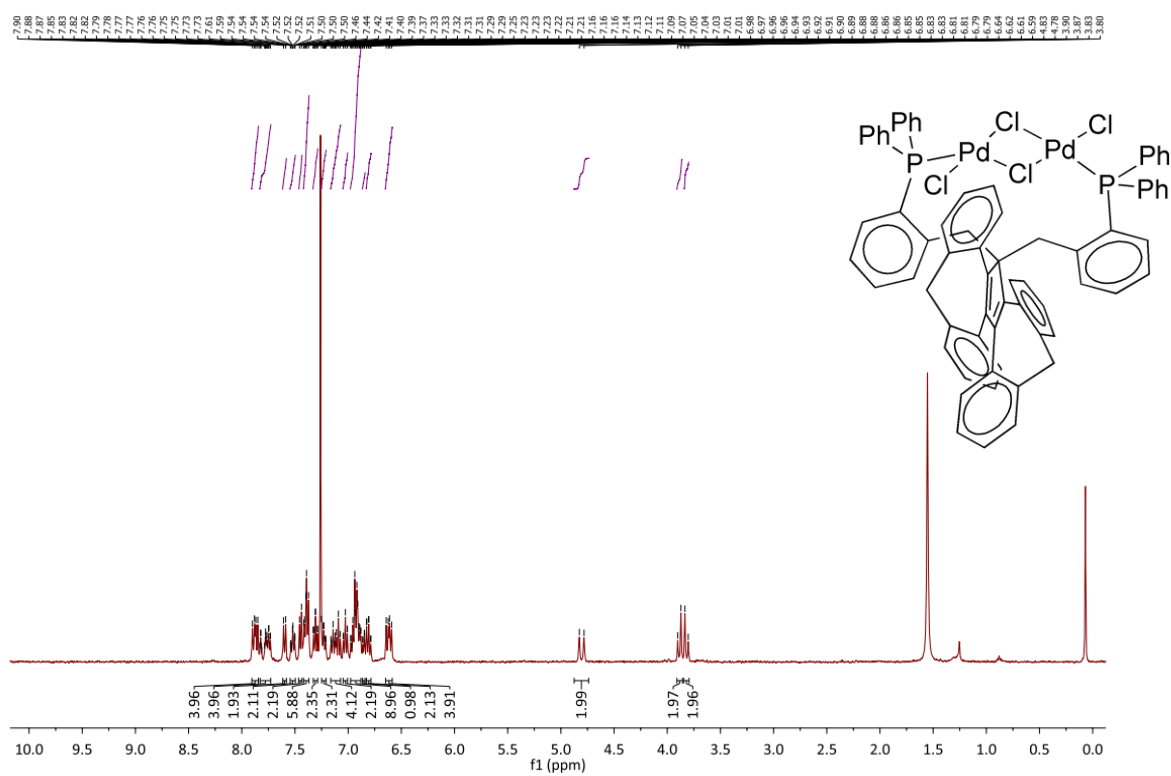


Figure S61: ^1H NMR spectrum of **8** (expanded).

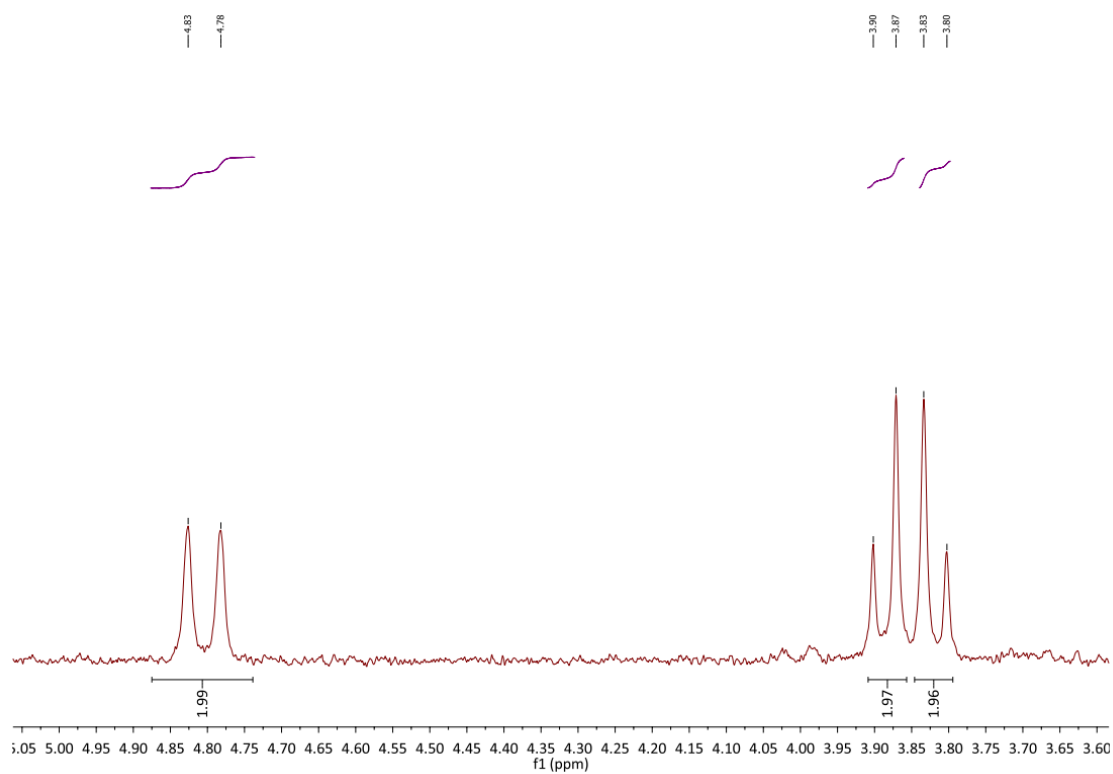


Figure S62: ^1H NMR spectrum of **8** (expanded).

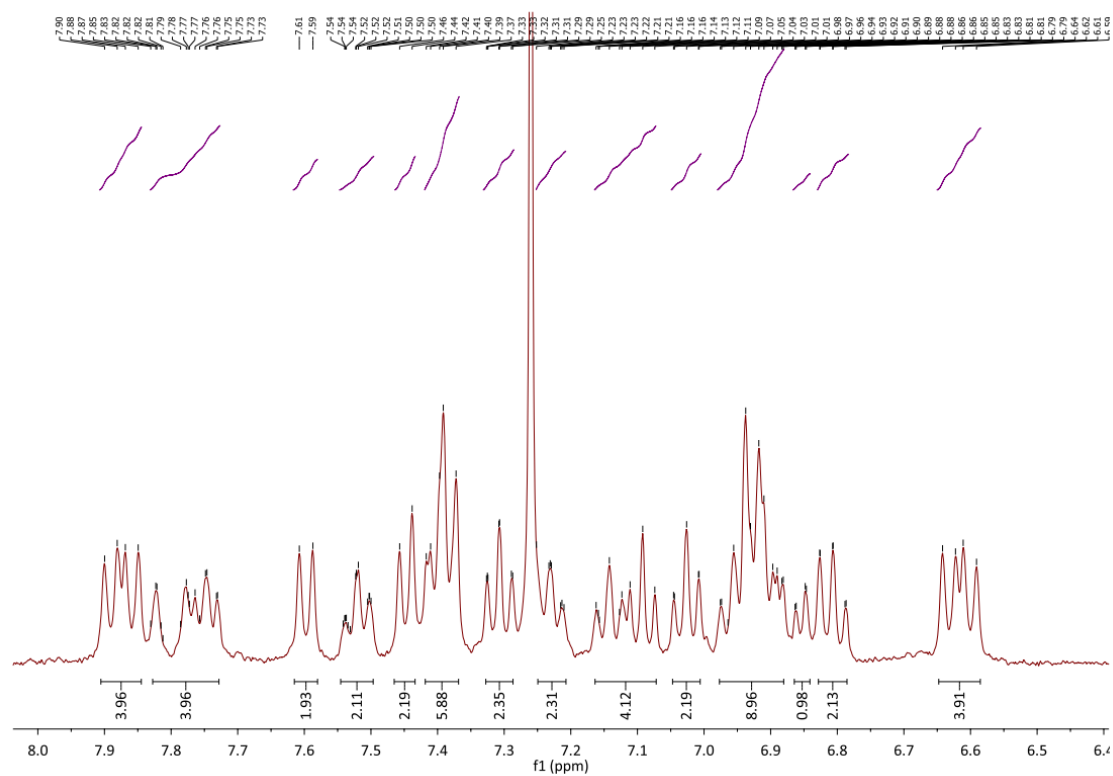


Figure S63: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **8**.

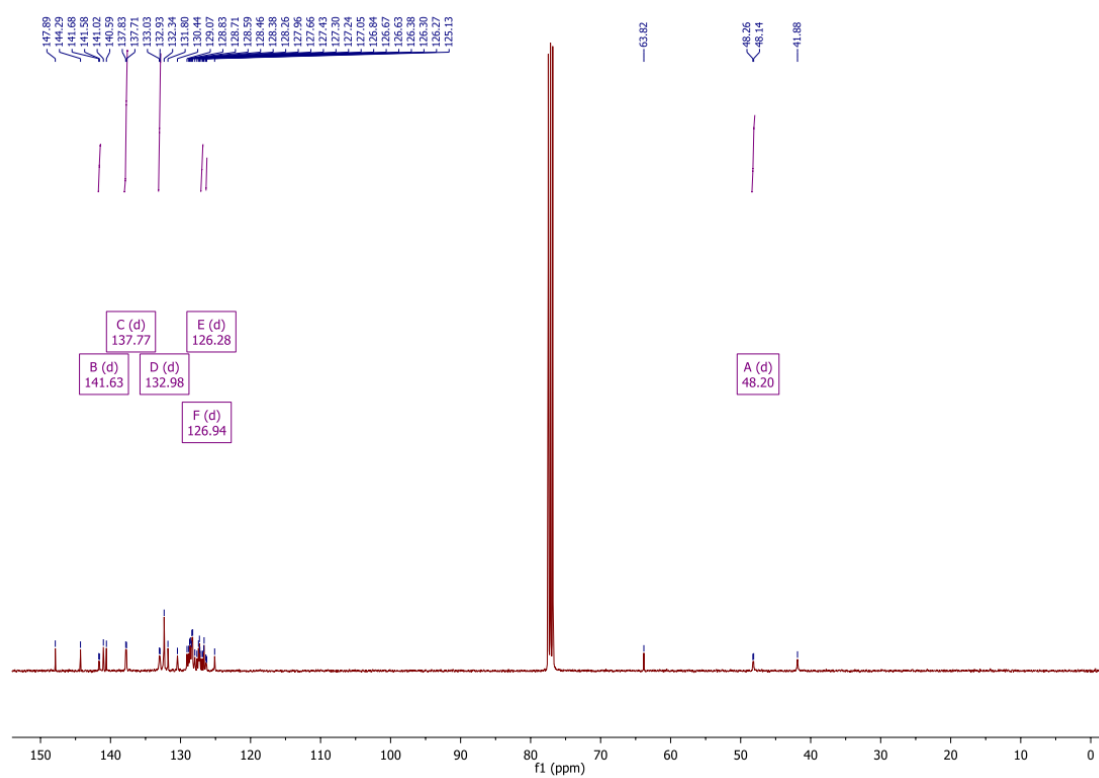


Figure S64: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **8** (expanded).

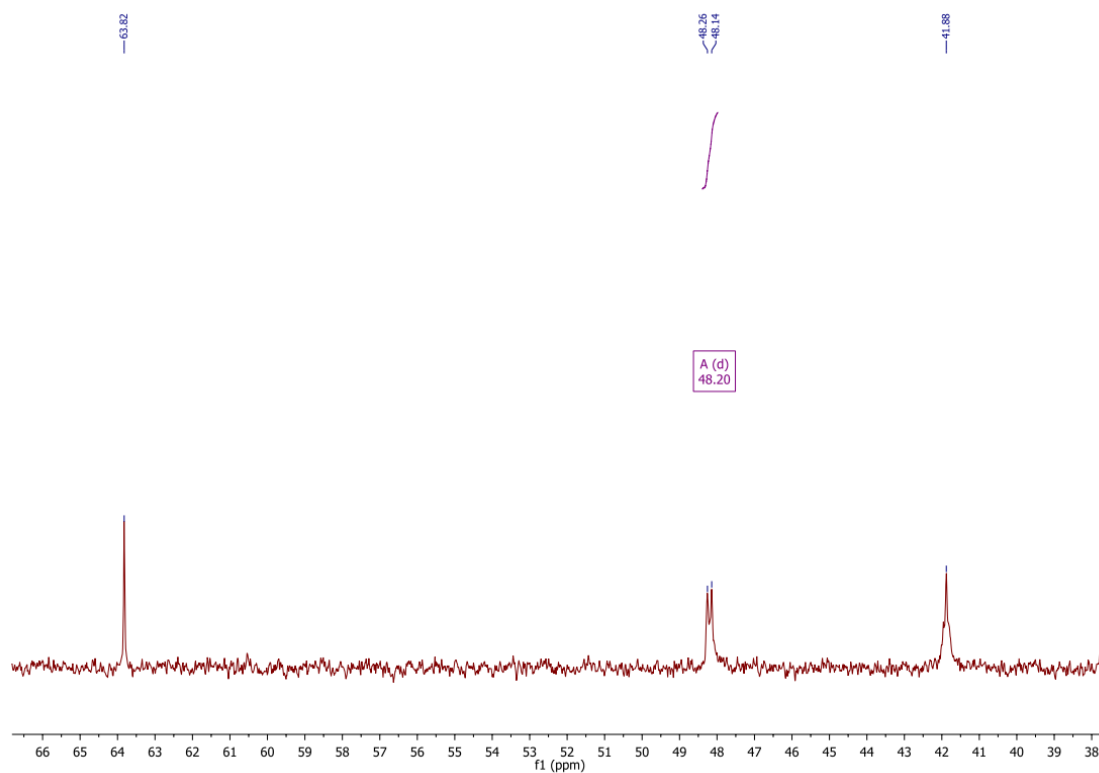


Figure S65: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **8** (expanded).

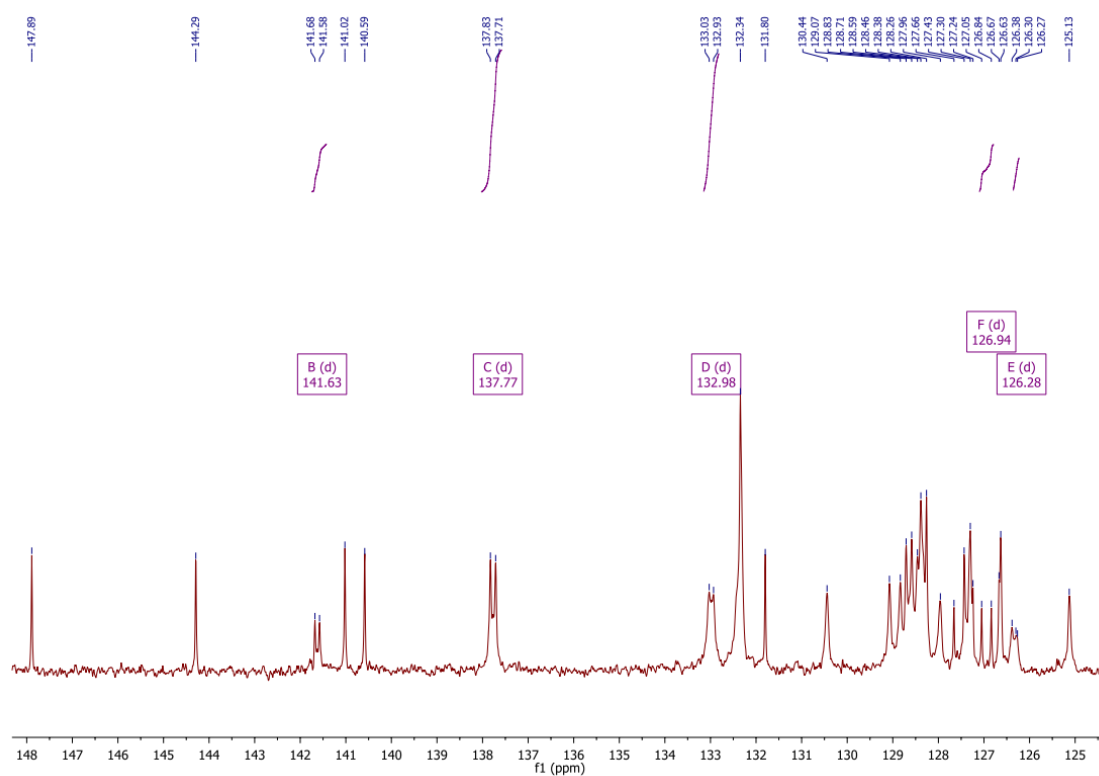


Figure S66: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **8**.

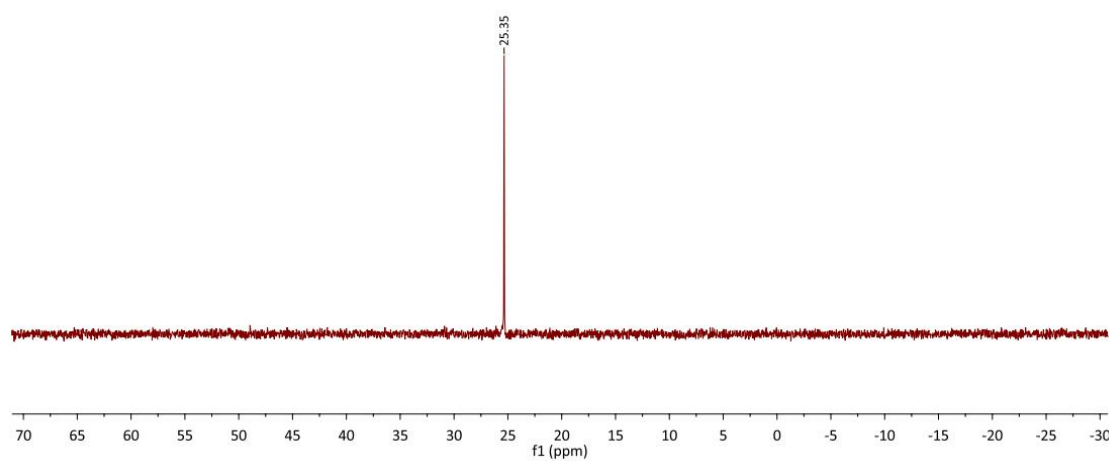


Figure S67: H,H-COSY NMR spectrum of **8**.

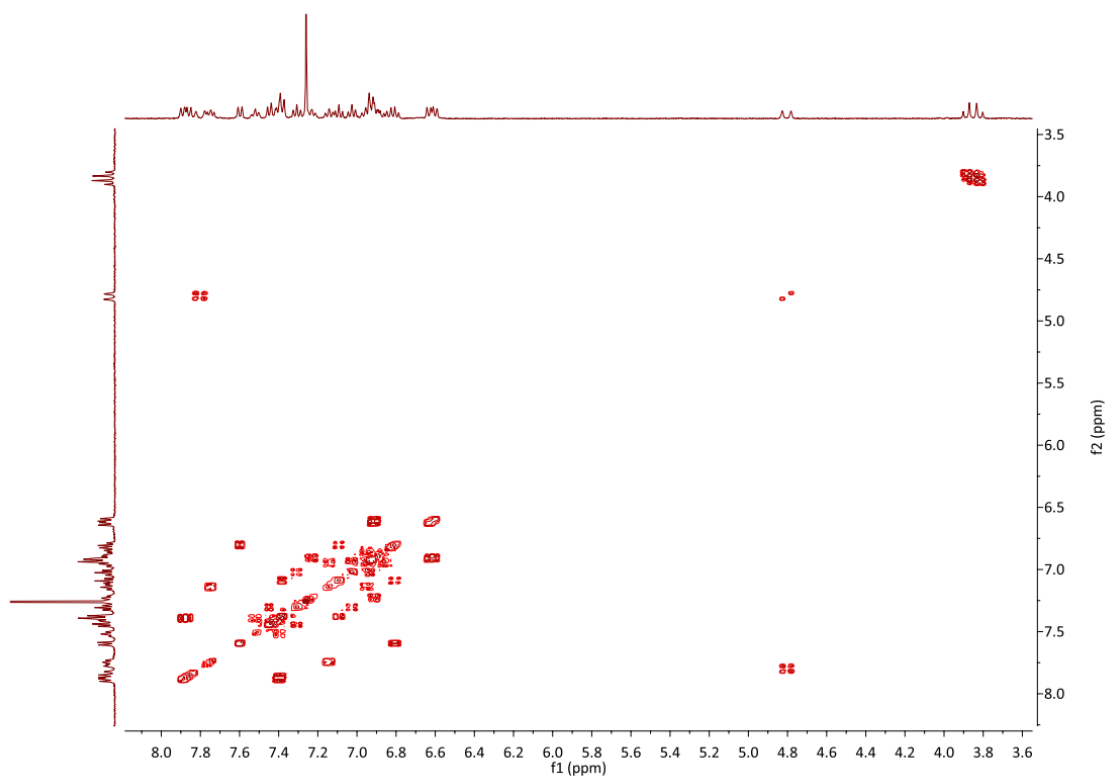


Figure S68: H,H-COSY NMR spectrum of **8** (expanded).

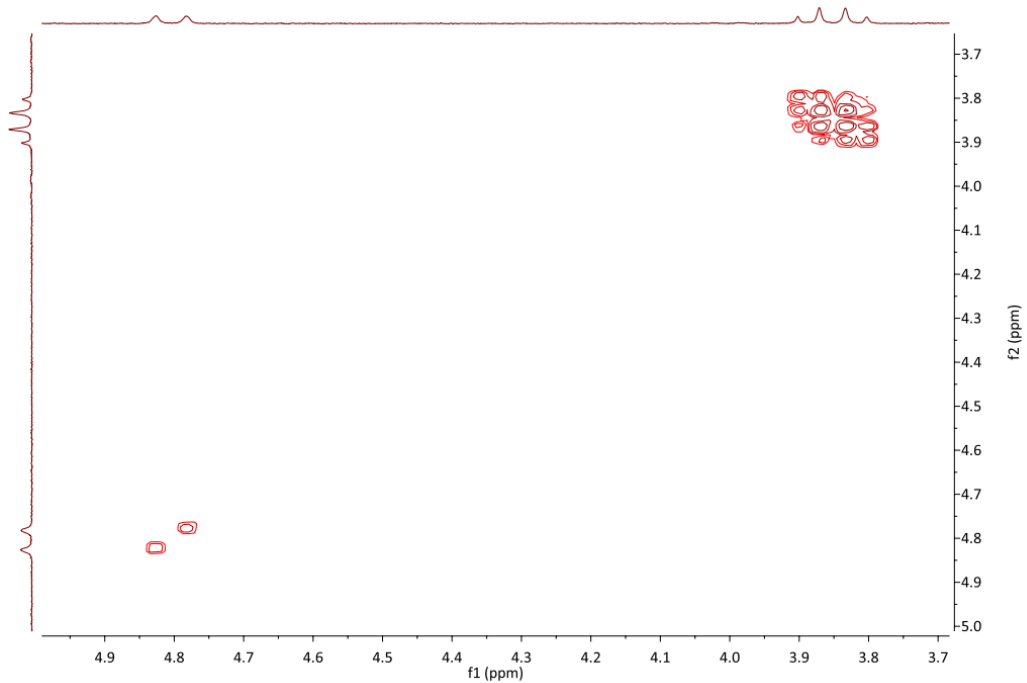


Figure S69: H,H-COSY NMR spectrum of **8** (expanded).

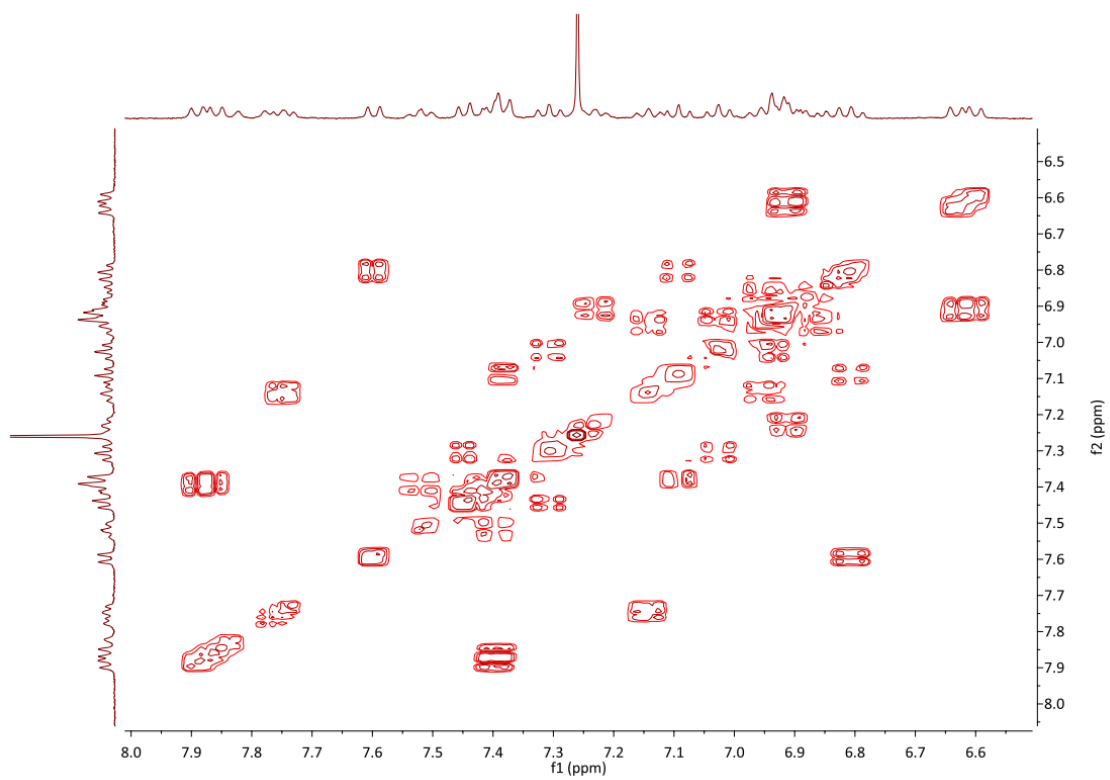


Figure S70: HMQC NMR spectrum of **8**.

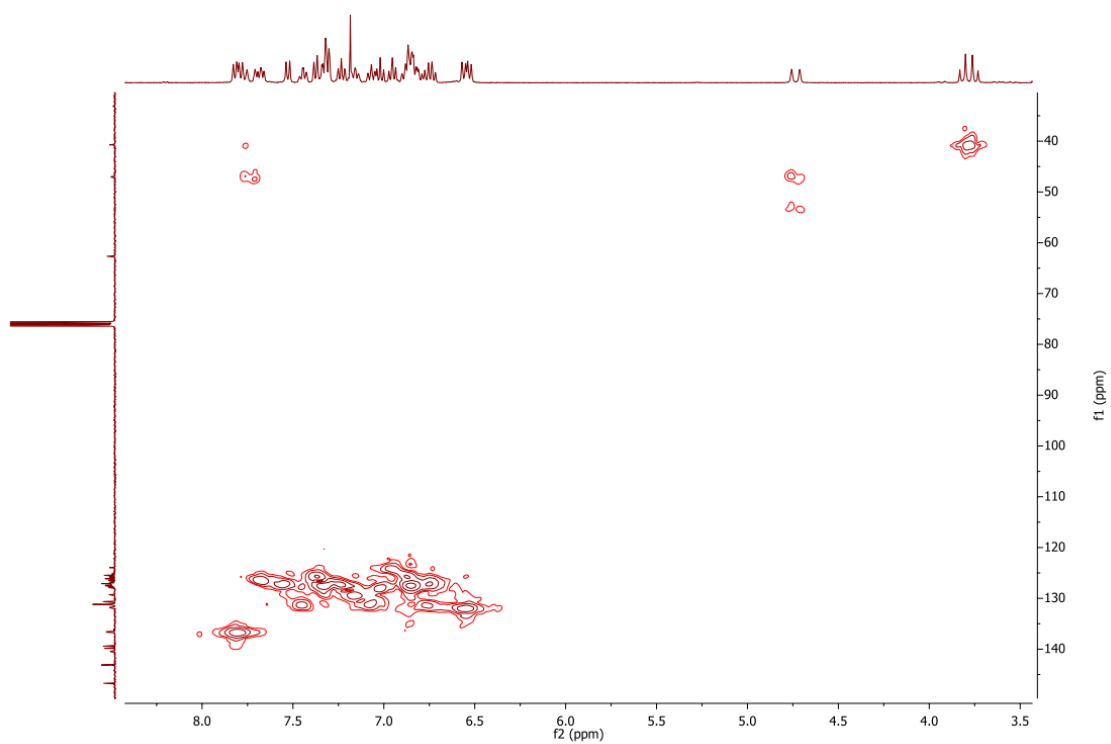
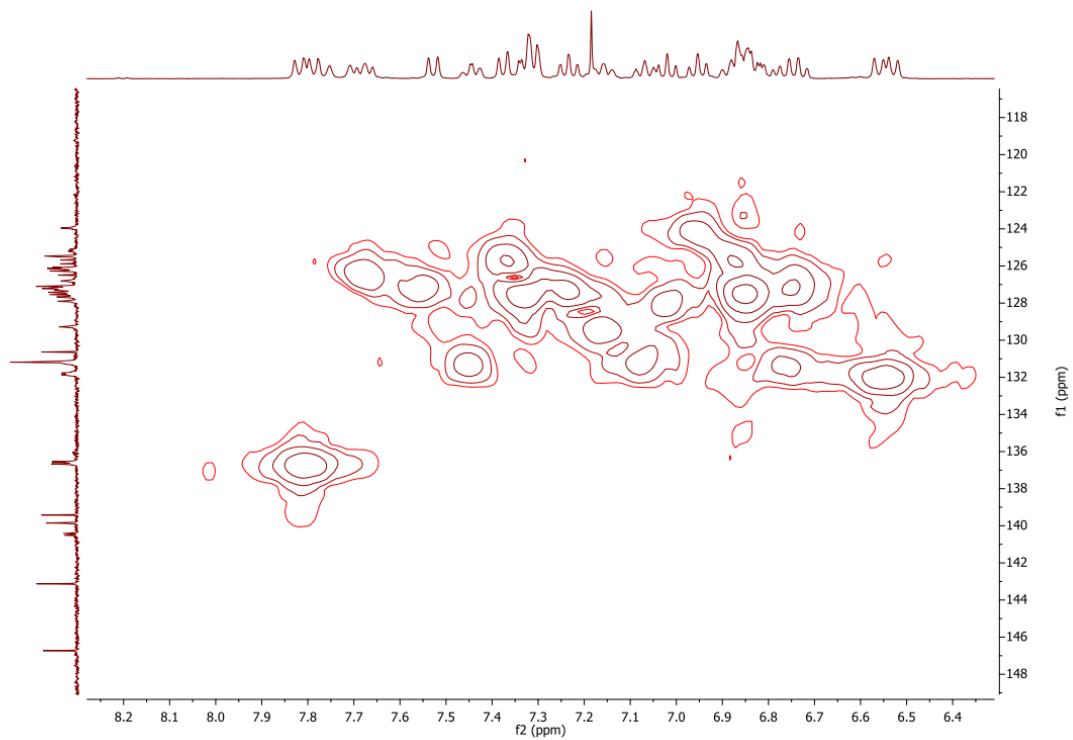


Figure S71: HMQC NMR spectrum of **8** (expanded).



[Cp^c(BzPPh₂)₂](Rh(μ²-Cl(CO))₂) (9):

Figure S72: ^1H NMR spectrum of **9**.

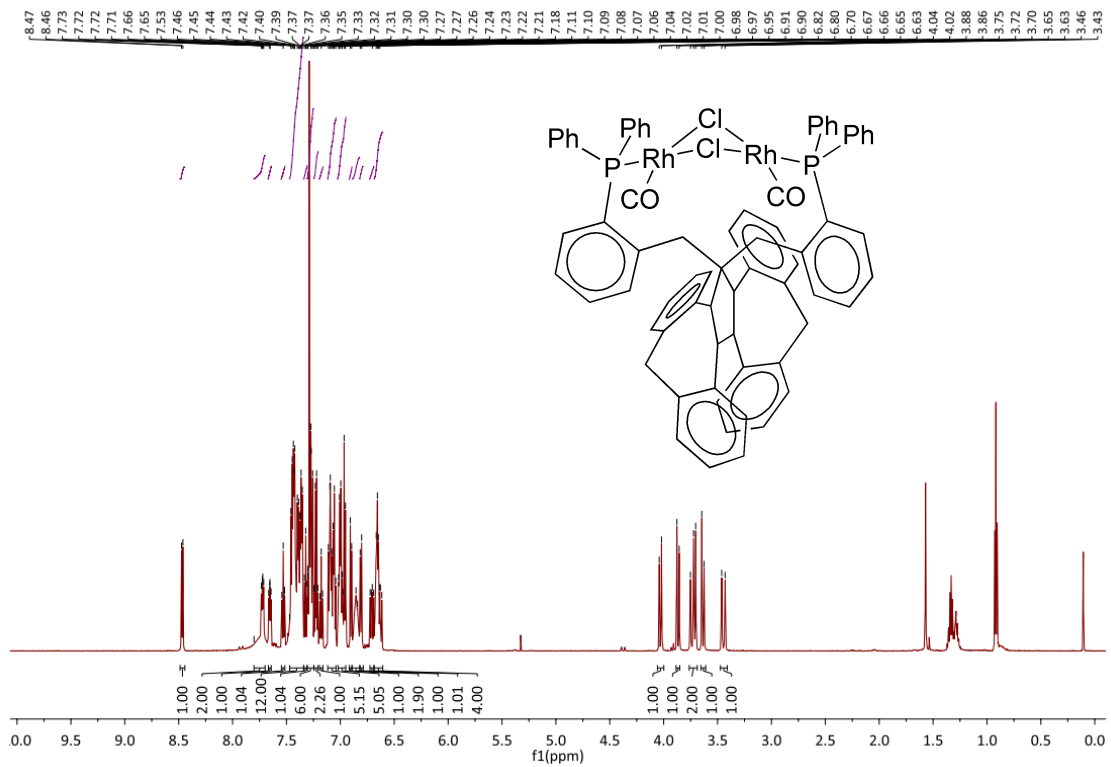


Figure S73: ^1H NMR spectrum of **9** (expanded).

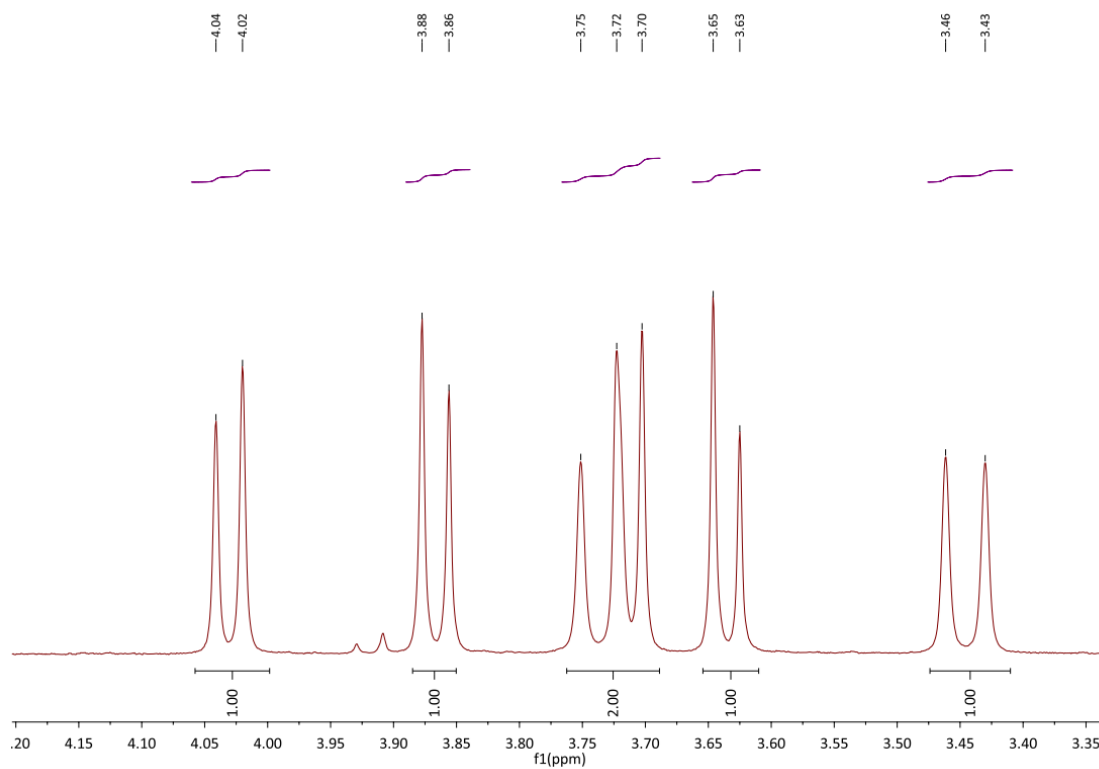


Figure S74: ^1H NMR spectrum of **9** (expanded).

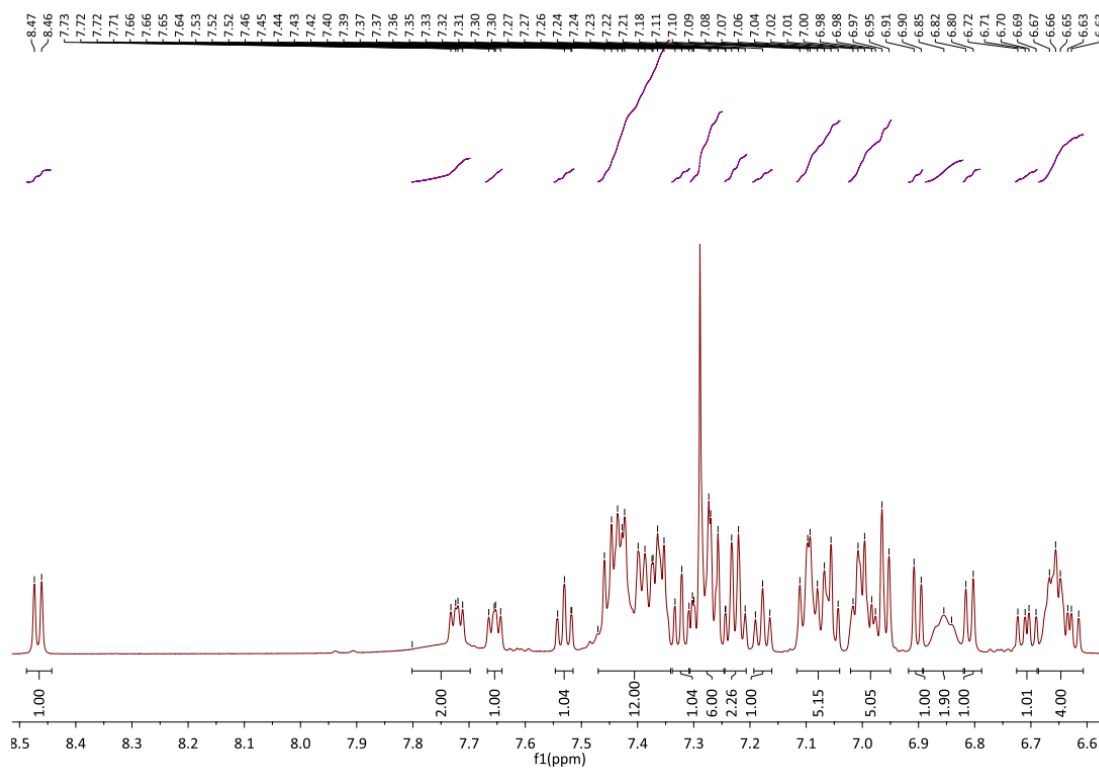


Figure S75: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9**.

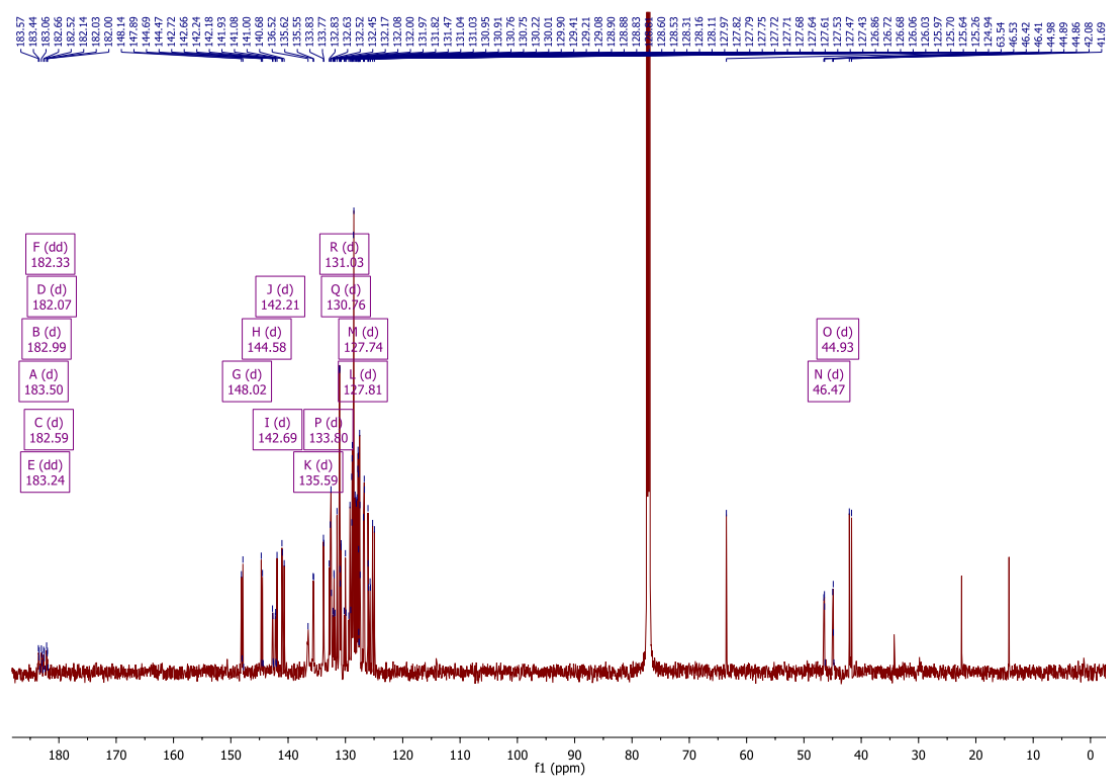


Figure S76: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9** (expanded).

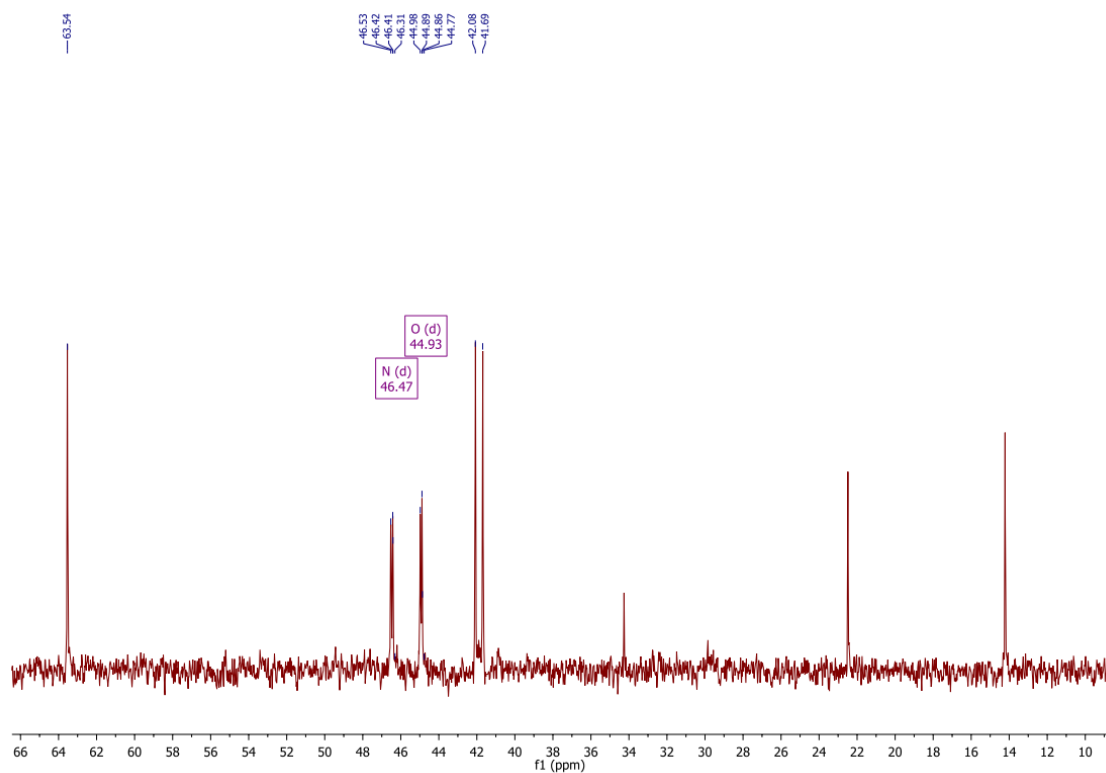


Figure S77: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9** (expanded).

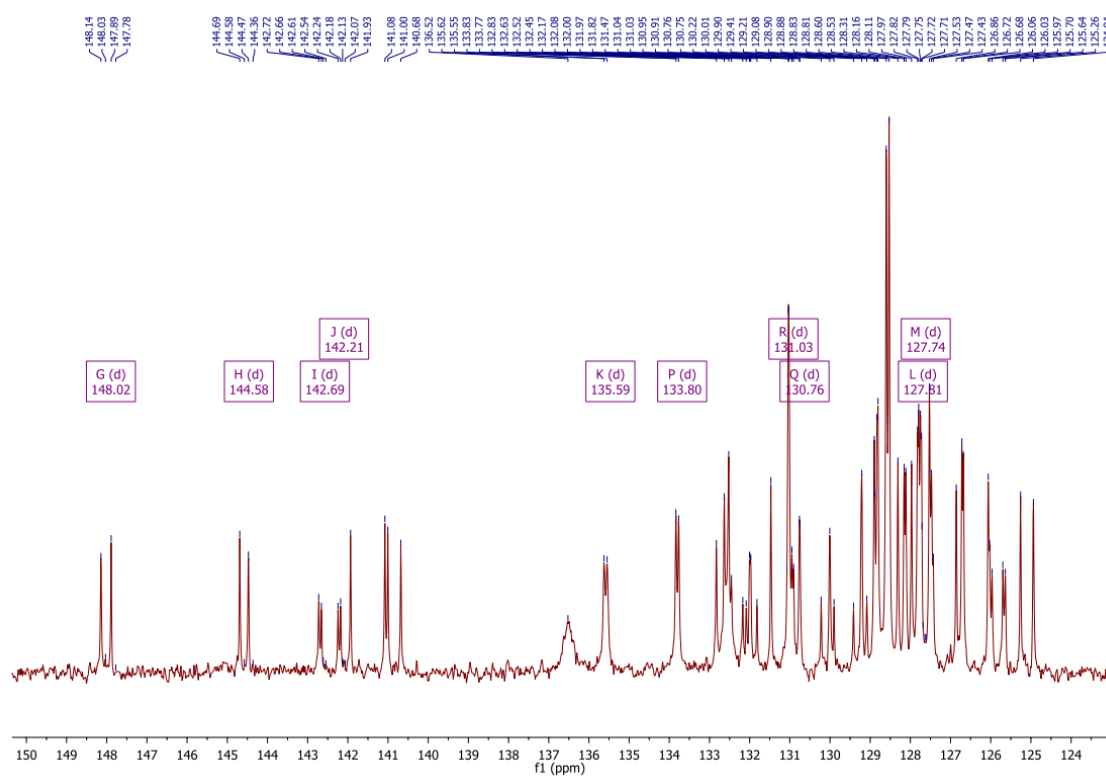


Figure S78: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9** (expanded).

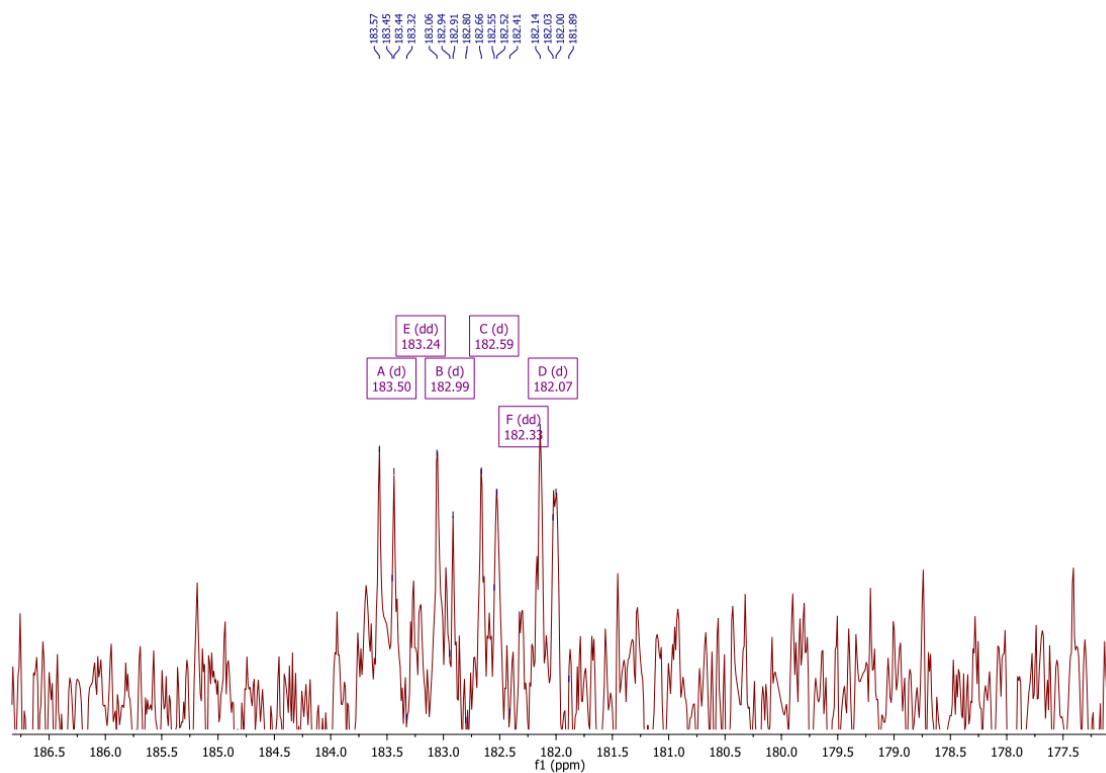


Figure S79: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **9**.

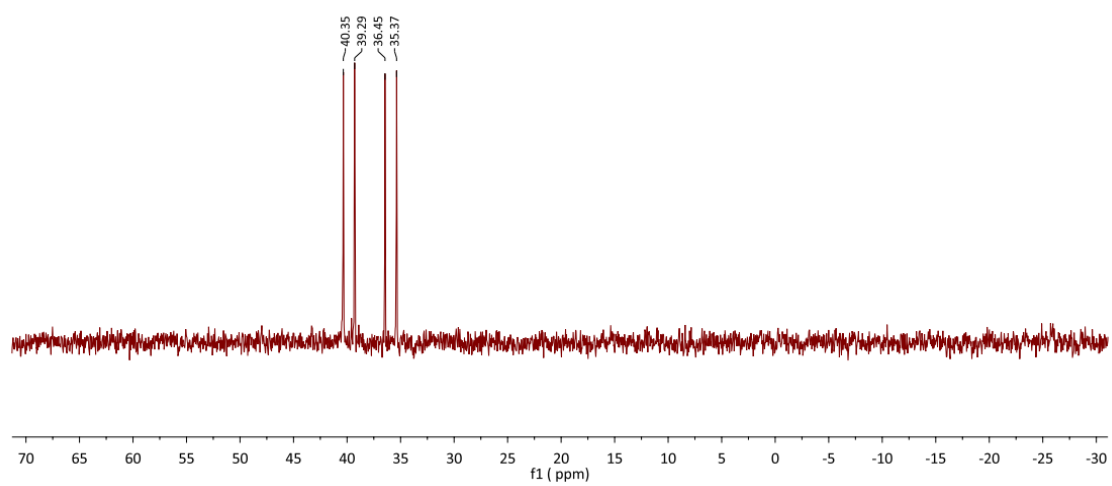


Figure S80: H,H-COSY NMR spectrum of **9**.

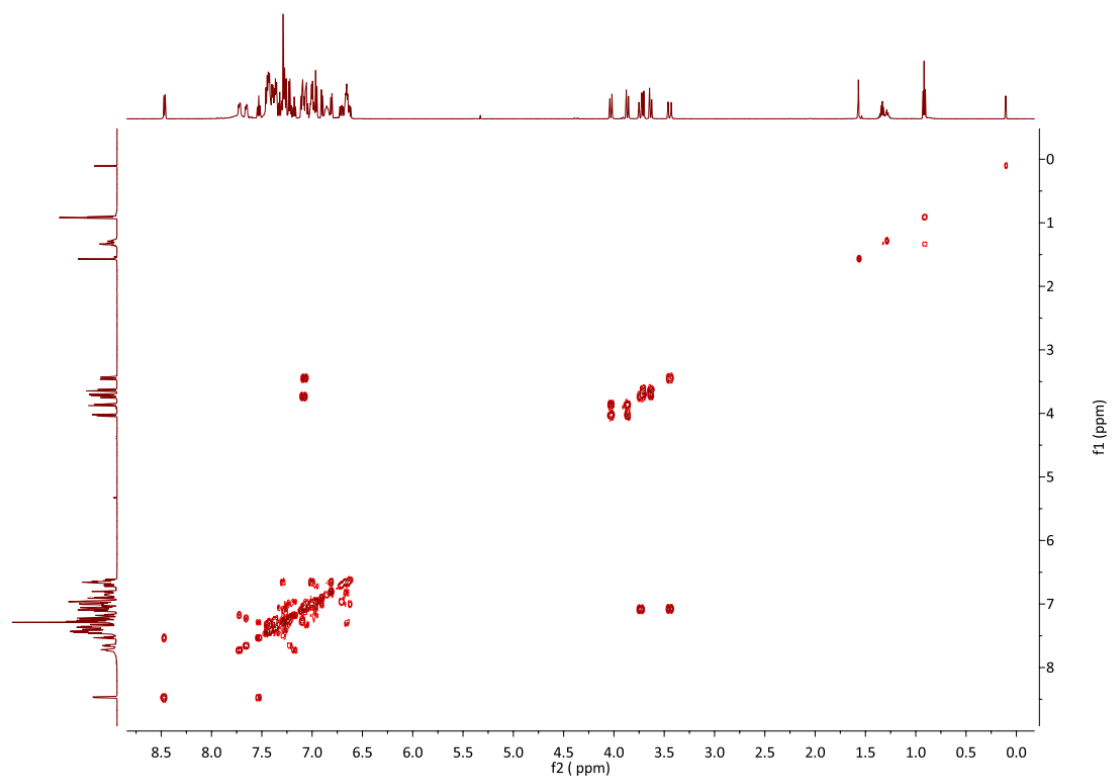


Figure S81: H,H-COSY NMR spectrum of **9** (expanded).

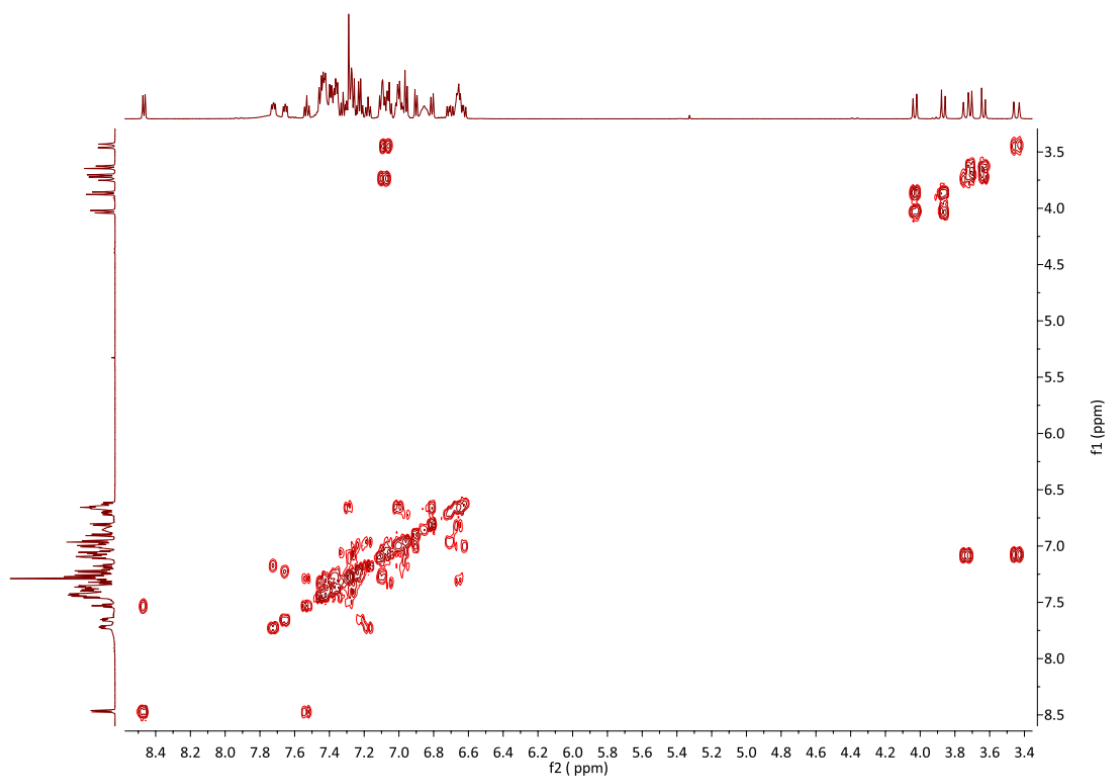


Figure S82: H,H-COSY NMR spectrum of **9** (expanded).

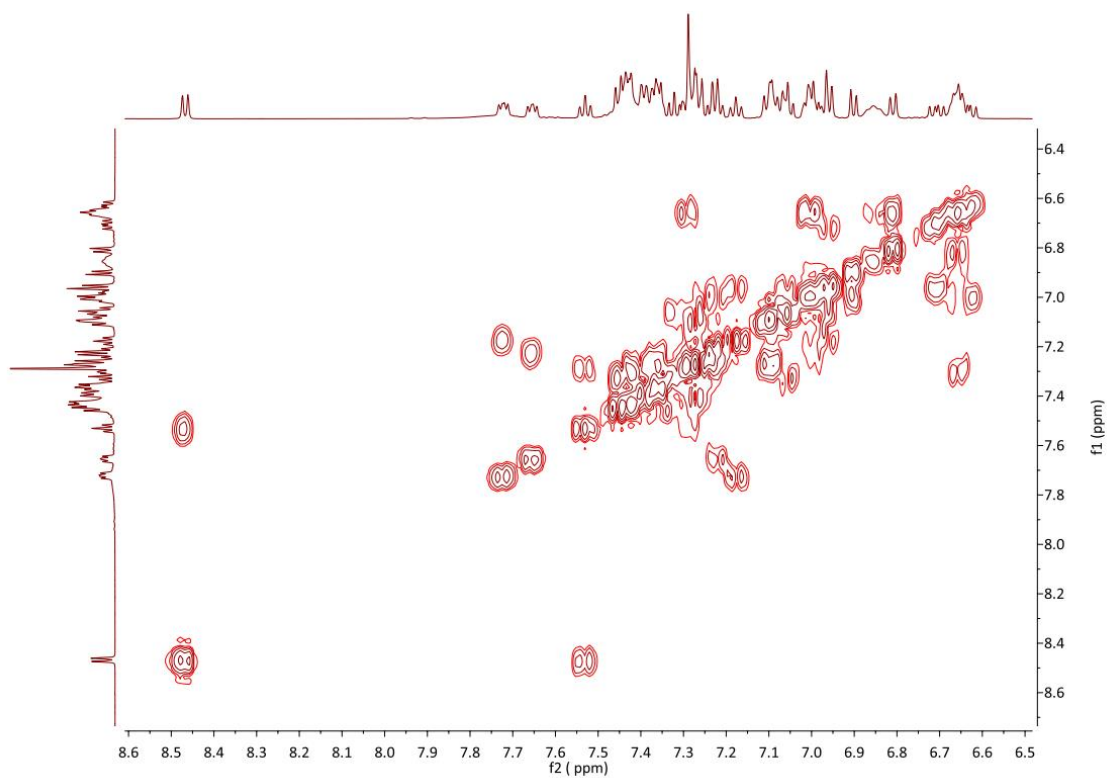


Figure S83: HMQC NMR spectrum of **9**.

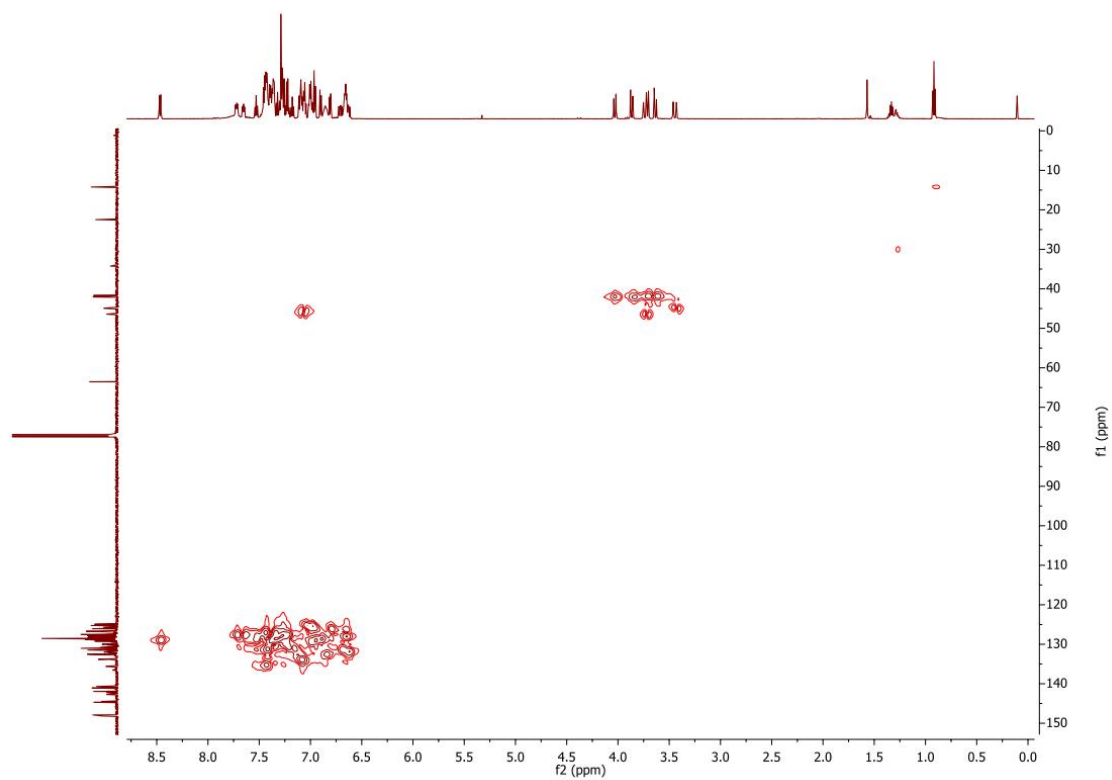
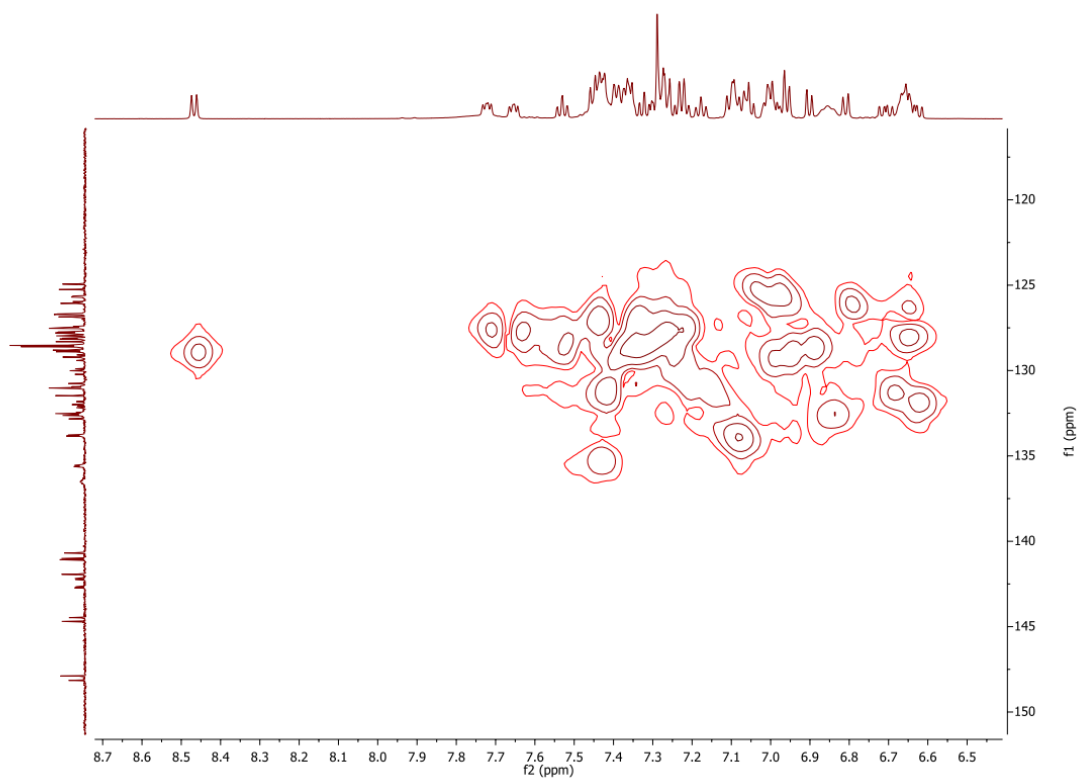


Figure S84: HMQC NMR spectrum of **9** (expanded).



[Cp^C(BzPPh₂)₂(RhCl(CO))] **(10):**

Figure S85: ¹H NMR spectrum of **10**.

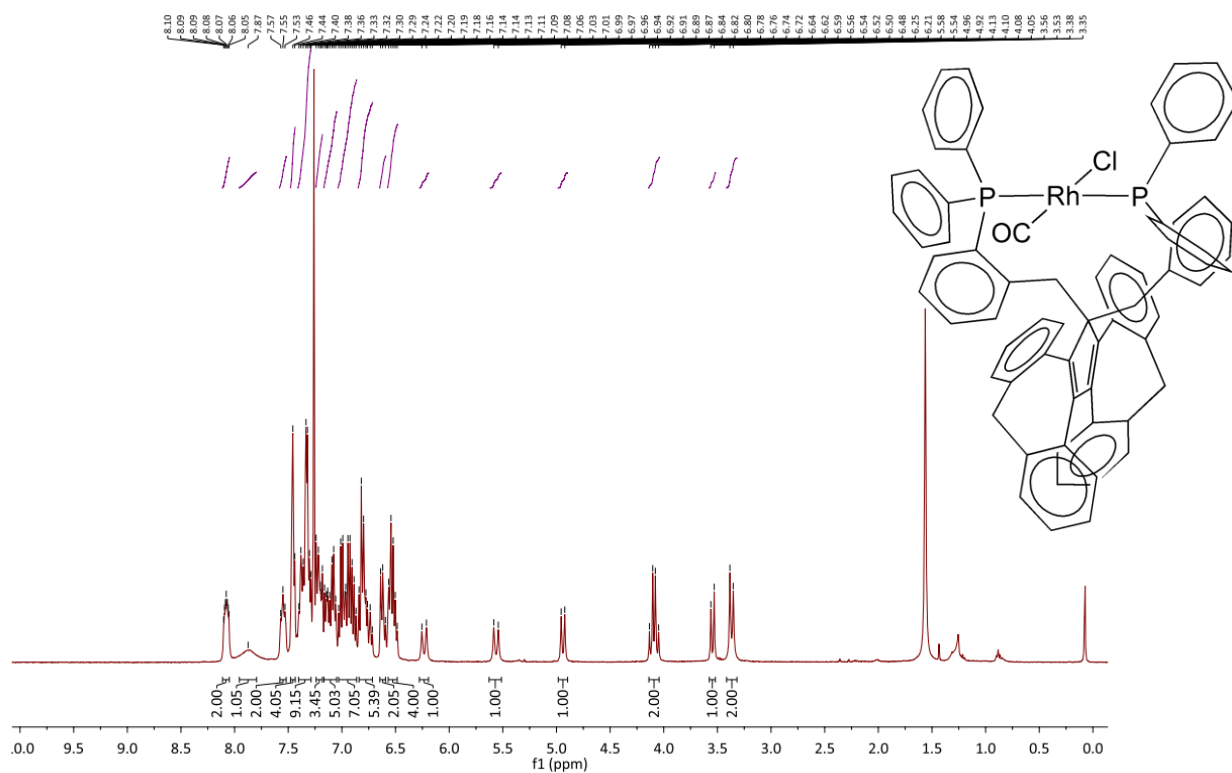


Figure S86: ¹H NMR spectrum of **10** (expanded).

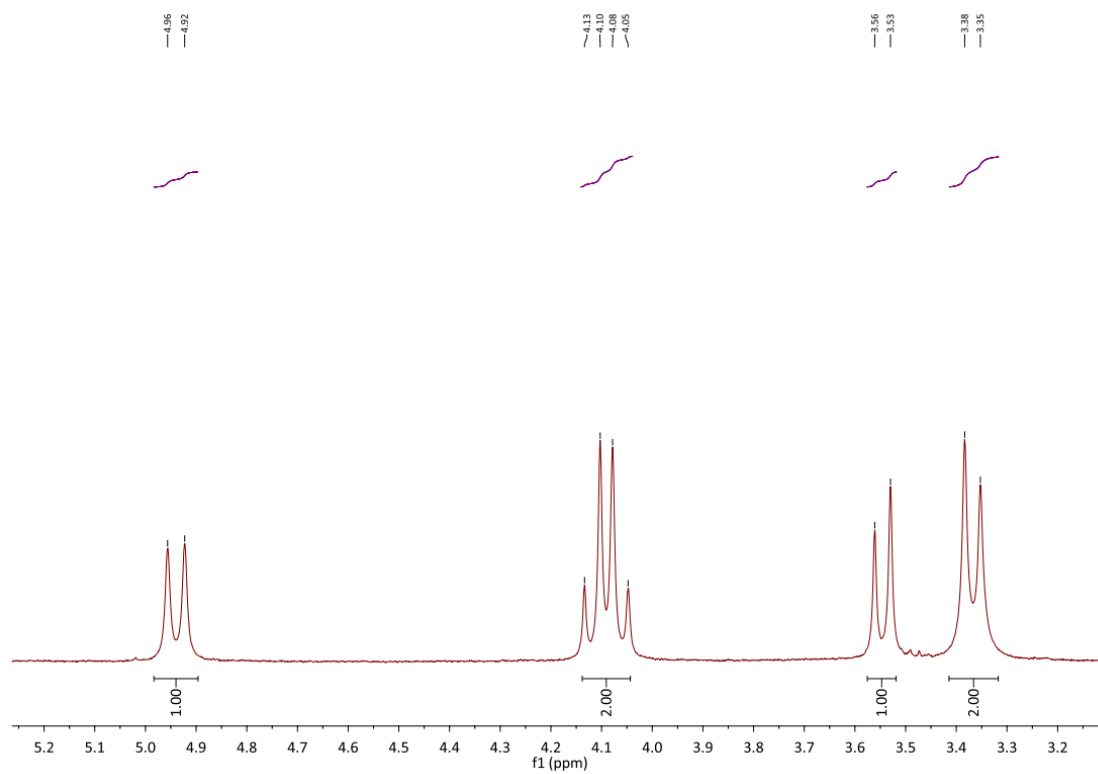


Figure S87: ^1H NMR spectrum of **10** (expanded).

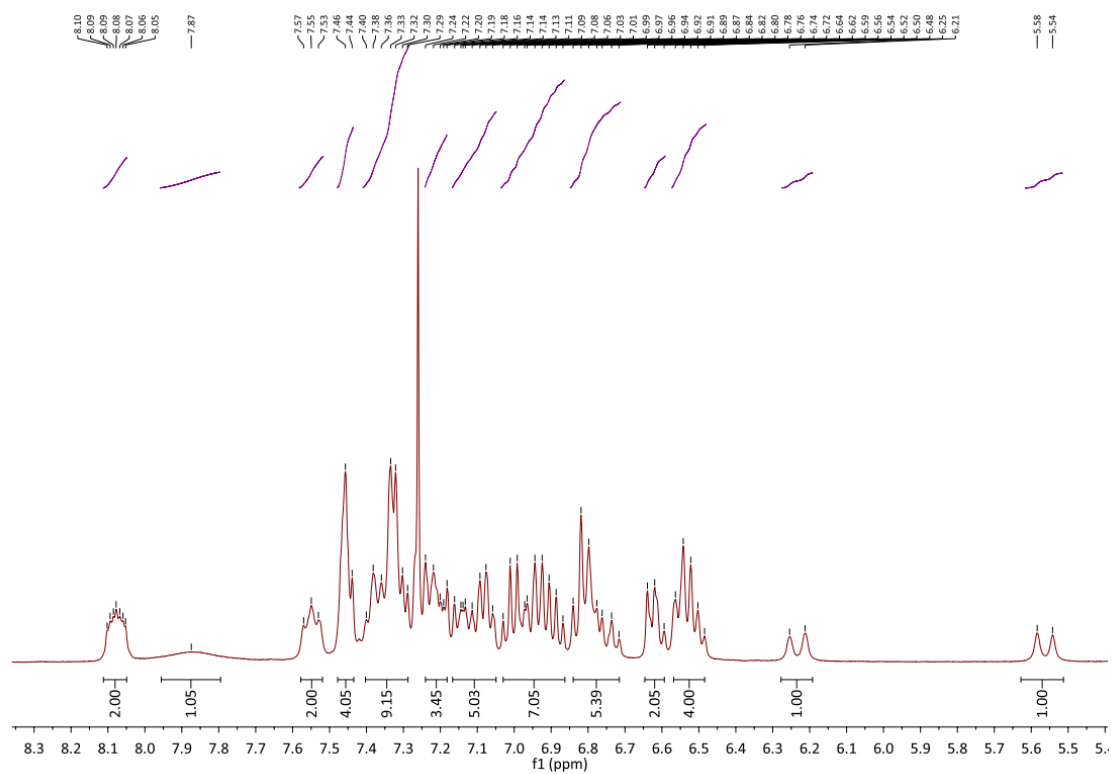


Figure S88: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **10**.

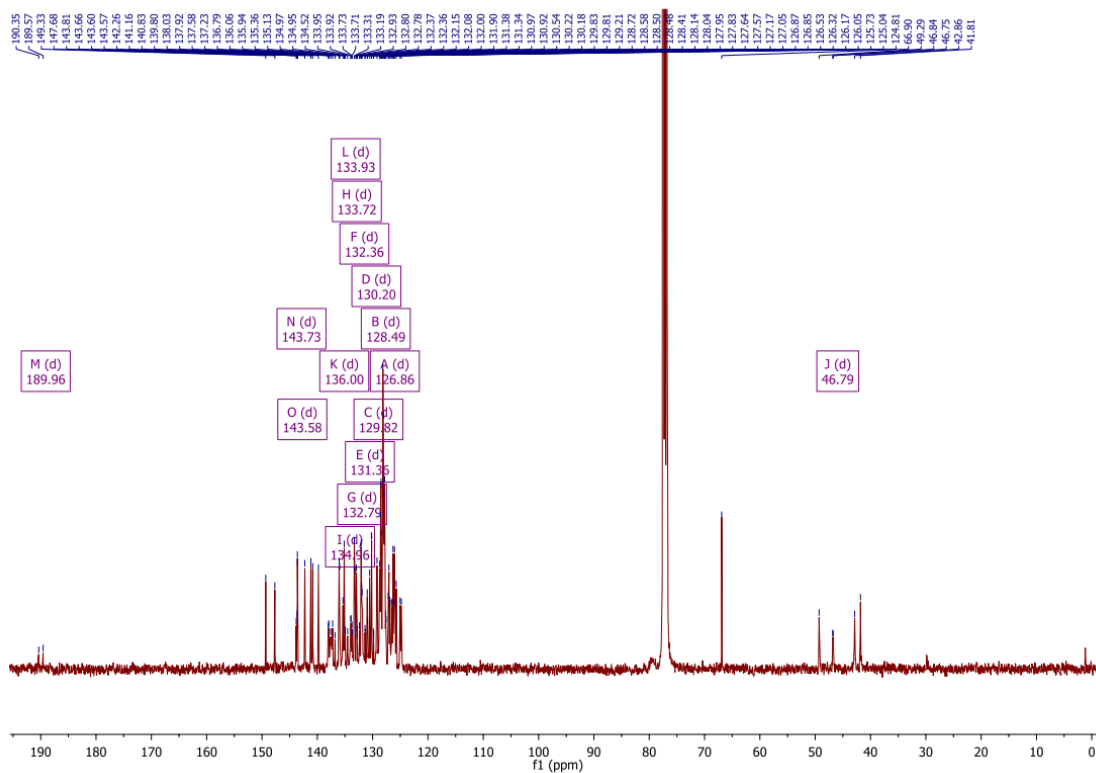


Figure S89: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **10** (expanded).

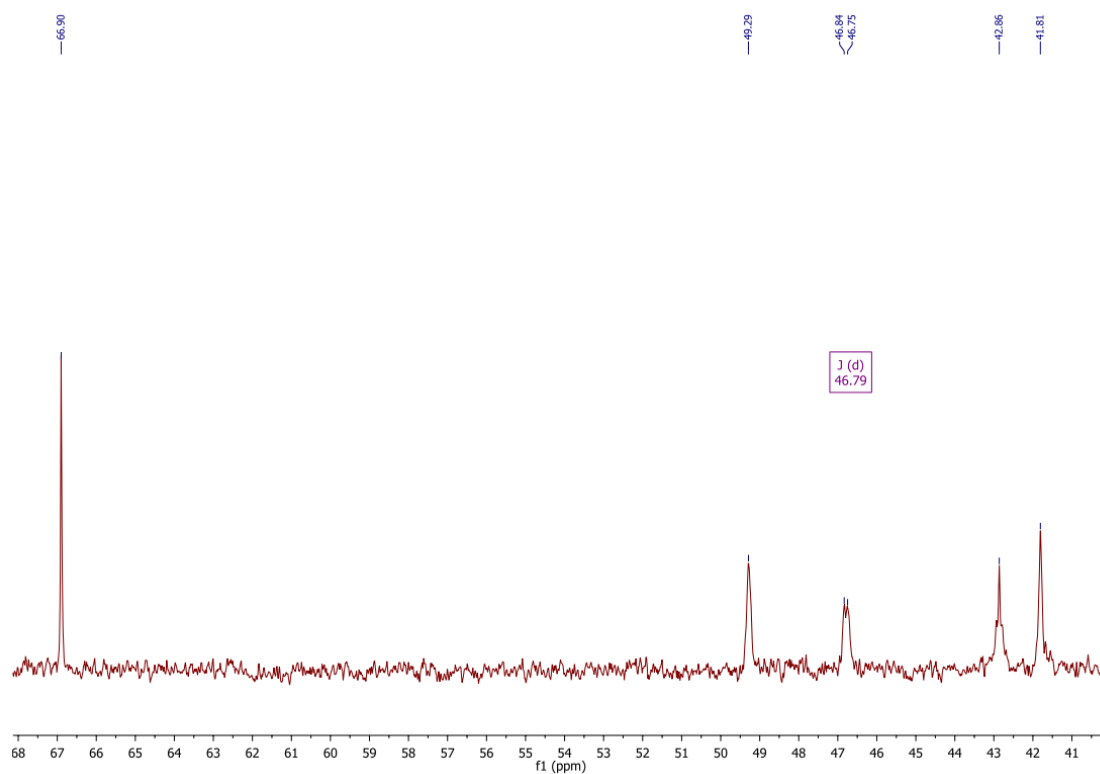


Figure S90: $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **10** (expanded).

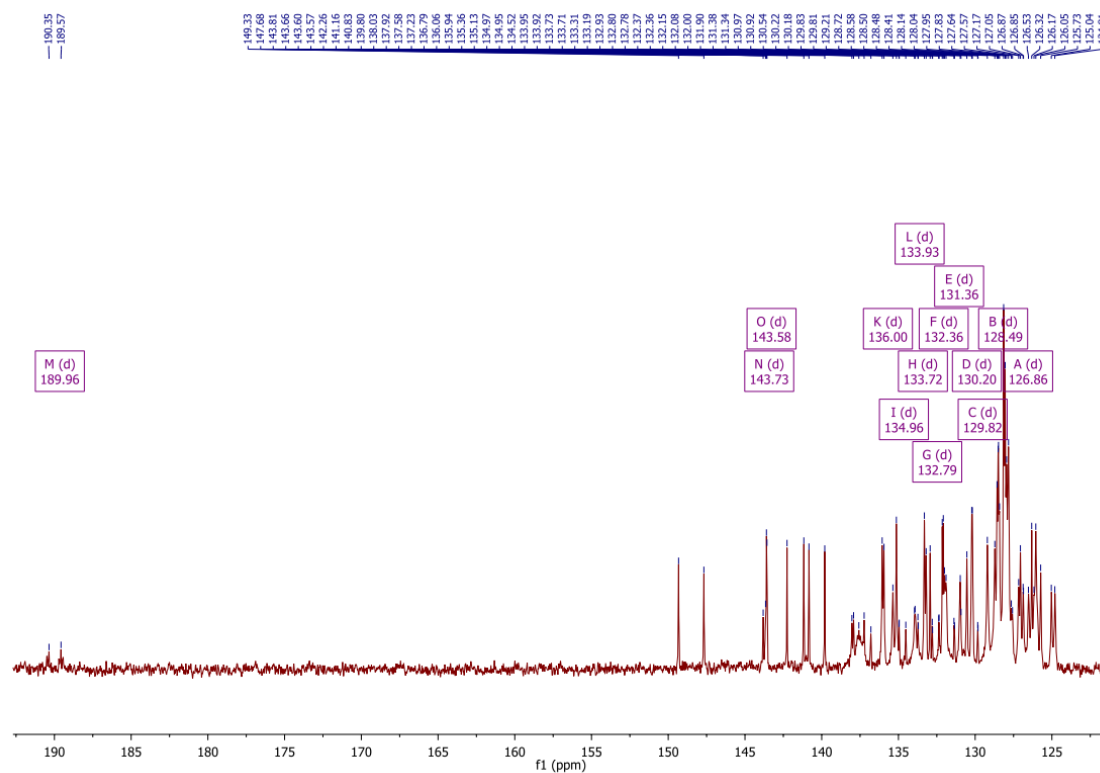


Figure S91: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **10**.

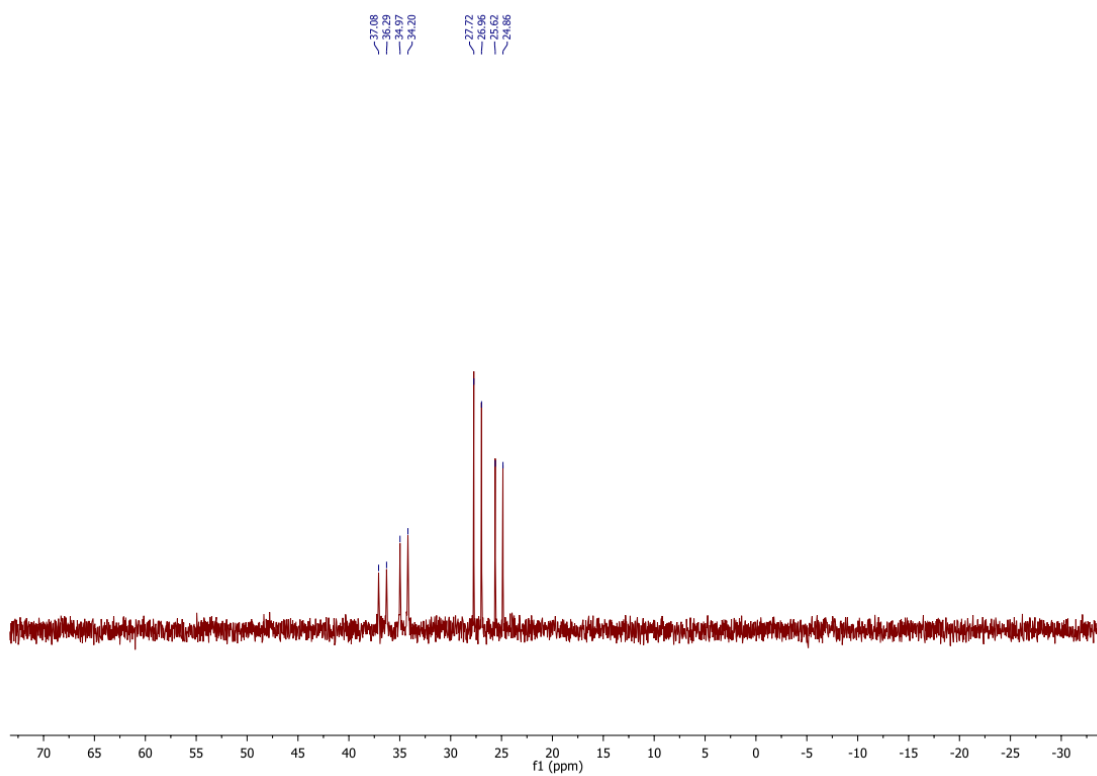


Figure S92: ^1H , ^1H -COSY NMR spectrum of **10**.

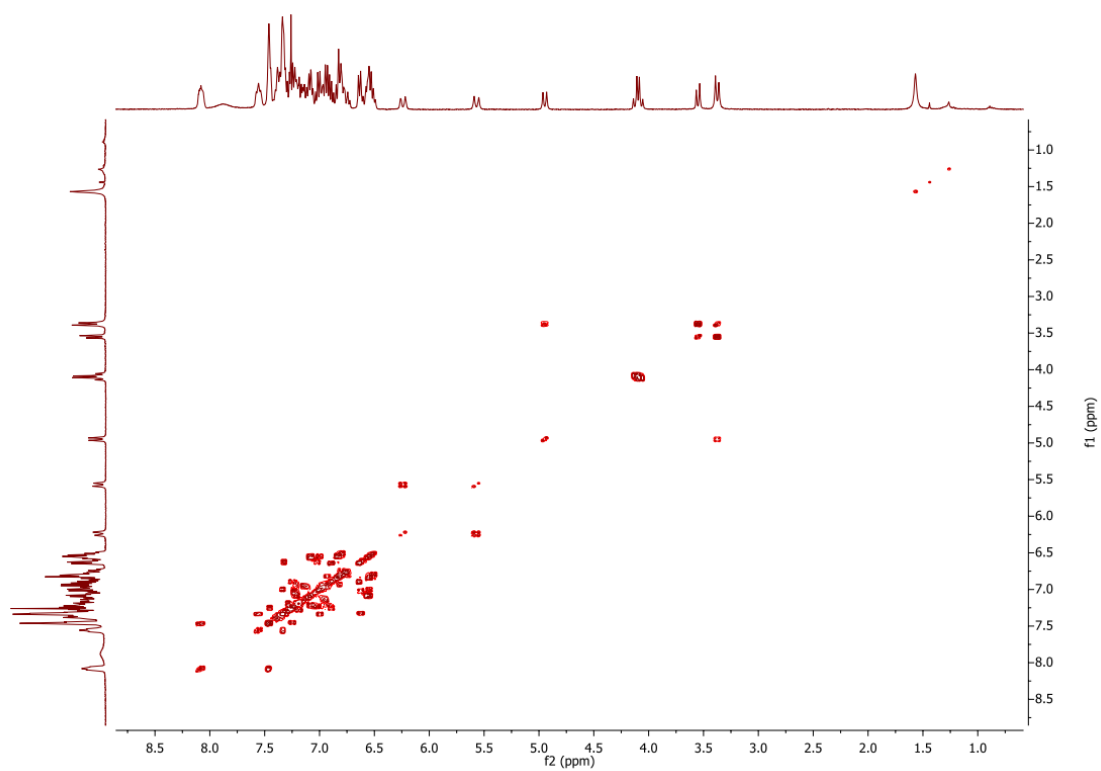


Figure S93: H,H-COSY NMR spectrum of **10** (expanded).

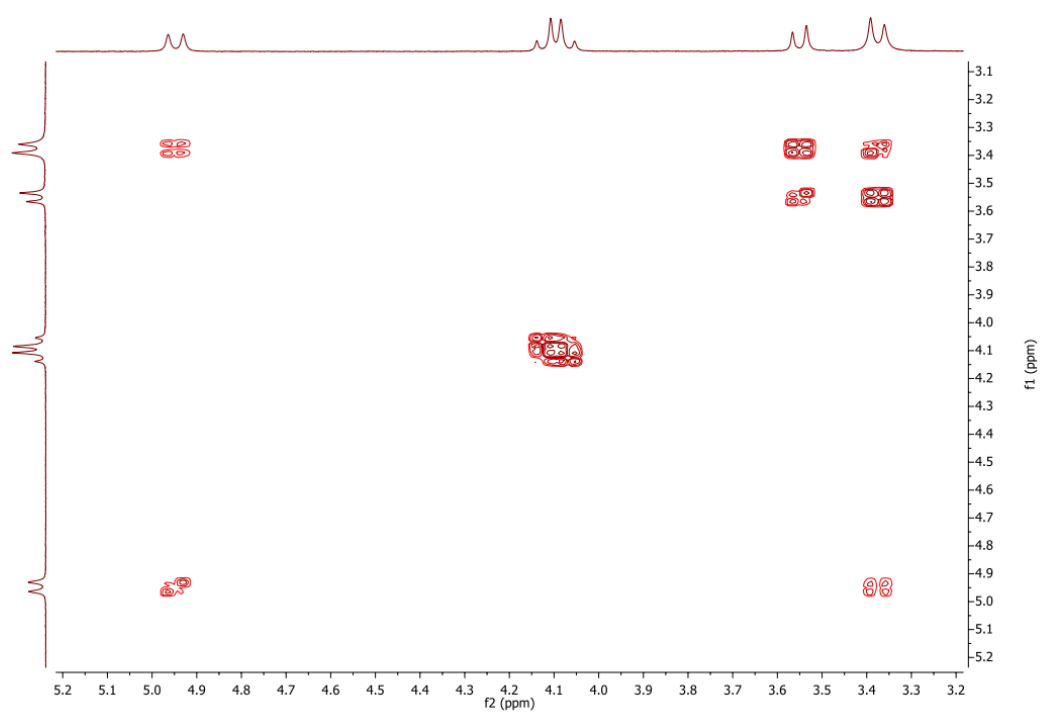


Figure S94: H,H-COSY NMR spectrum of **10** (expanded).

