

Supporting information for:

Platinum Complexes of a Boron-Rich Diphosphine Ligand

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1. Multinuclear NMR data	S2
2. Crystallography Discussion and Tables	S36
3. Density Functional Theory	S38

Figure S1. 1, ^1H NMR, C_6D_6 , 500 MHz, 298 K

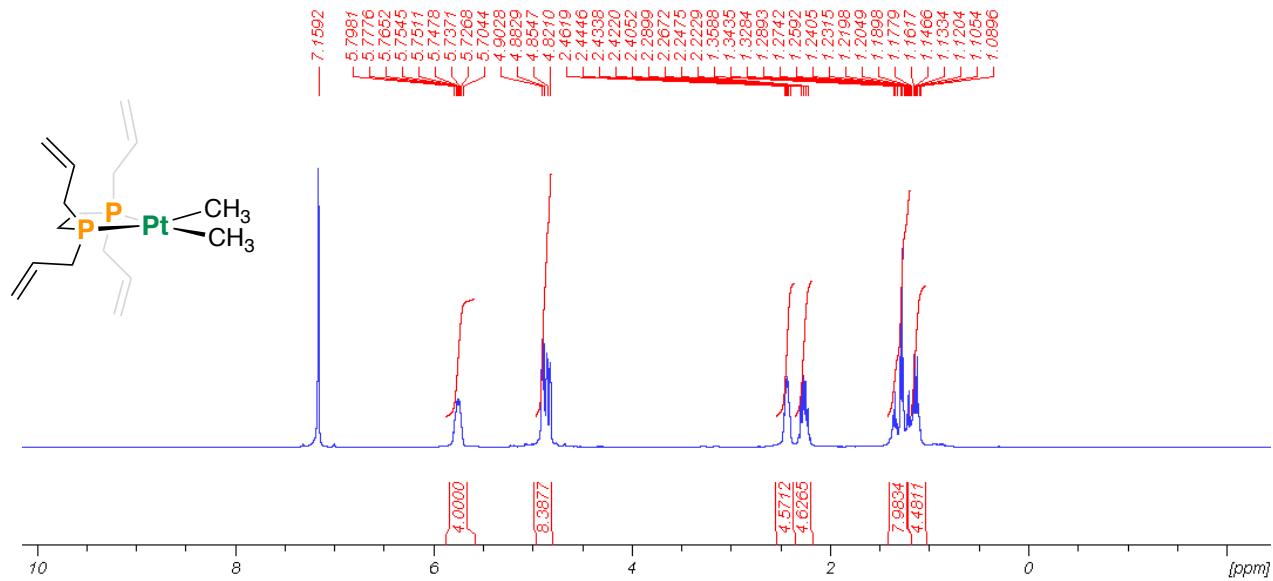


Figure S2. 1, ^1H NMR (expanded), C_6D_6 , 500 MHz, 298 K

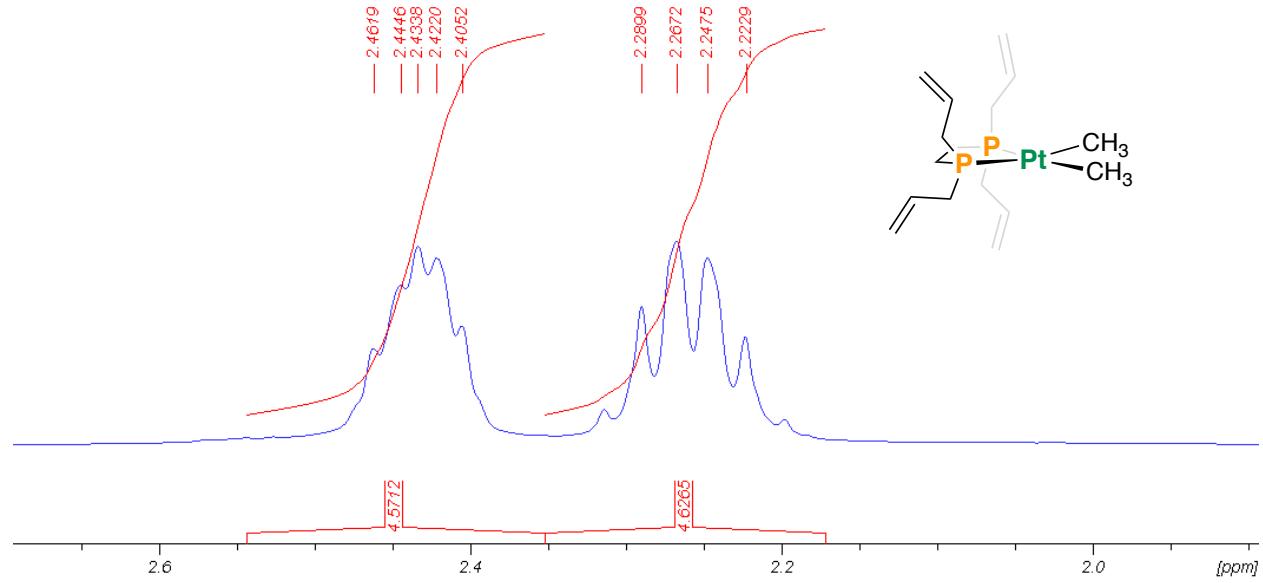


Figure S3. 1, ^1H NMR (expanded), C_6D_6 , 500 MHz, 298 K

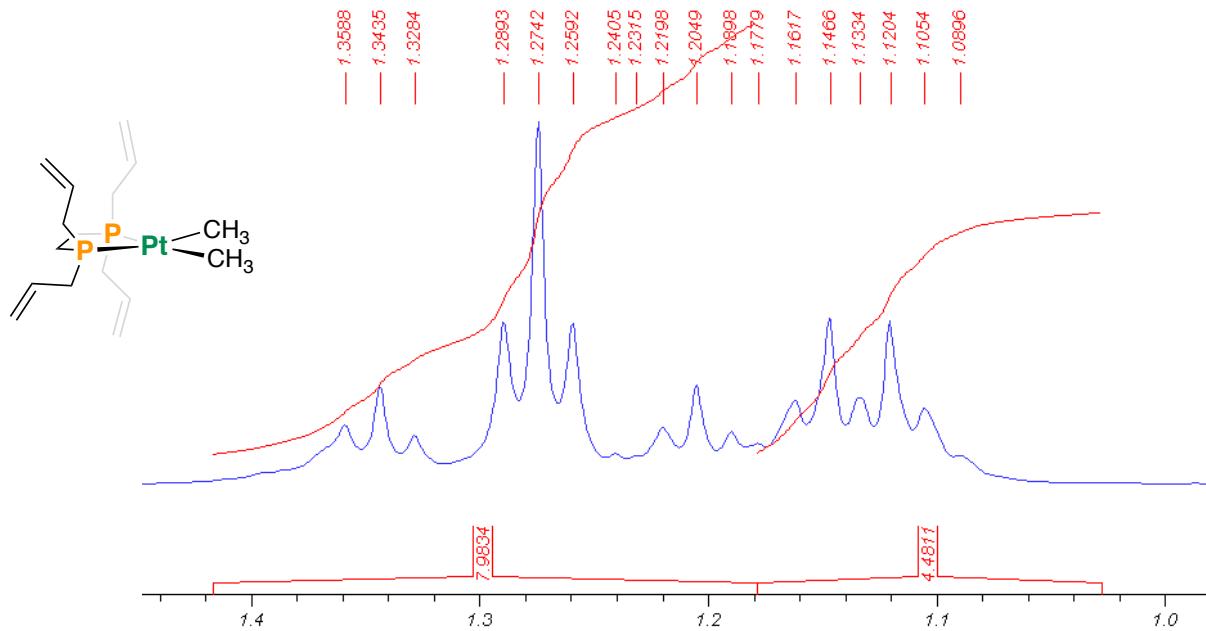


Figure S4. 1, $^{13}\text{C}\{^1\text{H}\}$ NMR, C_6D_6 , 125 MHz, 298 K

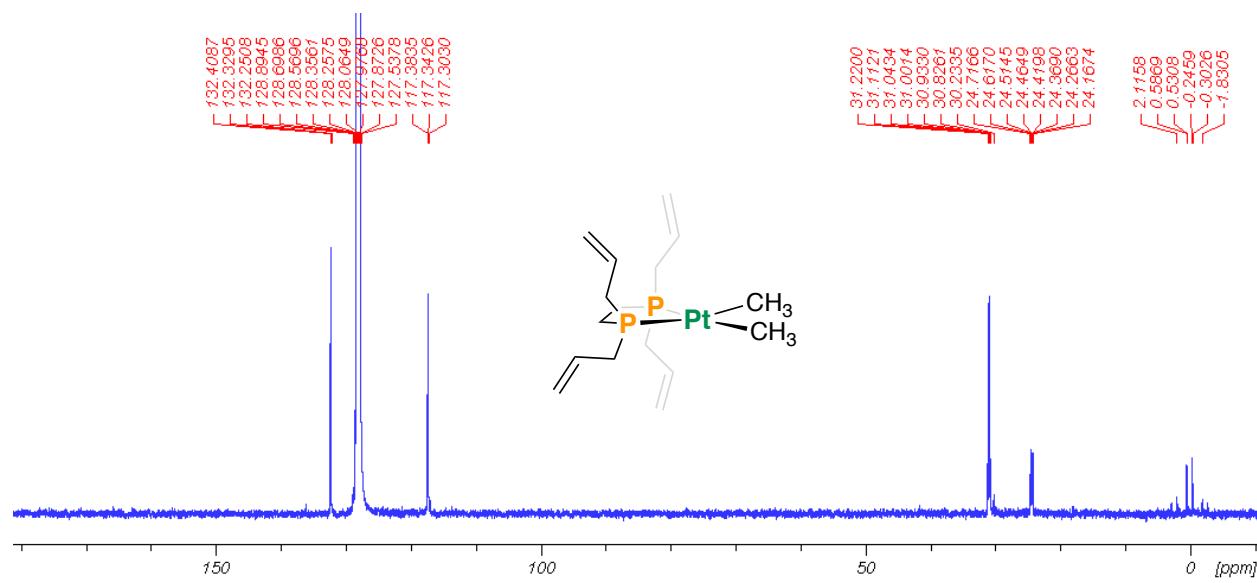


Figure S5. 1, $^{13}\text{C}\{^1\text{H}\}$ NMR (expanded), C_6D_6 , 125 MHz, 298 K

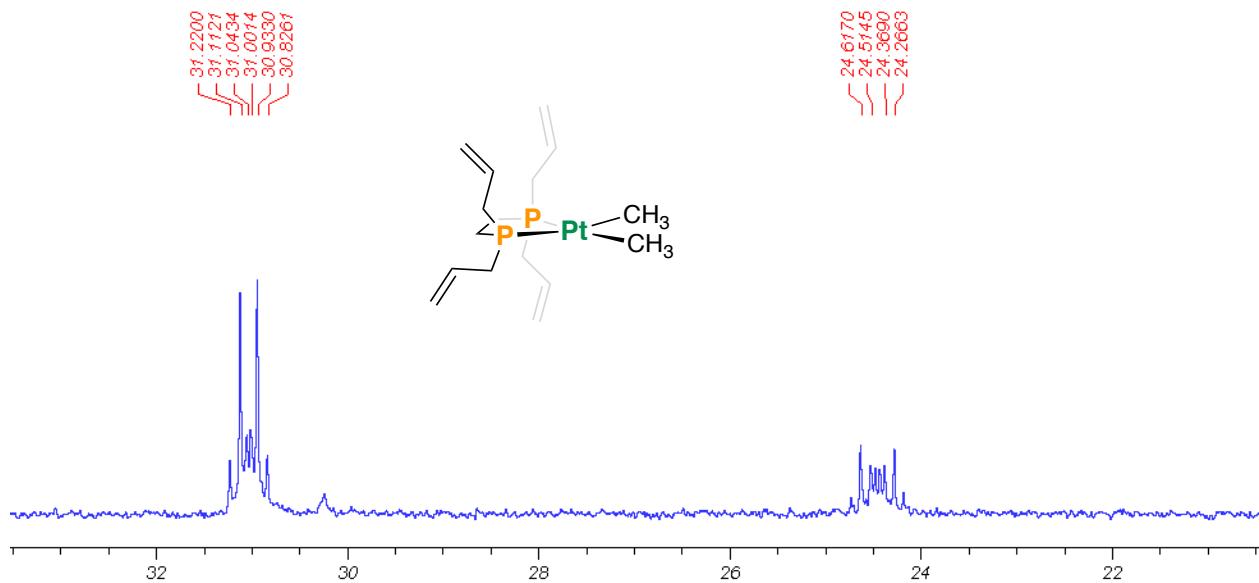


Figure S6. 1, $^{13}\text{C}\{^1\text{H}\}$ NMR (expanded), C_6D_6 , 125 MHz, 298 K for $[\text{Pt}] \text{-CH}_3$ resonance.

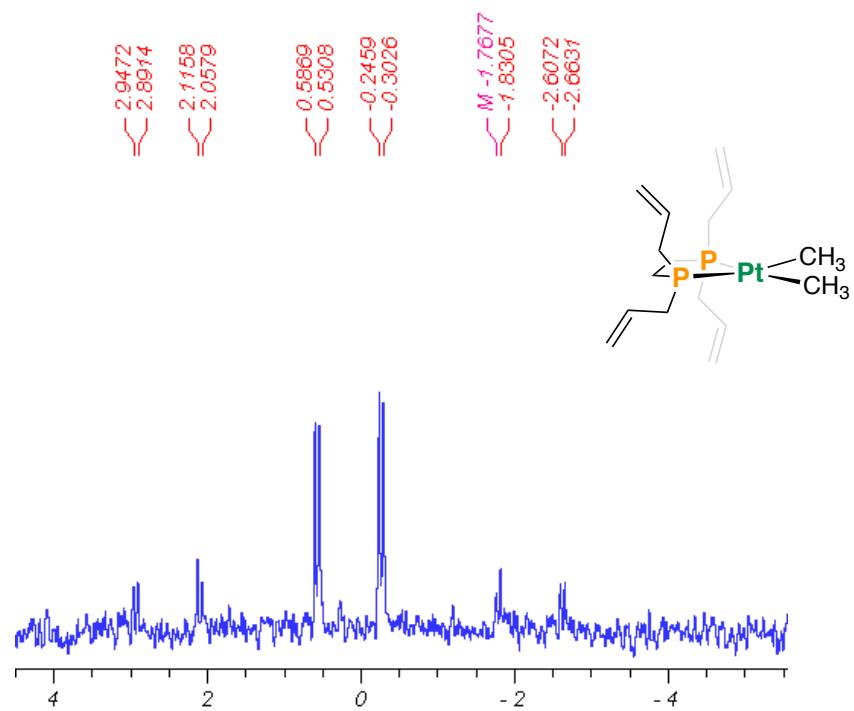


Figure S7. 1, $^{31}\text{P}\{\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K

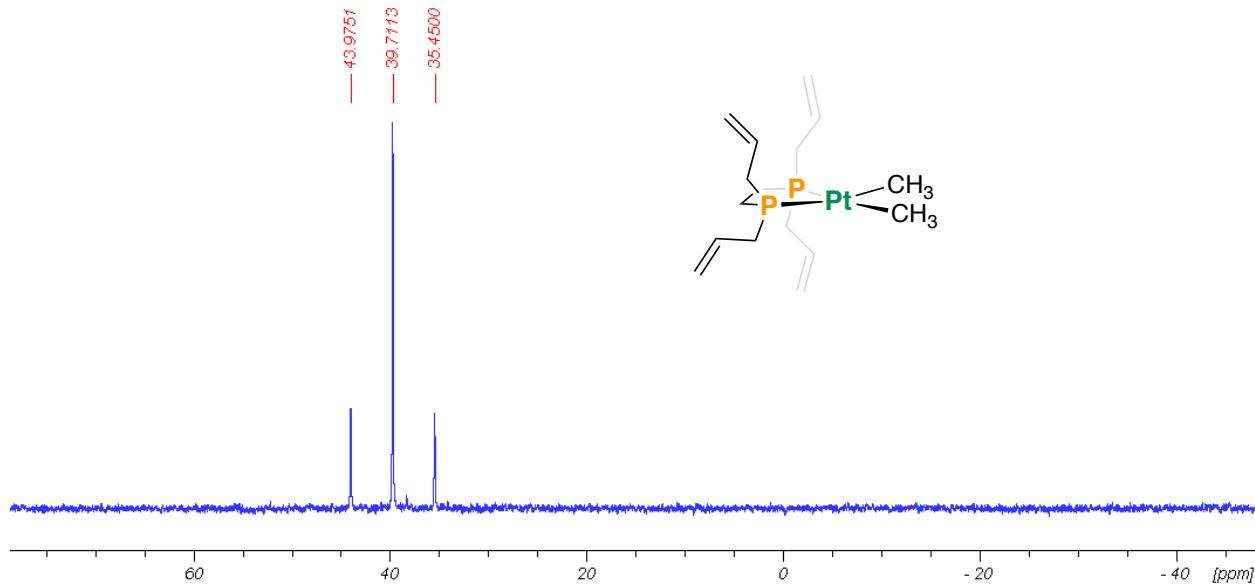


Figure S8. 2, ^1H NMR, C_6D_6 , 500 MHz, 298 K

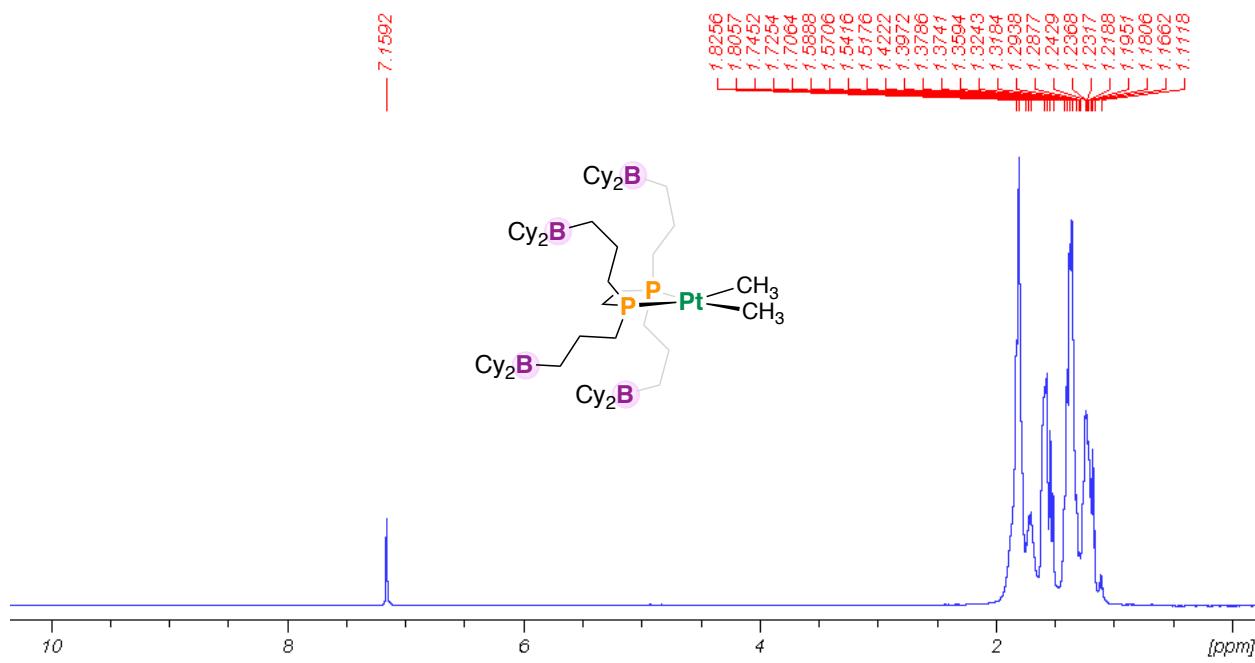


Figure S9. 2, ^1H NMR (expanded), C_6D_6 , 500 MHz, 298 K

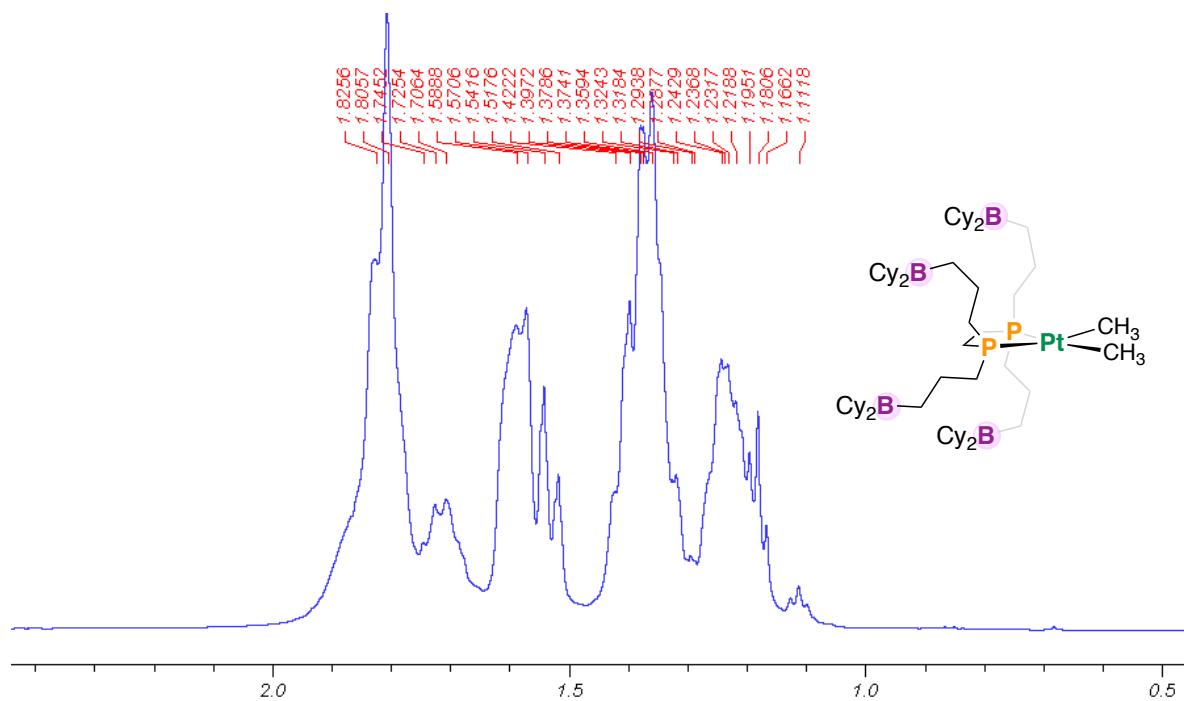


Figure S10. 2, ^1H NMR and $^1\text{H}\{^{31}\text{P}\}$ NMR, C_6D_6 , 500 MHz, 298 K. Note collapse of the $\text{Pt}-\text{CH}_3$ signal at $\delta = 1.17$ ppm.

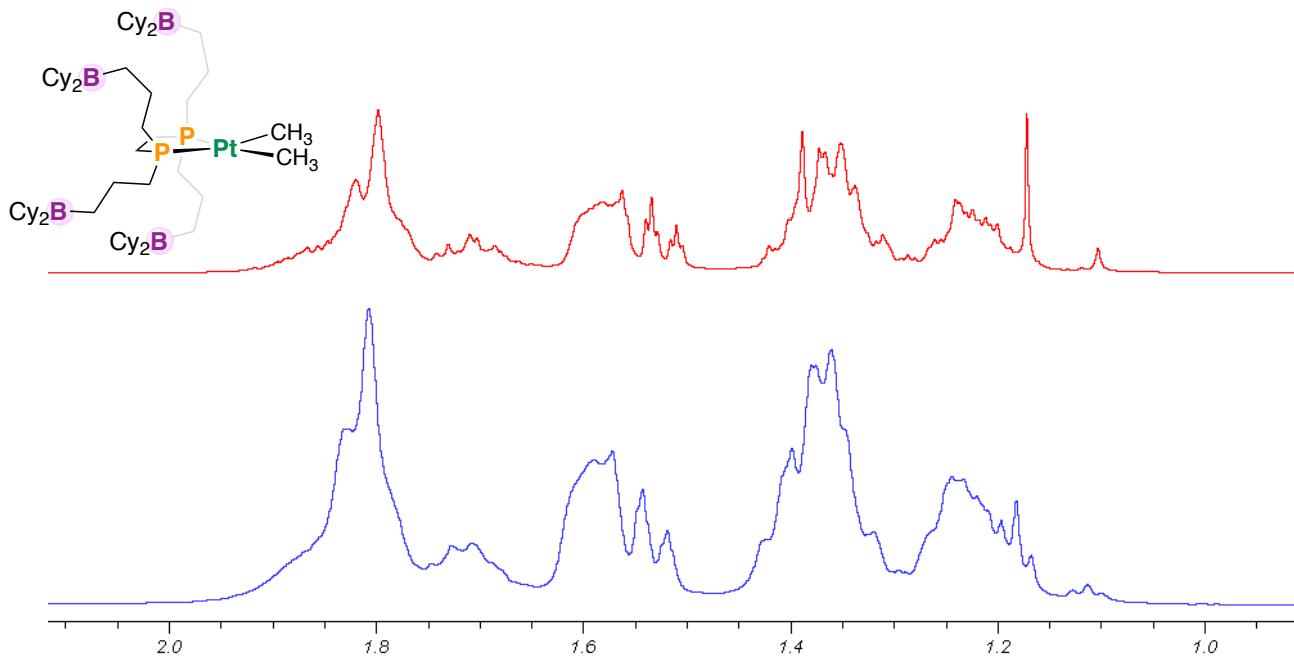


Figure S11. 2, $^{13}\text{C}\{^1\text{H}\}$ NMR, C_6D_6 , 125 MHz, 298 K

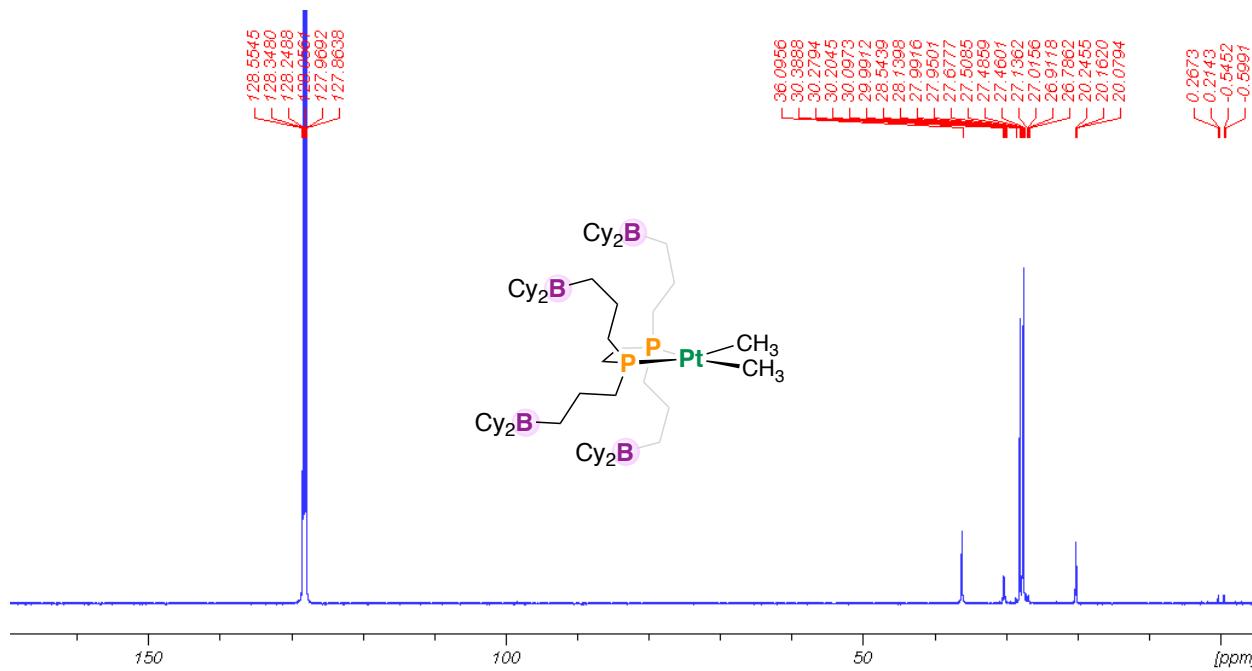


Figure S12. 2, $^{13}\text{C}^{\{1\text{H}\}}$ NMR (expanded), C_6D_6 , 125 MHz, 298 K

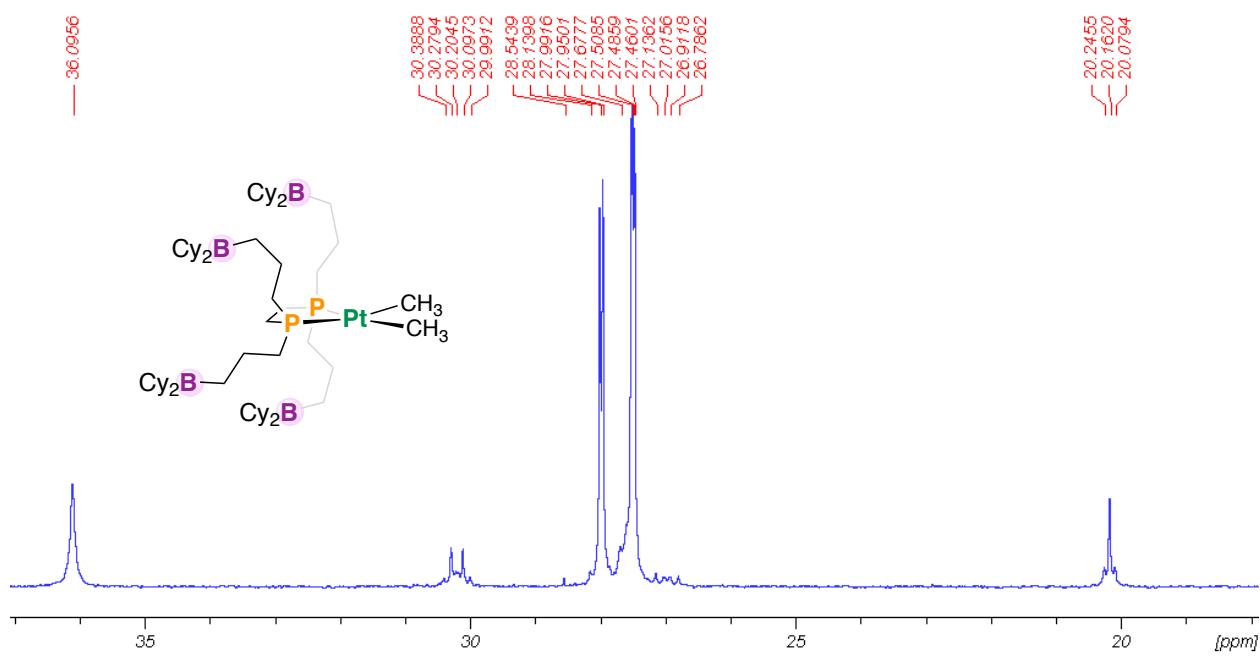


Figure S13. 2, $^{13}\text{C}\{\text{H}\}$ NMR (expanded), C_6D_6 , 125 MHz, 298 K for [Pt]- CH_3 resonance.

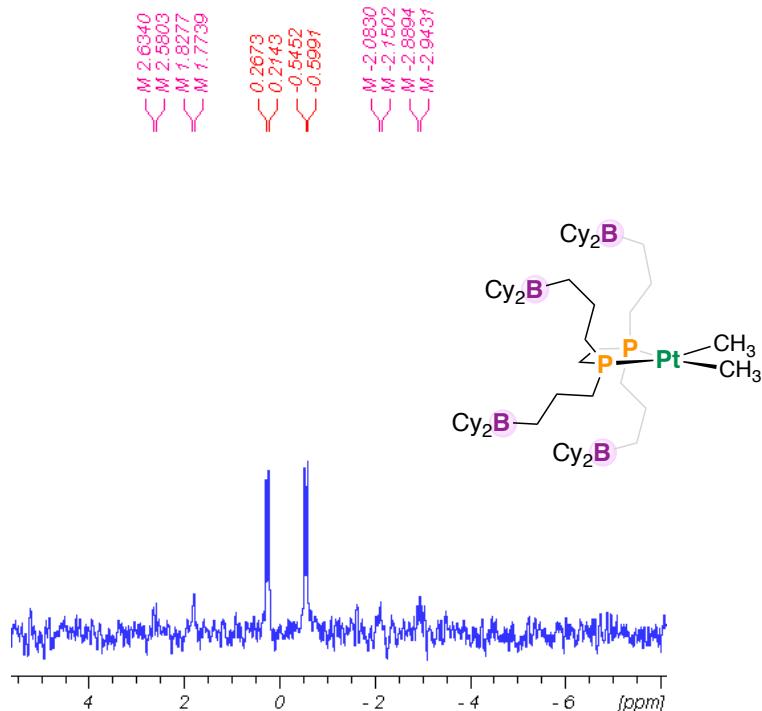


Figure S14. 2, $^{31}\text{P}\{\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K

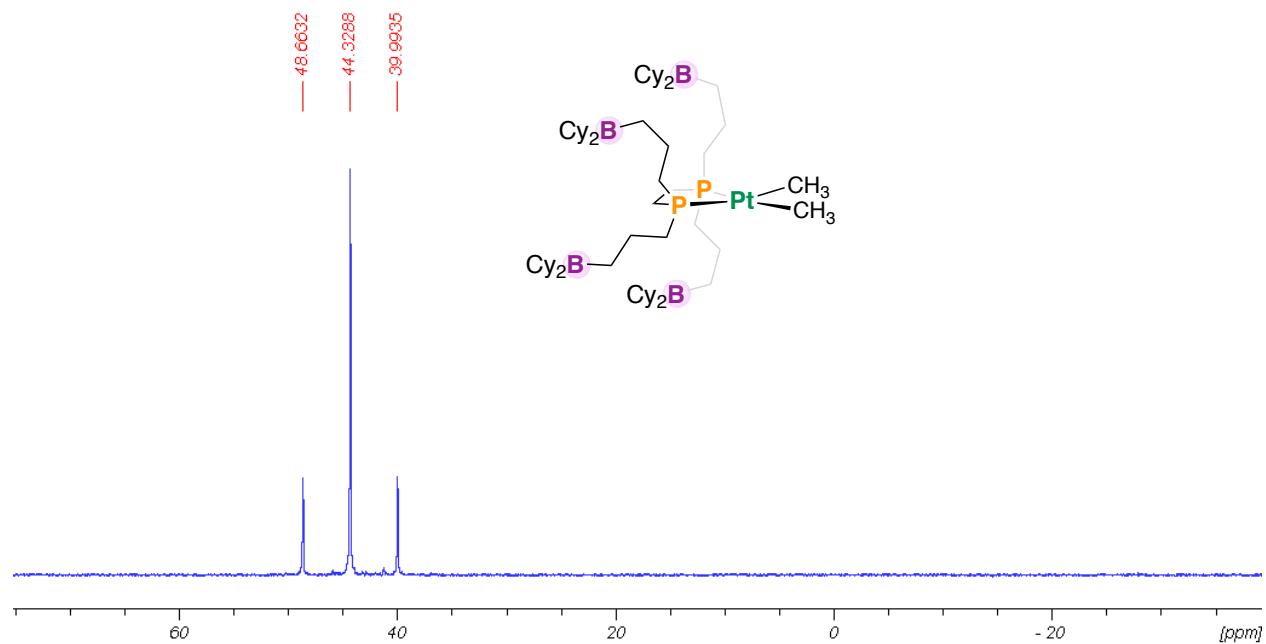


Figure S15. 2, $^{11}\text{B}\{\text{H}\}$ NMR, C_6D_6 , 160.5 MHz, 298 K

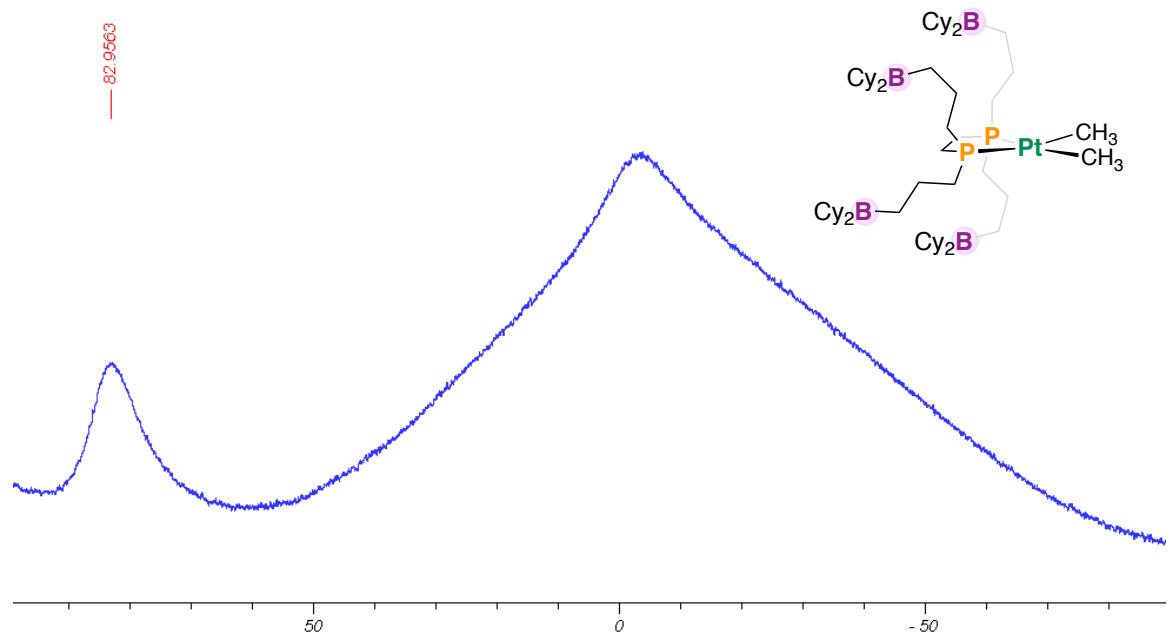


Figure S16. 3, ^1H NMR, C_6D_6 , 500 MHz, 298 K

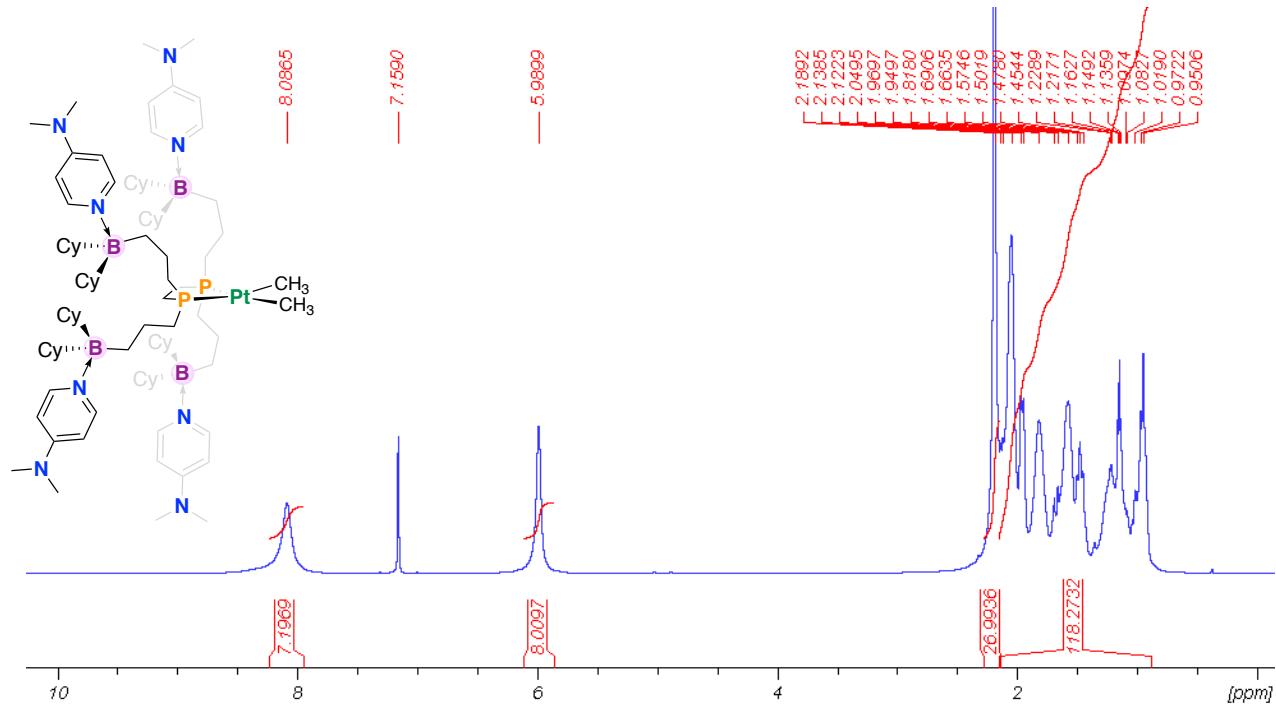


Figure S17. 3, ^1H NMR (expanded), C_6D_6 , 500 MHz, 298 K

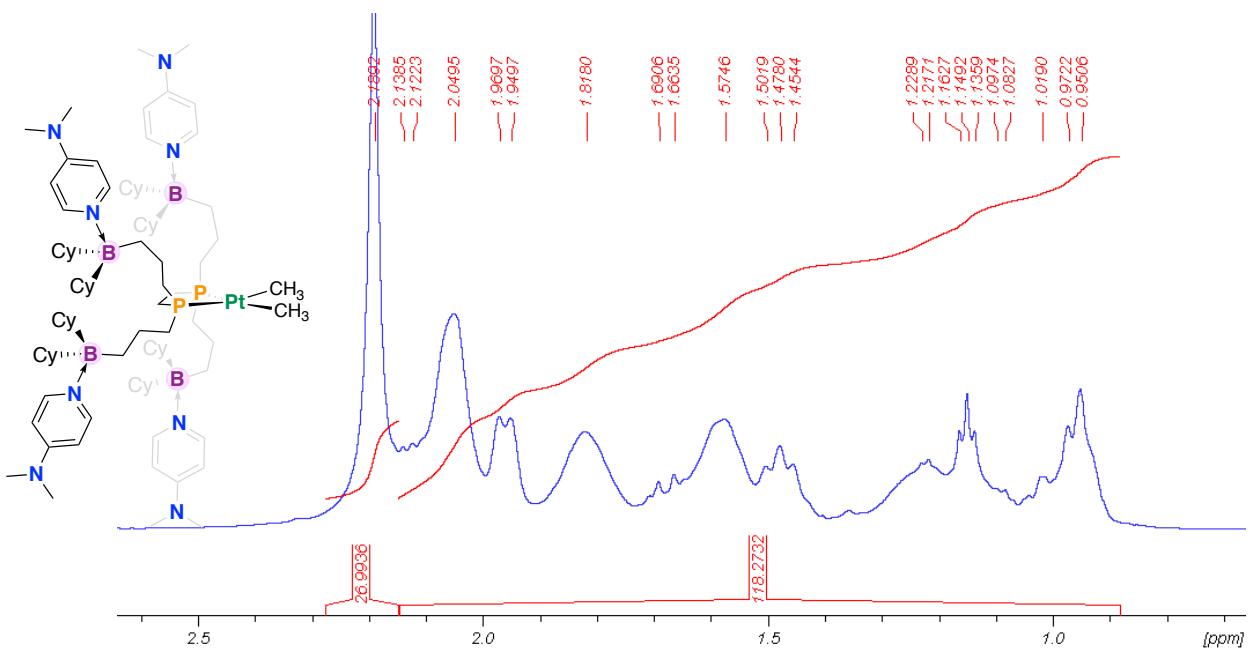


Figure S18. 3, ^1H NMR and $^1\text{H}\{^{31}\text{P}\}$ NMR, C_6D_6 , 500 MHz, 298 K. Note collapse of the $\text{Pt}-\text{CH}_3$ signal at $\delta = 1.15$ ppm.

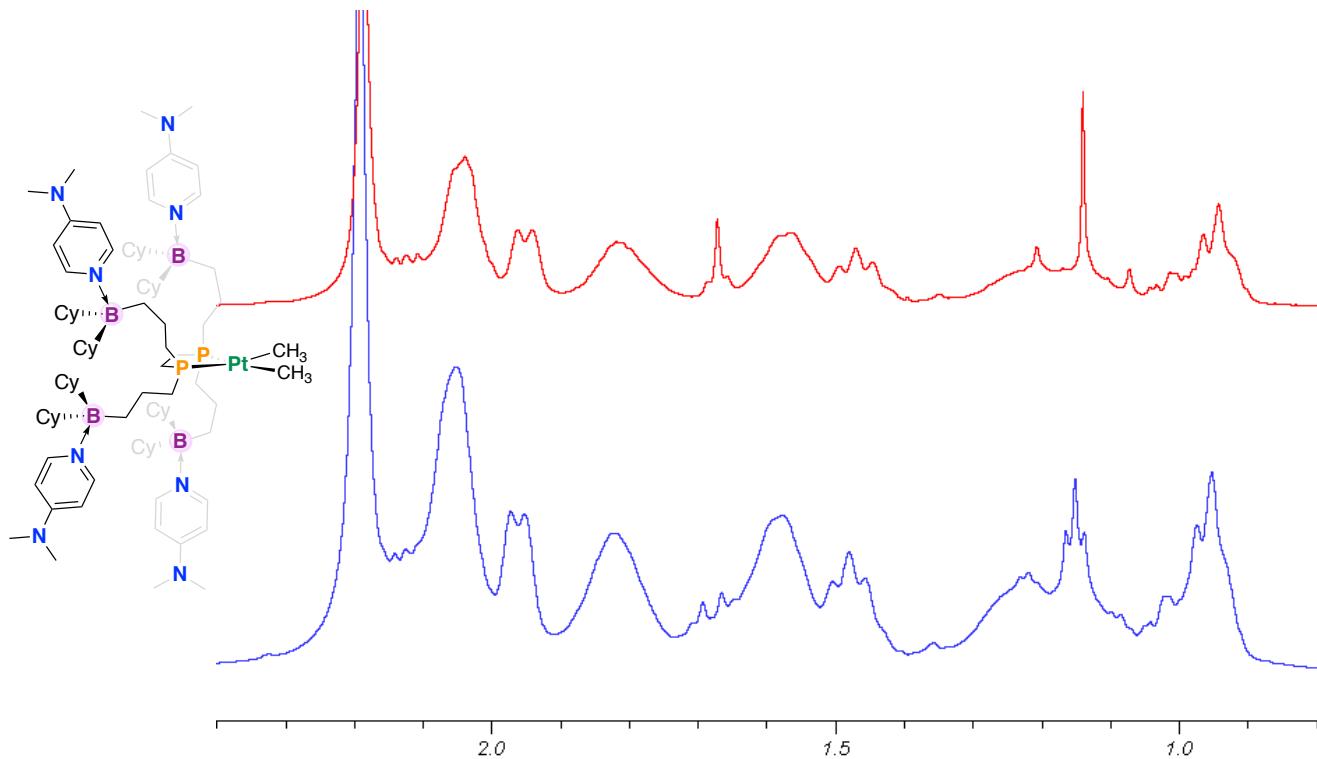


Figure S19. 3, $^{13}\text{C}\{^1\text{H}\}$ NMR, C_6D_6 , 125 MHz, 298 K

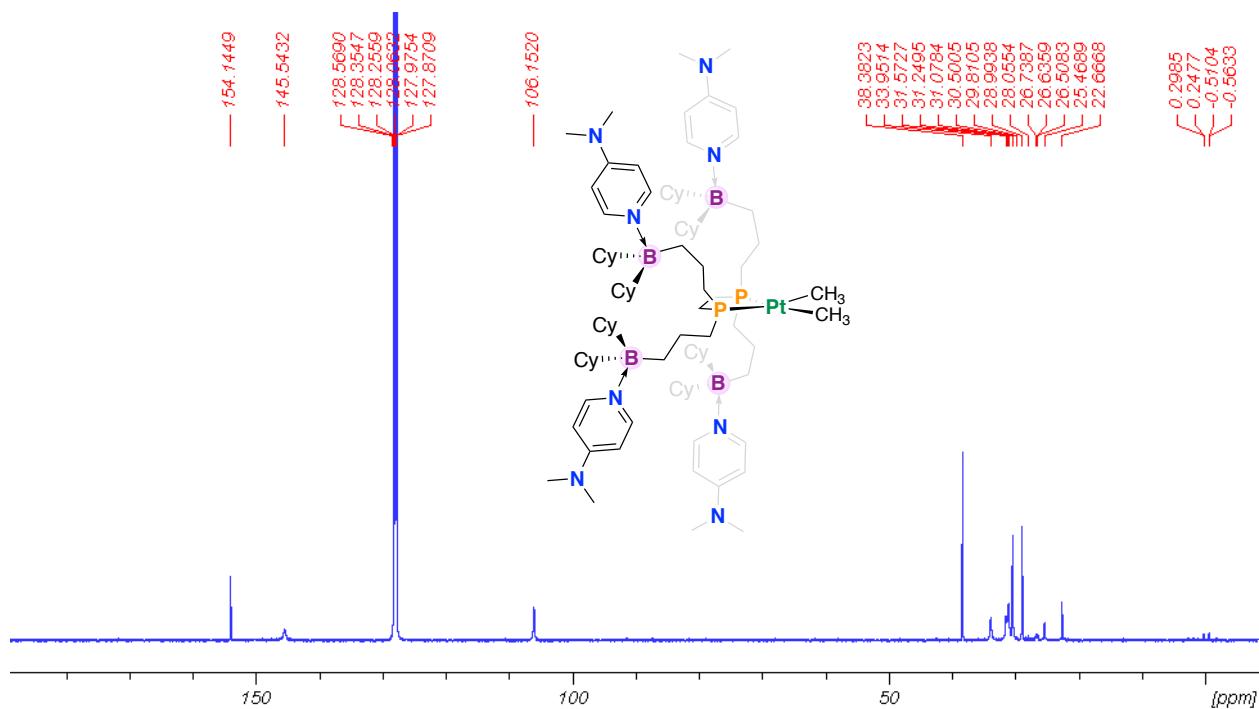


Figure S20. 3, $^{13}\text{C}\{^1\text{H}\}$ NMR (expanded), C_6D_6 , 125 MHz, 298 K

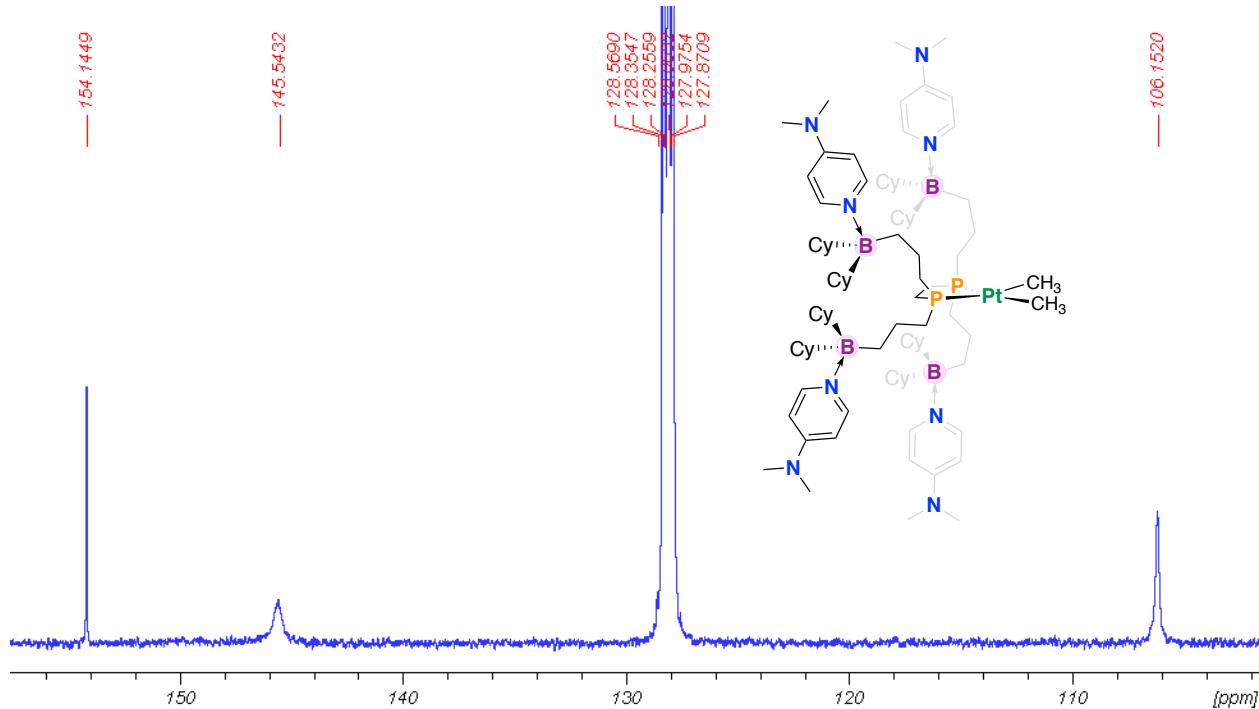


Figure S21. 3, $^{13}\text{C}\{\text{H}\}$ NMR (expanded), C_6D_6 , 125 MHz, 298 K

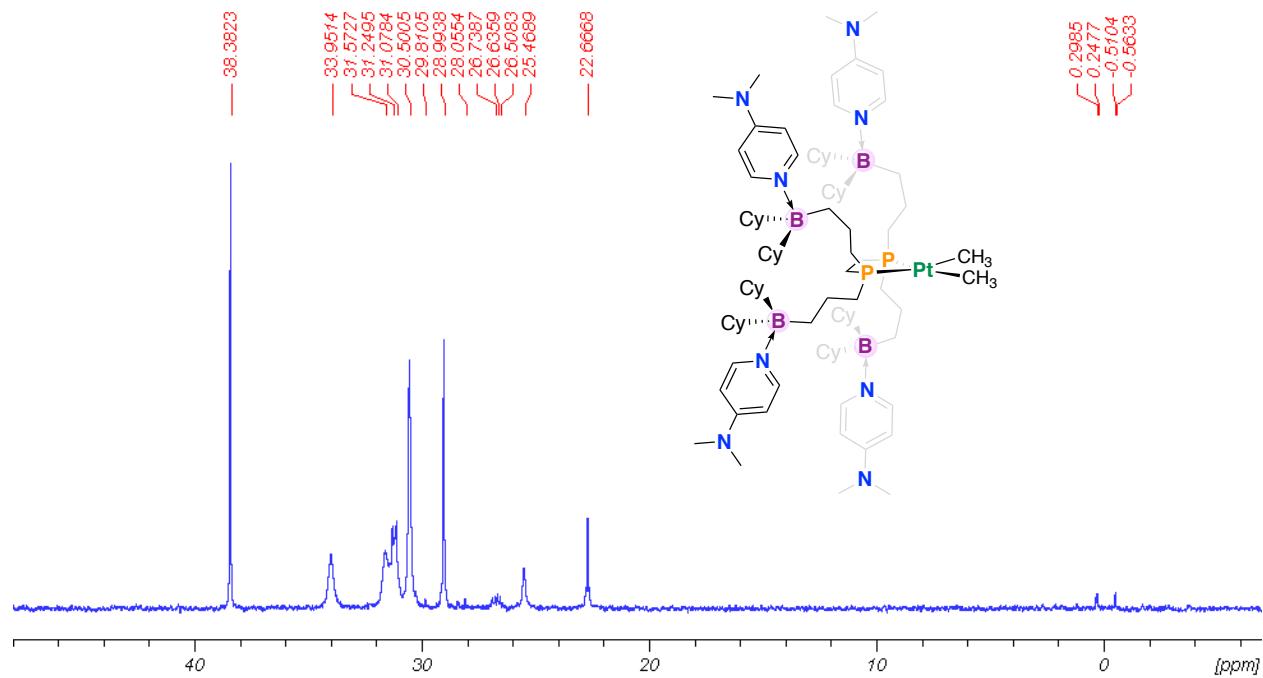


Figure S22. 3, $^{31}\text{P}\{\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K

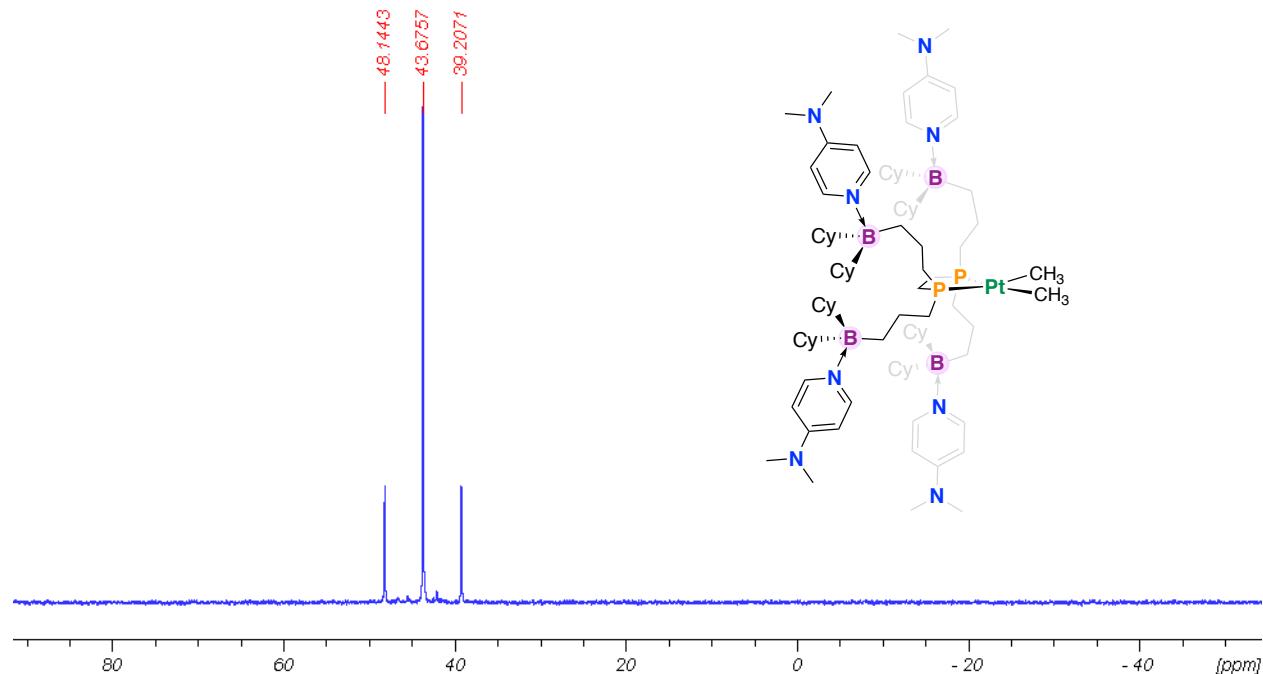


Figure S23. 3, $^{11}\text{B}\{\text{H}\}$ NMR, C_6D_6 , 160.5 MHz, 298 K

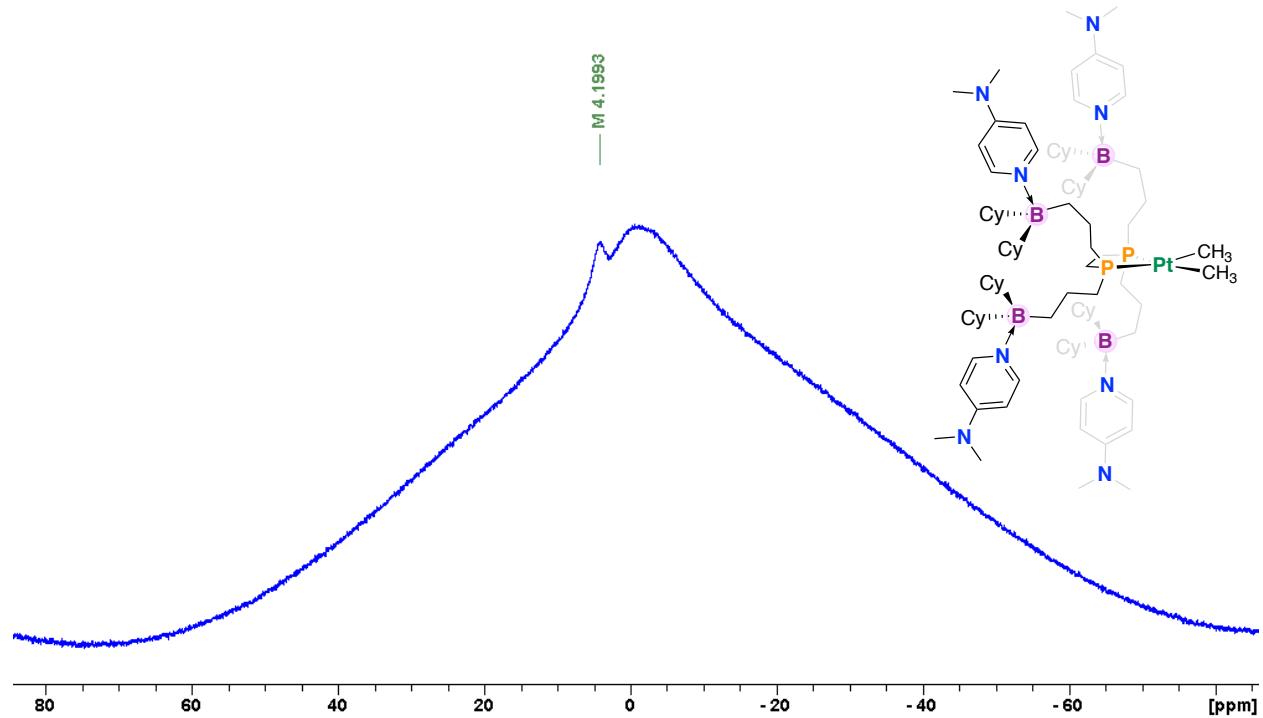


Figure S24. Stacked ^1H NMR of **2** and **3** (C_6D_6 , 500 MHz, 298 K), showing dispersion of ^1H NMR signals associated with propyl linkers and Cy rings, following binding of DMAP.

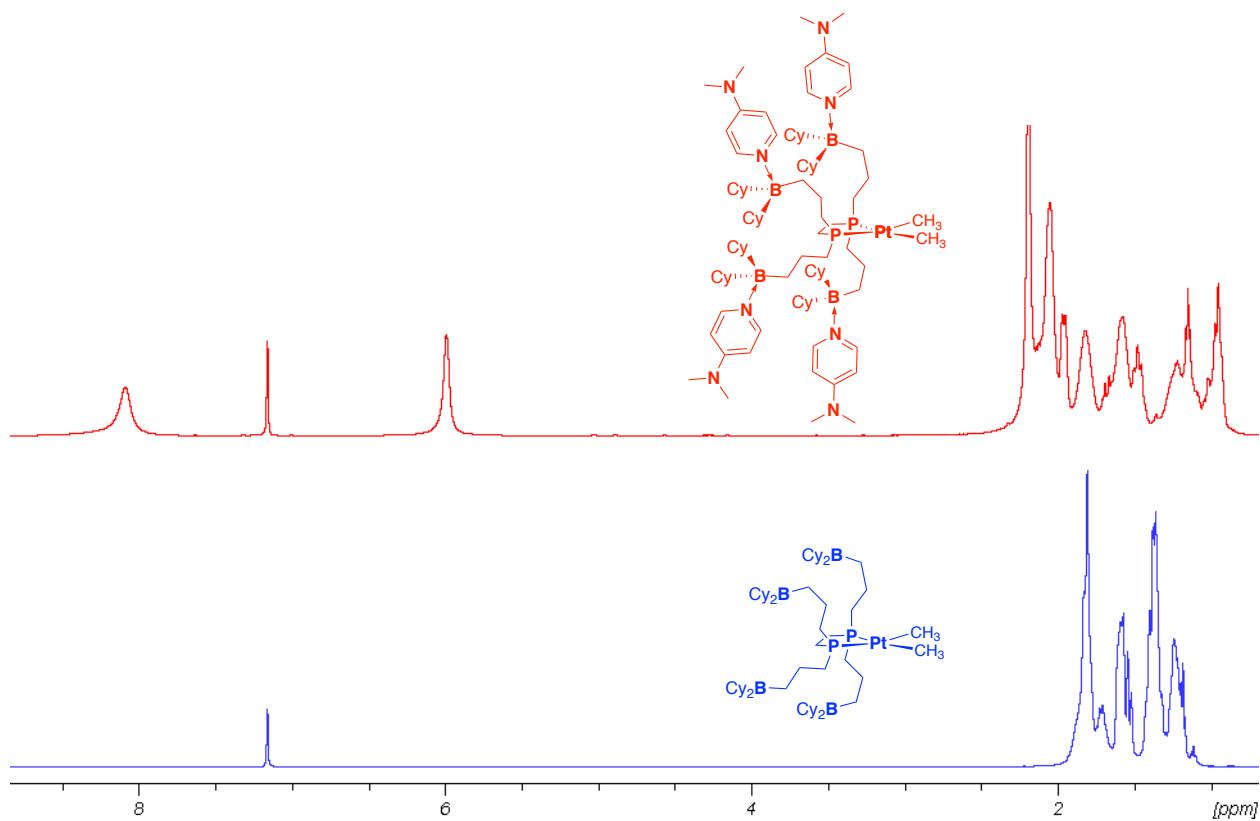


Figure S25. Stacked $^{13}\text{C}\{^1\text{H}\}$ NMR of **2** and **3**, 125 MHz, 298 K (signal at $\delta = 38.38$ in blue spectrum due to coordinated DMAP), showing dispersion of ^{13}C NMR signals associated with propyl linkers and Cy rings, following binding of DMAP.

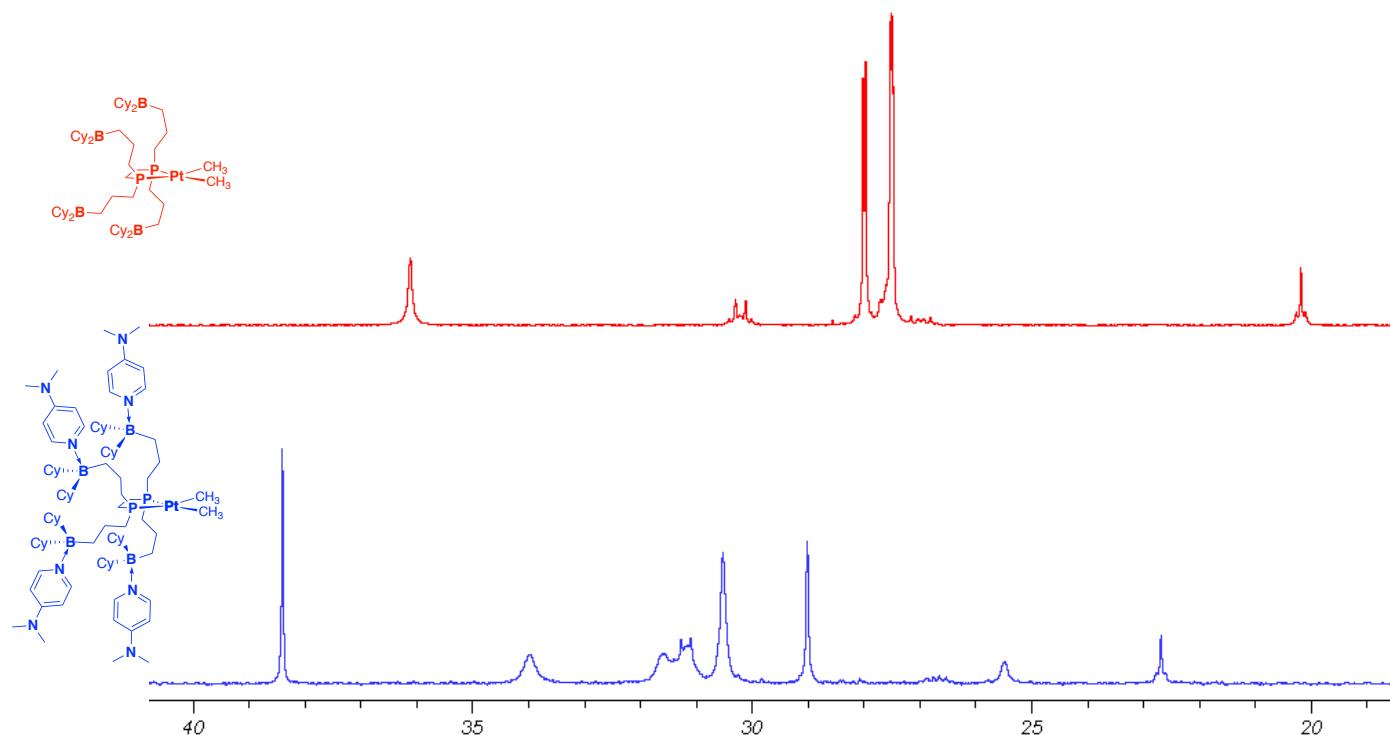


Figure S26. Stacked $^{31}\text{P}\{\text{H}\}$ NMR of **1**, **2**, and **3** (C_6D_6 , 203 MHz, 298 K).

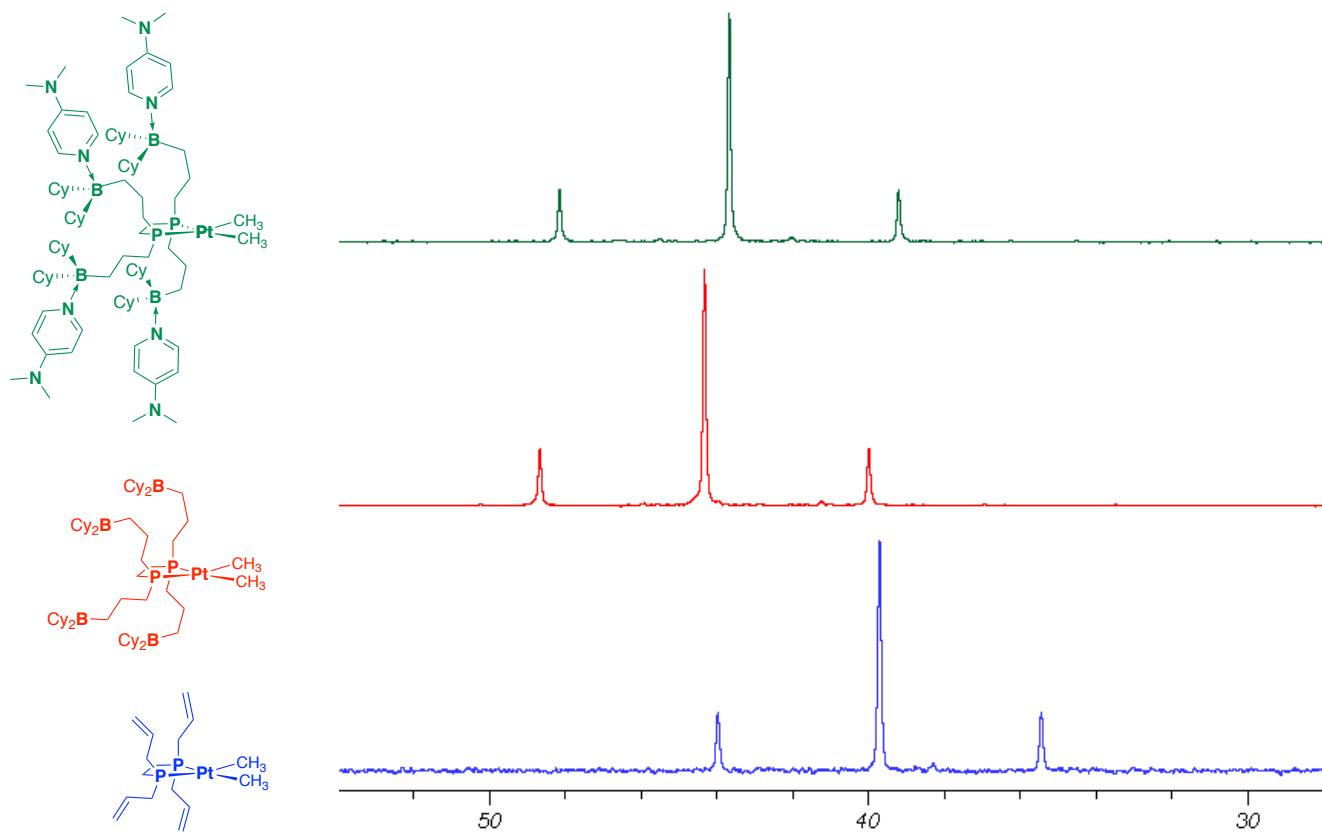


Figure S27. 4, ^1H NMR, C_6D_6 , 500 MHz, 298 K

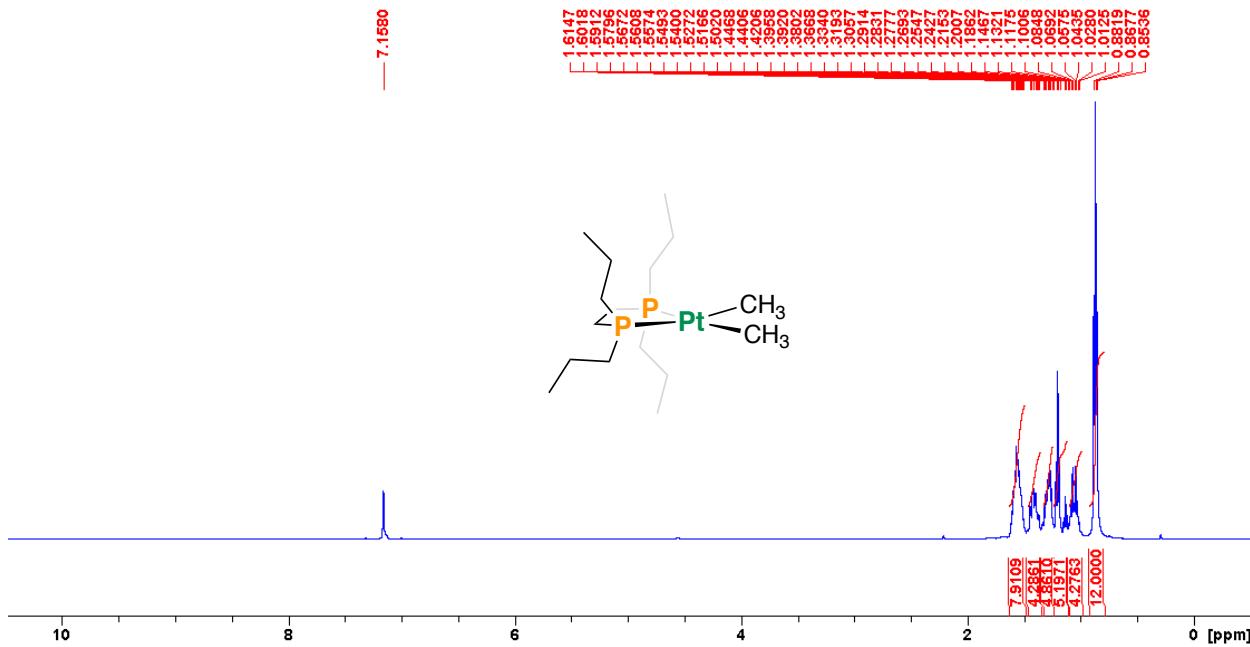


Figure S28. 4. $^{13}\text{C}\{\text{H}\}$ NMR, C_6D_6 , 125 MHz, 298 K

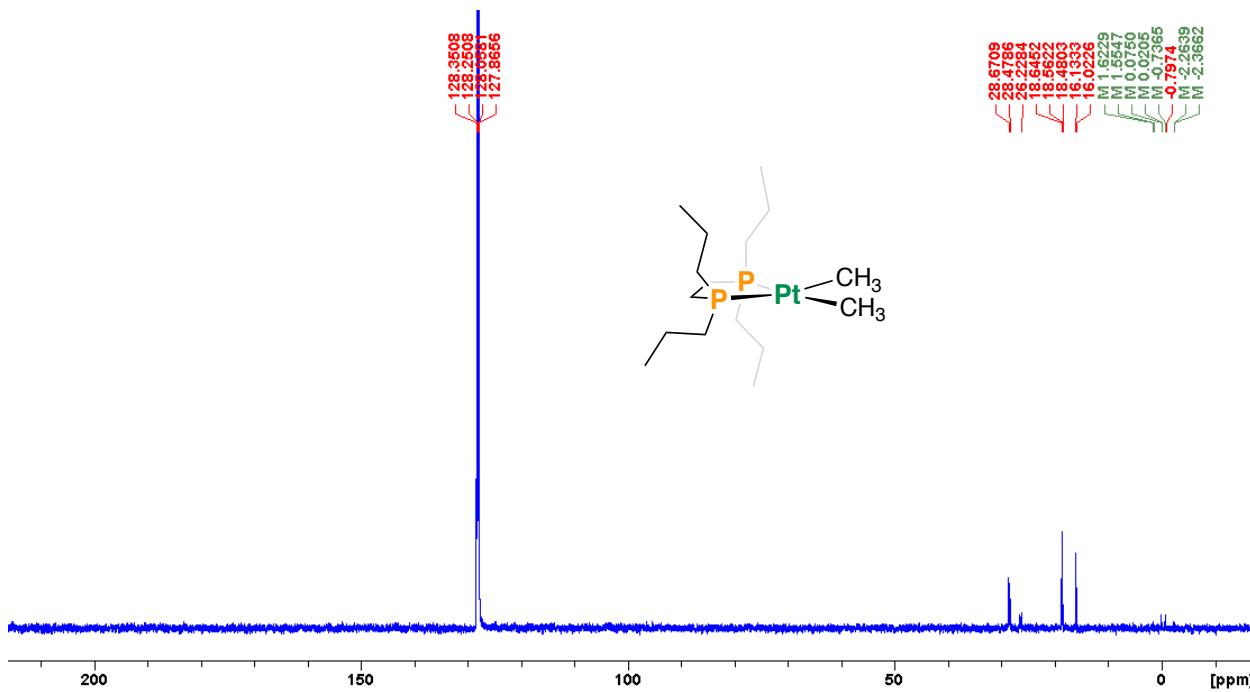


Figure S29. 4, $^{31}\text{P}\{\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K

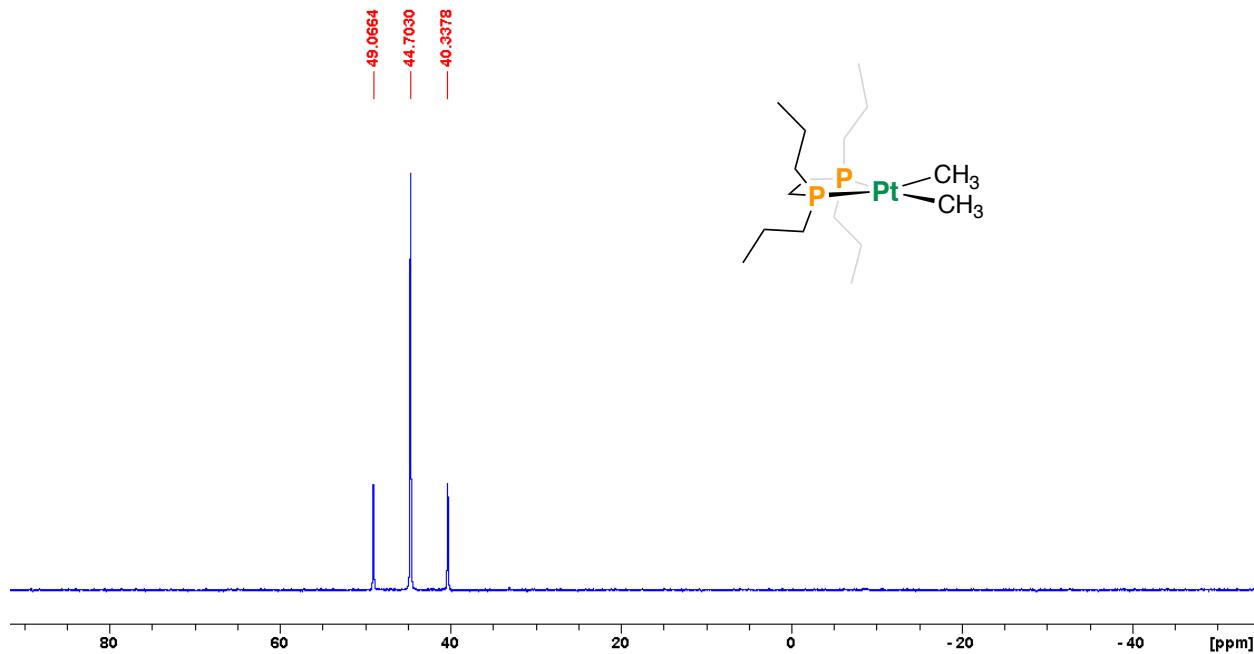


Figure S30. 5, ^1H NMR, C_6D_6 , 500 MHz, 298 K

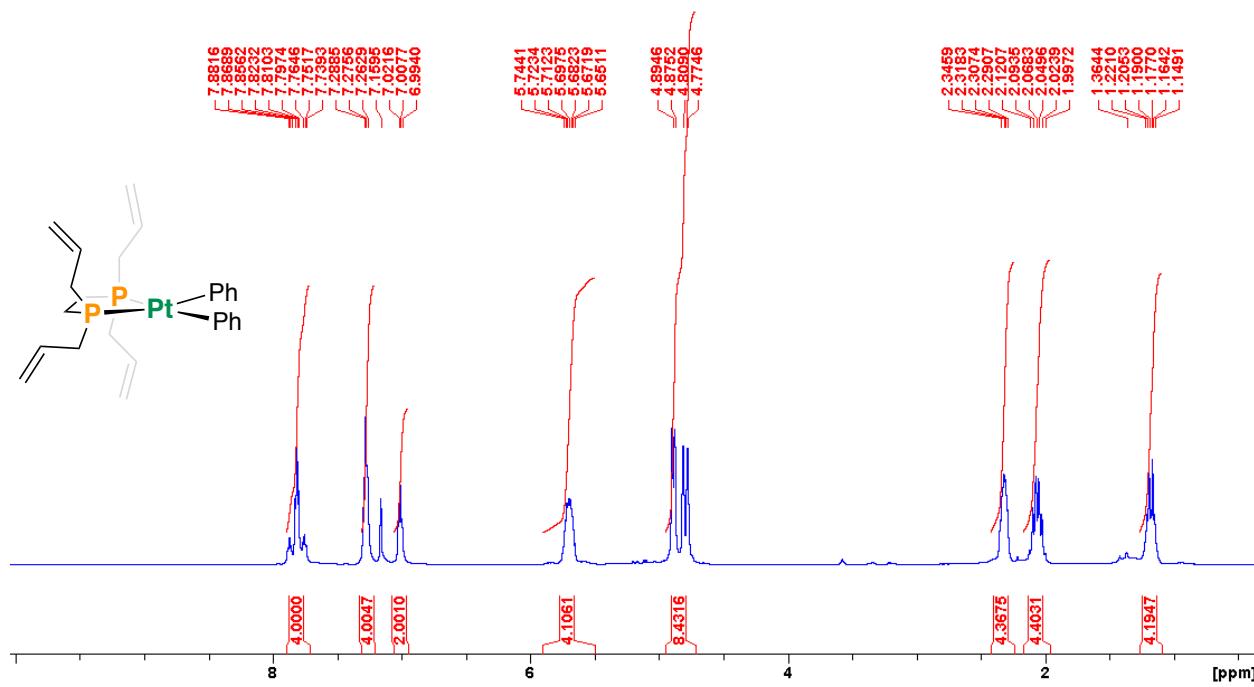


Figure S31. 5. $^{13}\text{C}\{\text{H}\}$ NMR, C_6D_6 , 125 MHz, 298 K

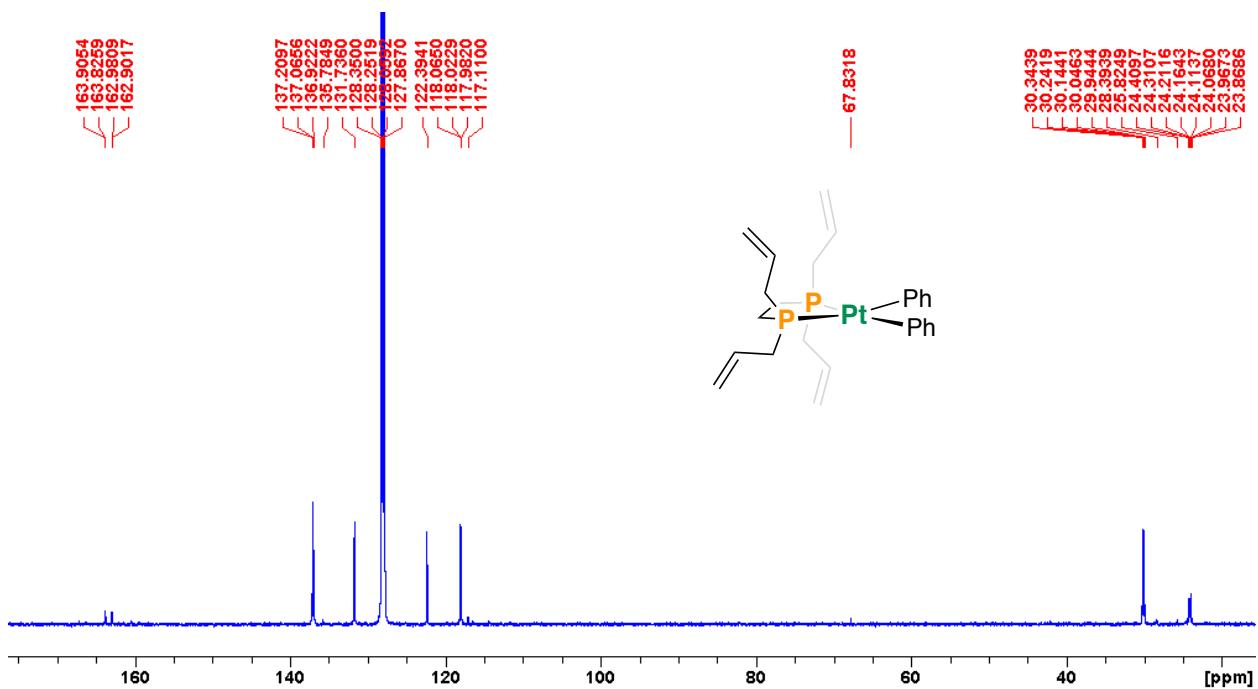


Figure S32. 5. $^{31}\text{P}\{\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K

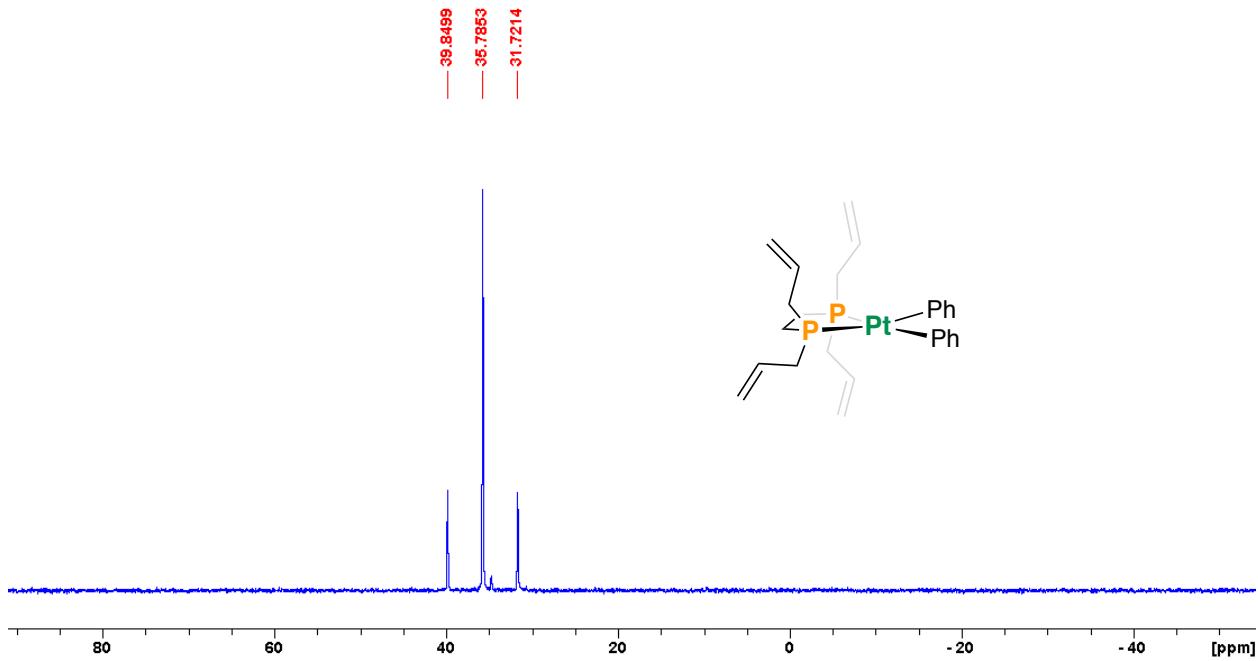


Figure S33. 6, ^1H NMR, C_6D_6 , 500 MHz, 298 K

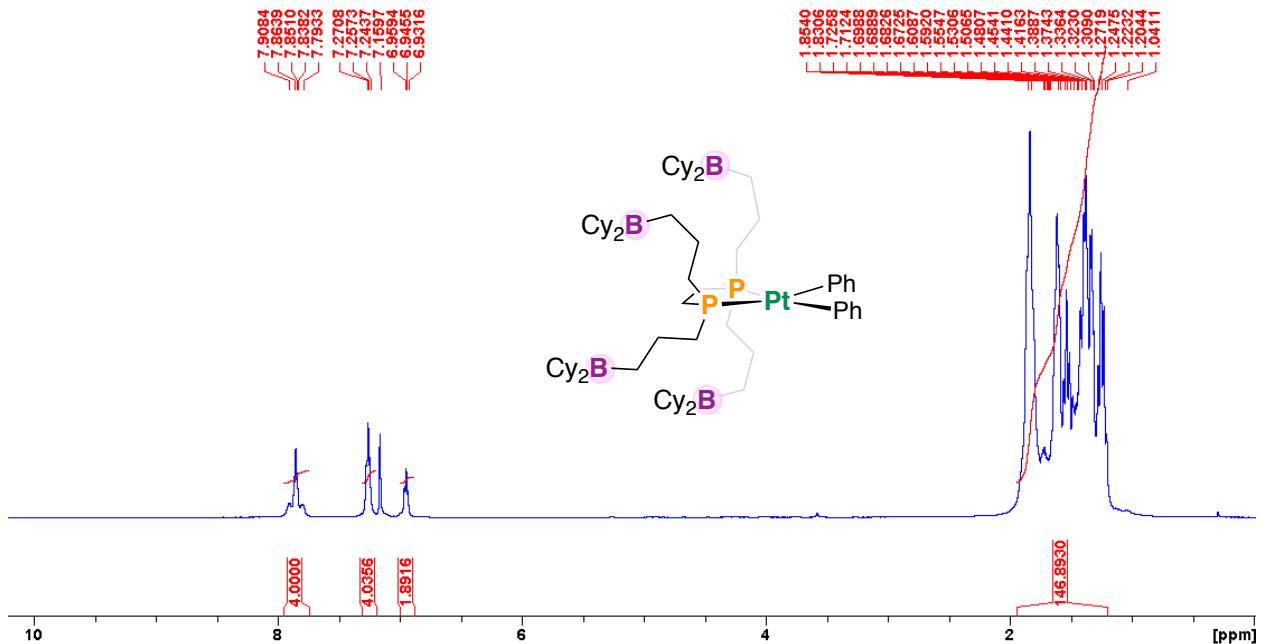


Figure S34. 6, $^{13}\text{C}\{\text{H}\}$ NMR, C_6D_6 , 125 MHz, 298 K

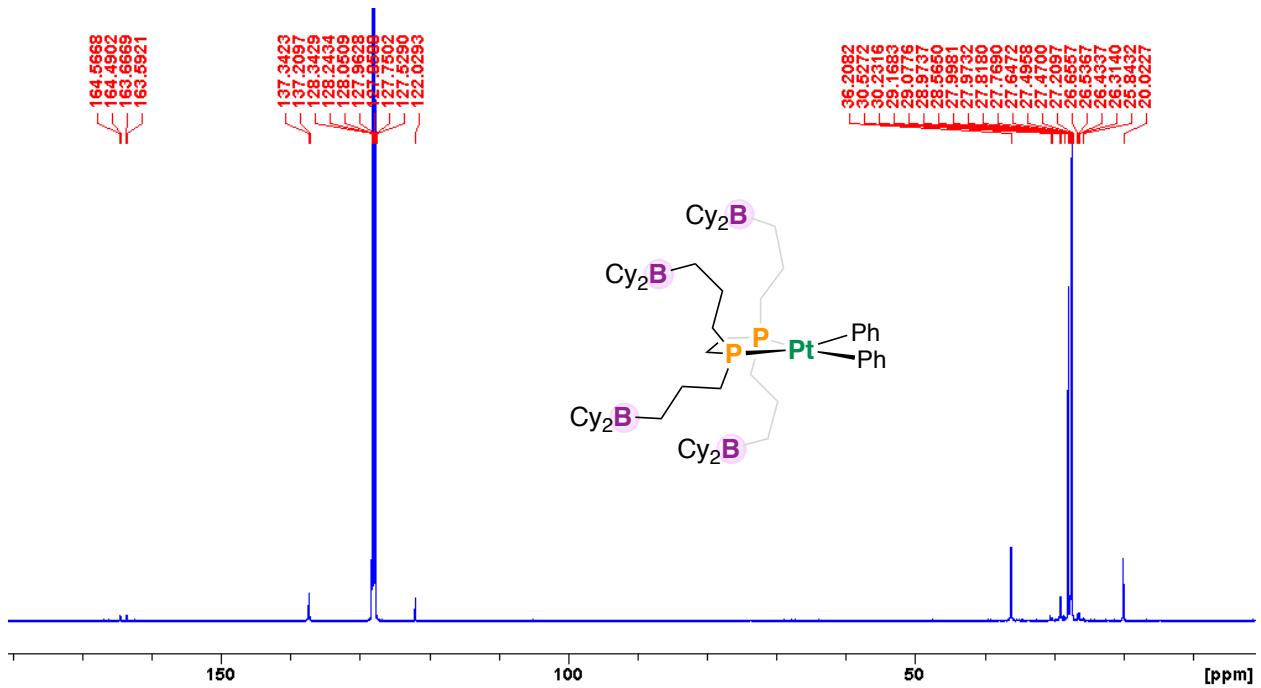


Figure S35. 6, $^{31}\text{P}\{\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K

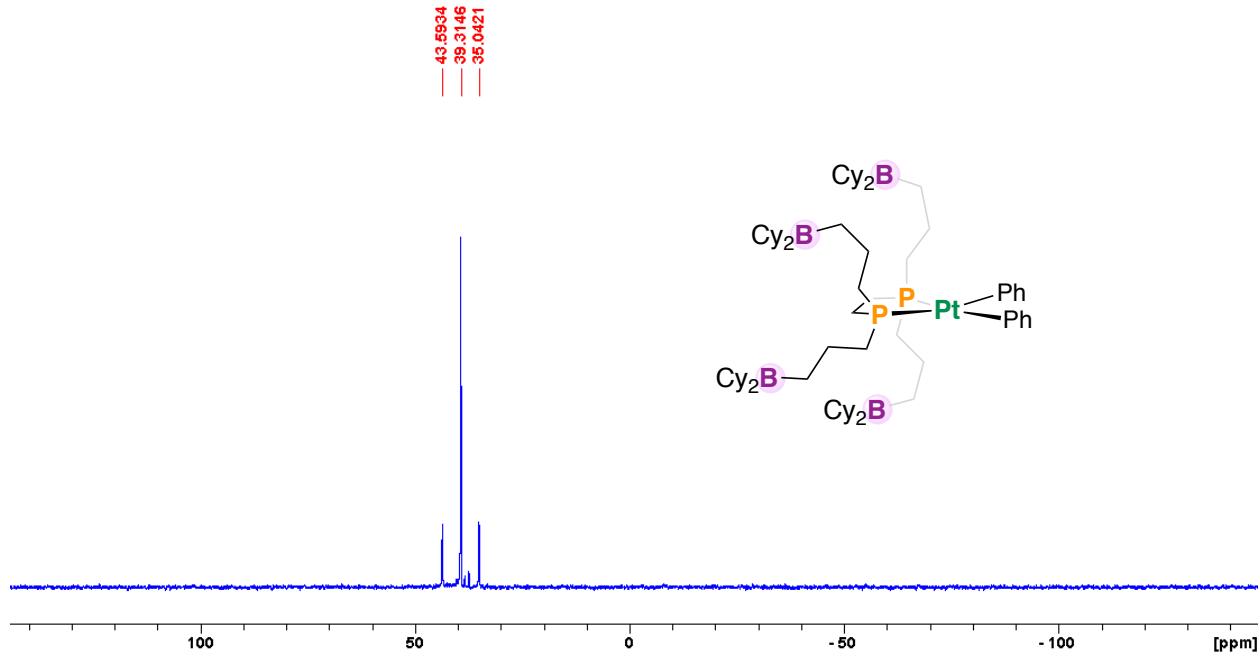


Figure S36. 6, $^{11}\text{B}\{\text{H}\}$ NMR, C_6D_6 , 160.5 MHz, 298 K

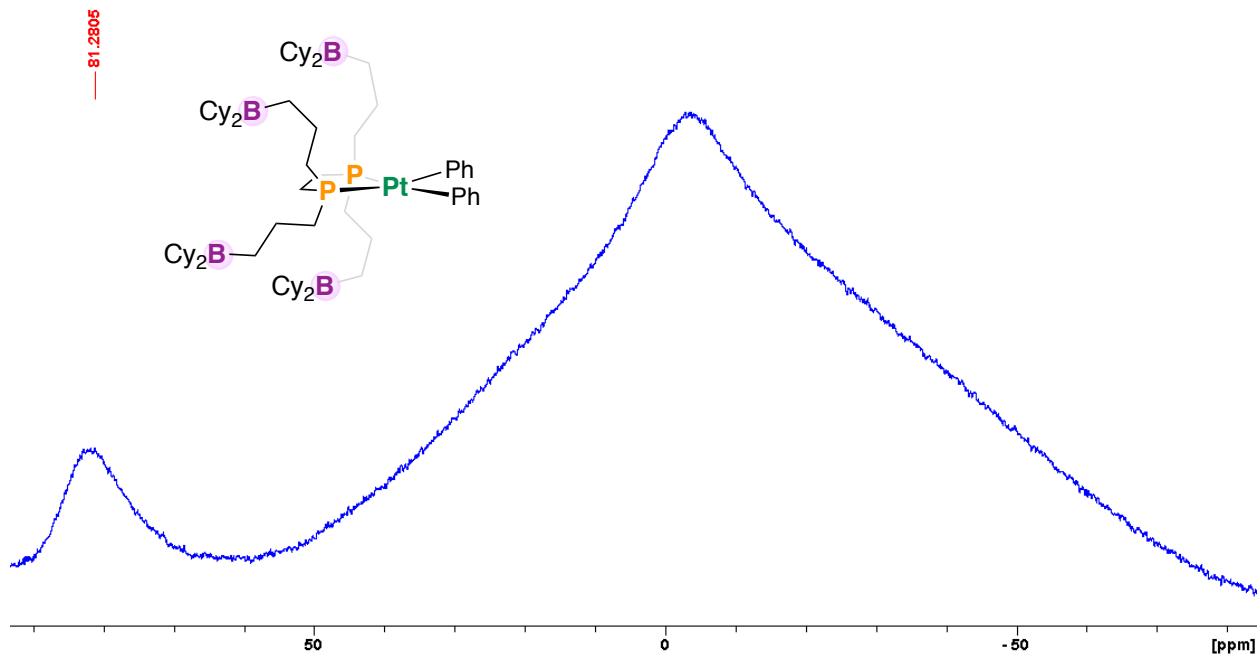


Figure S37. 7. ^1H NMR, C_6D_6 , 500 MHz, 298 K

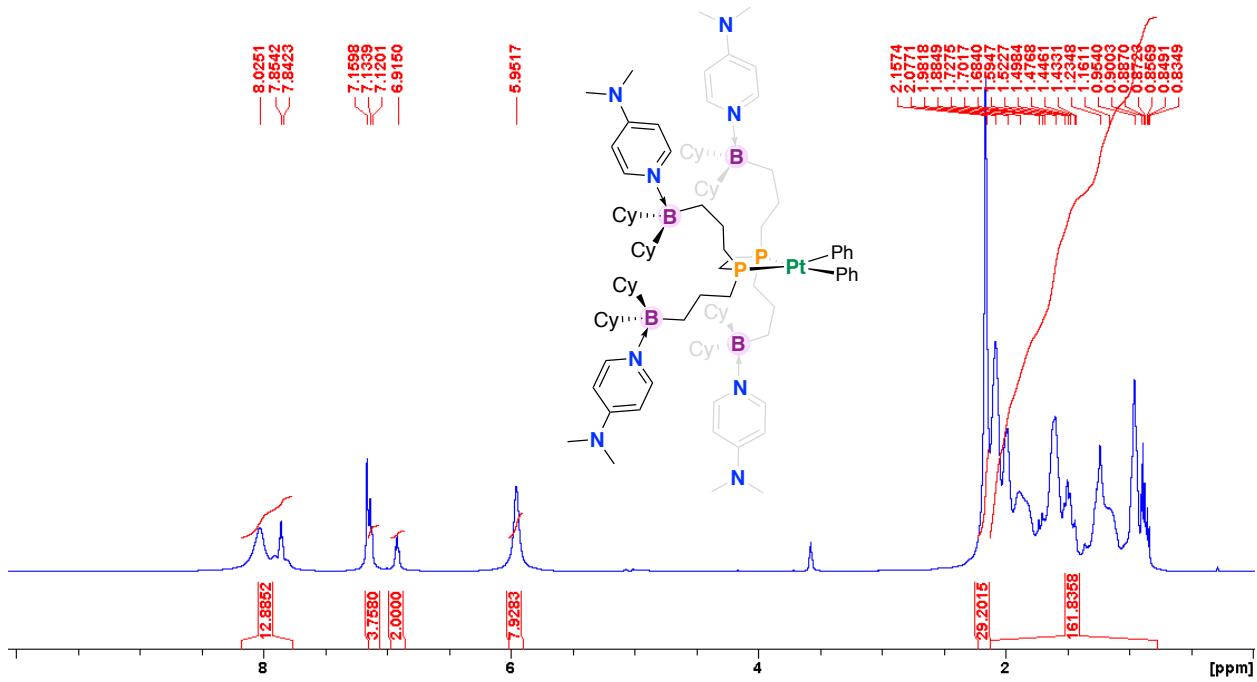


Figure S38. 7. ^1H NMR (expanded), C_6D_6 , 500 MHz, 298 K

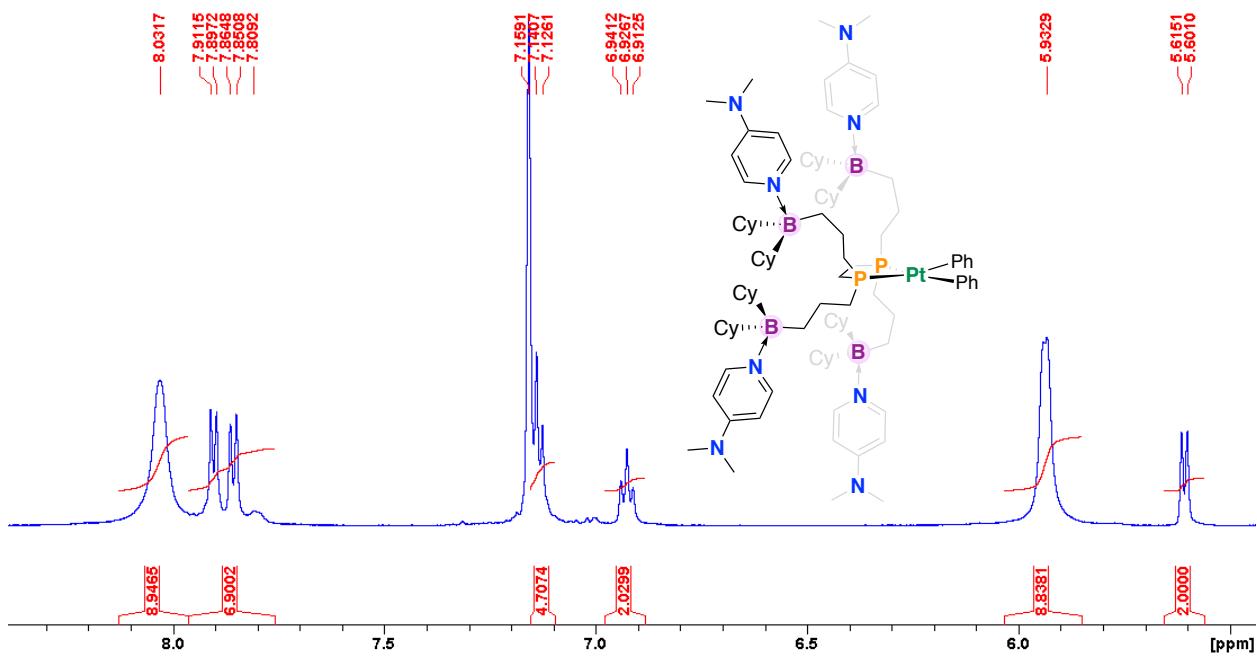


Figure S39. 7, $^{13}\text{C}\{\text{H}\}$ NMR, C_6D_6 , 125 MHz, 298 K

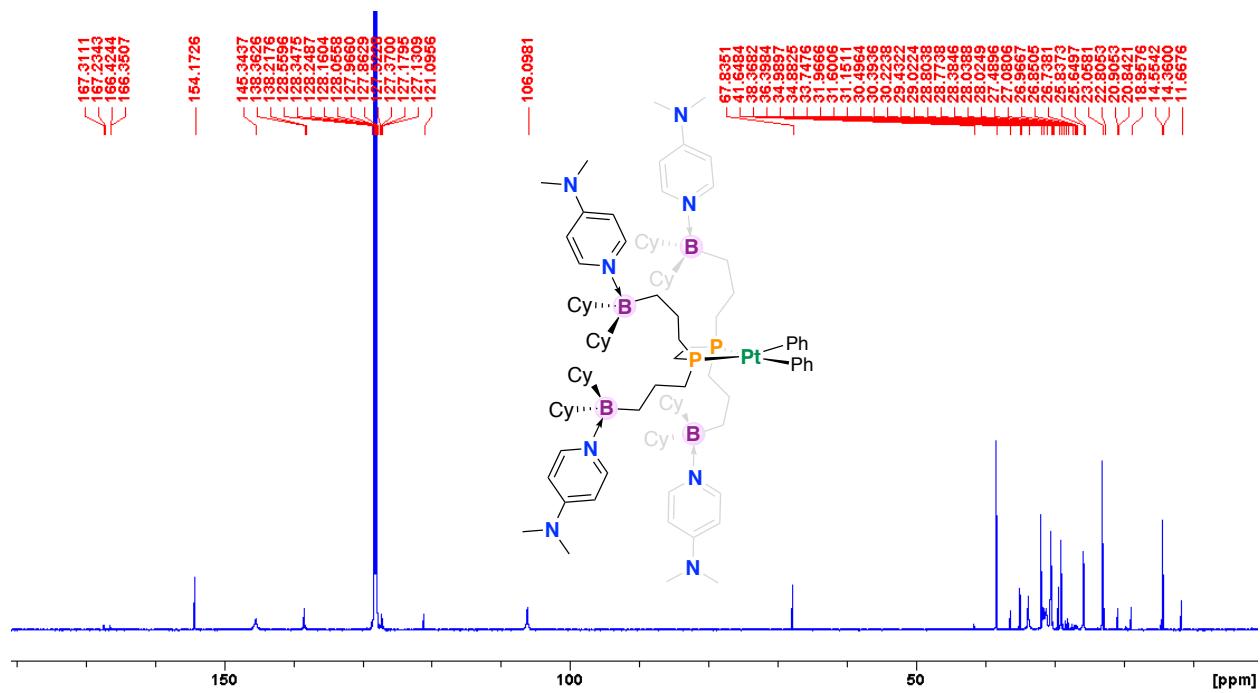


Figure S40. 7, $^{31}\text{P}\{\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K

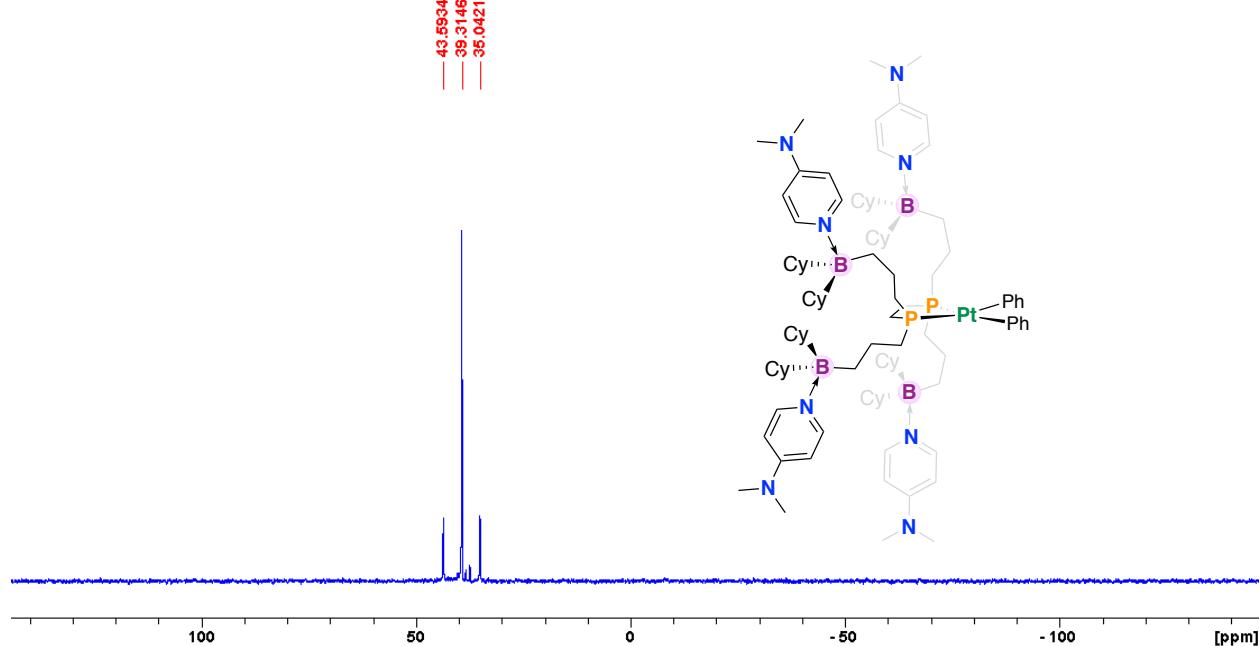


Figure S41. 7, ^{11}B { ^1H } NMR, C_6D_6 , 160.5 MHz, 298 K

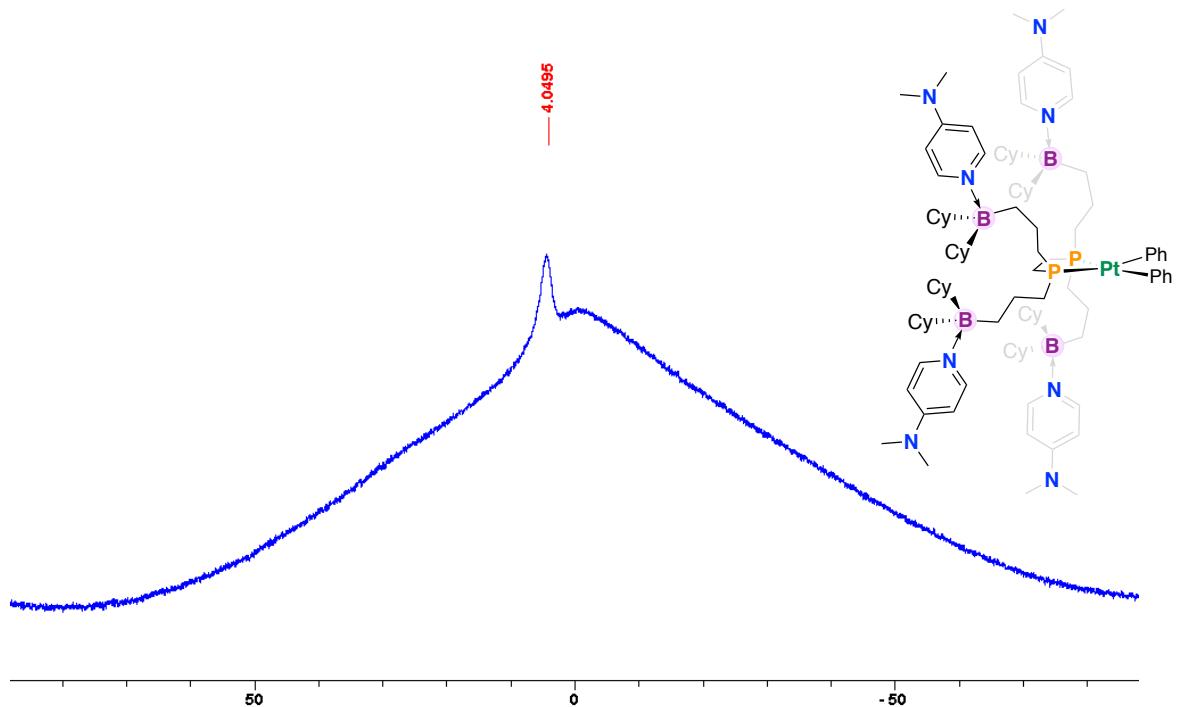


Figure S42. 8. ^1H NMR, C_6D_6 , 500 MHz, 298 K

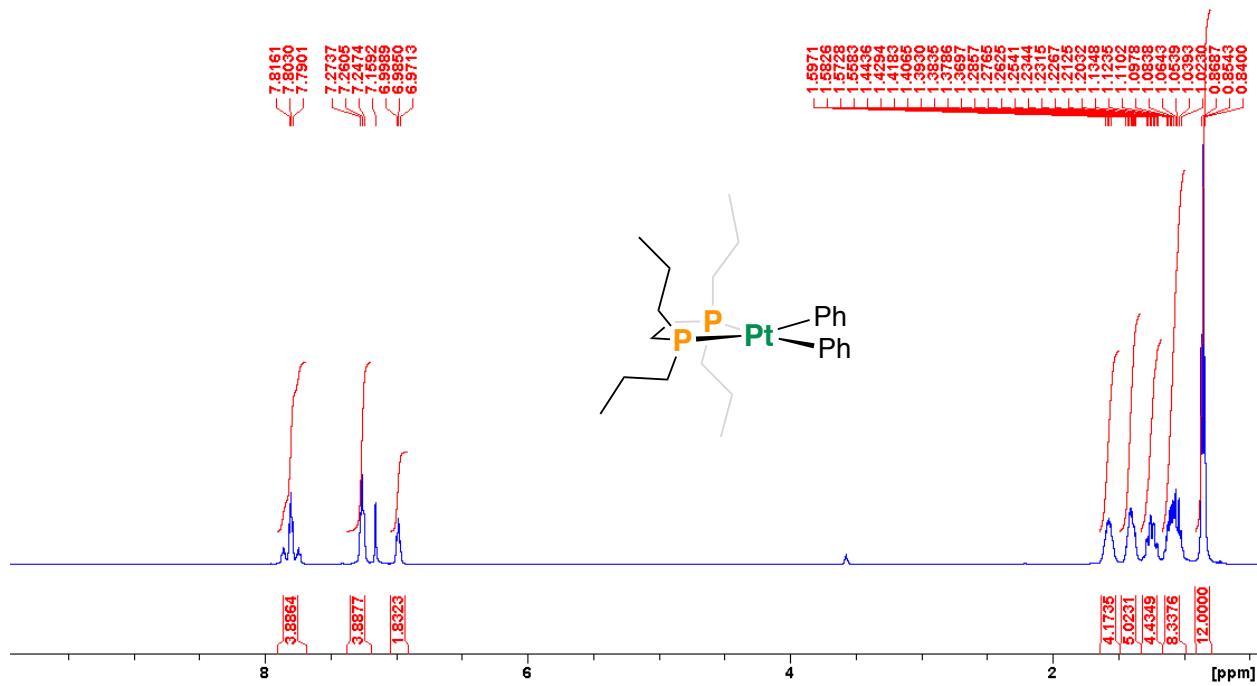


Figure S43. 8, $^{13}\text{C}\{\text{H}\}$ NMR, C_6D_6 , 125 MHz, 298 K

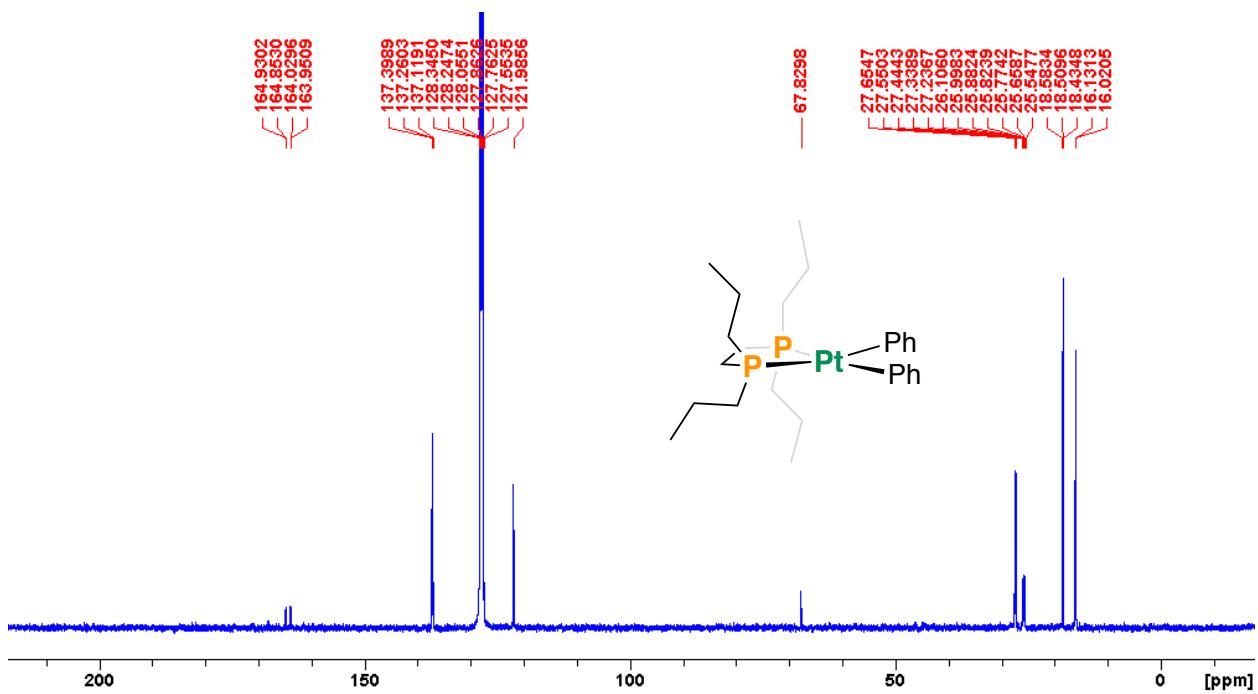


Figure S44. 8. $^{31}\text{P}\{\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K

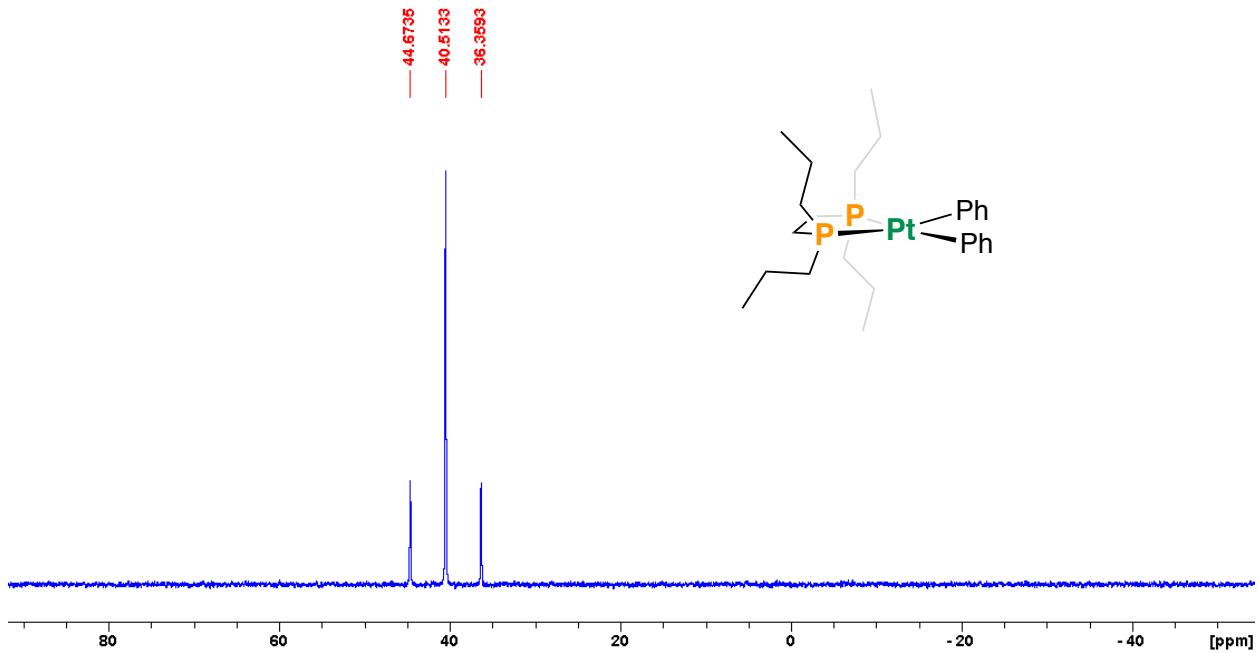


Figure S45. Thermolysis of **2** (100 °C), ^1H NMR, C_6D_6 , 500 MHz, 298 K showing appearance of signals at $\delta_{\text{H}} = 5.69$ (cyclohexene), 0.68 (B- CH_3), and 0.16 (CH_4).

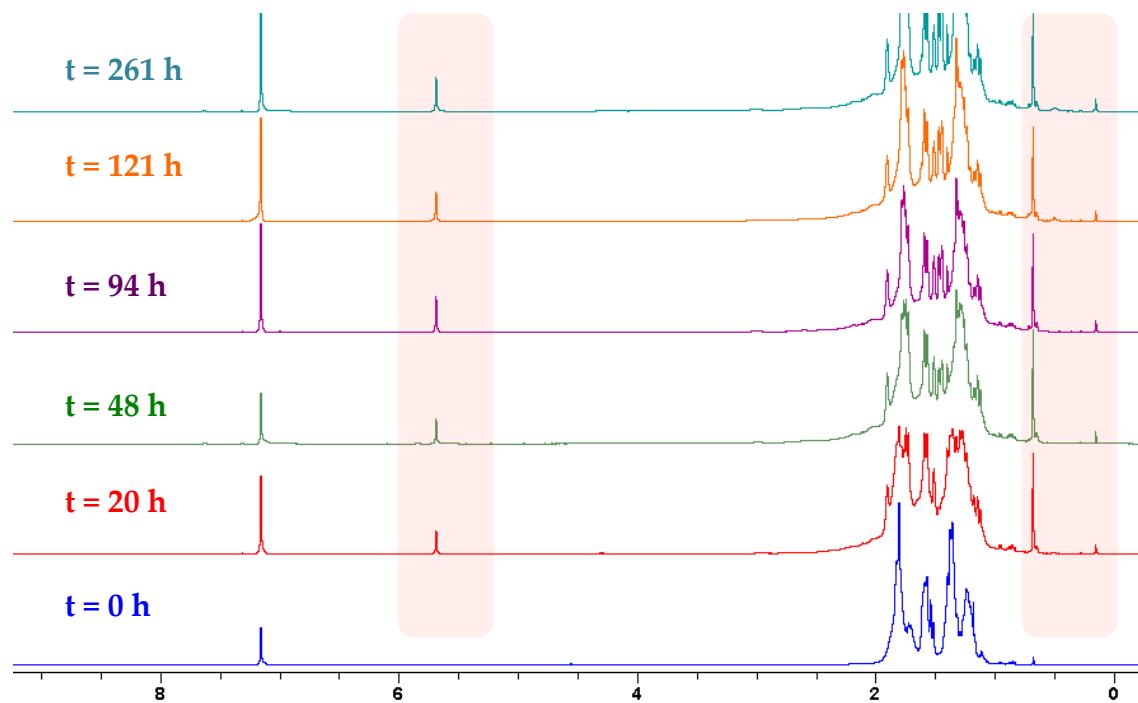


Figure S46. Thermolysis of **2** (100 °C), ^1H NMR, C_6D_6 , 500 MHz, 298 K (expanded) showing appearance of signals at $\delta_{\text{H}} = 0.68$ (B- CH_3) and 0.16 (CH_4).

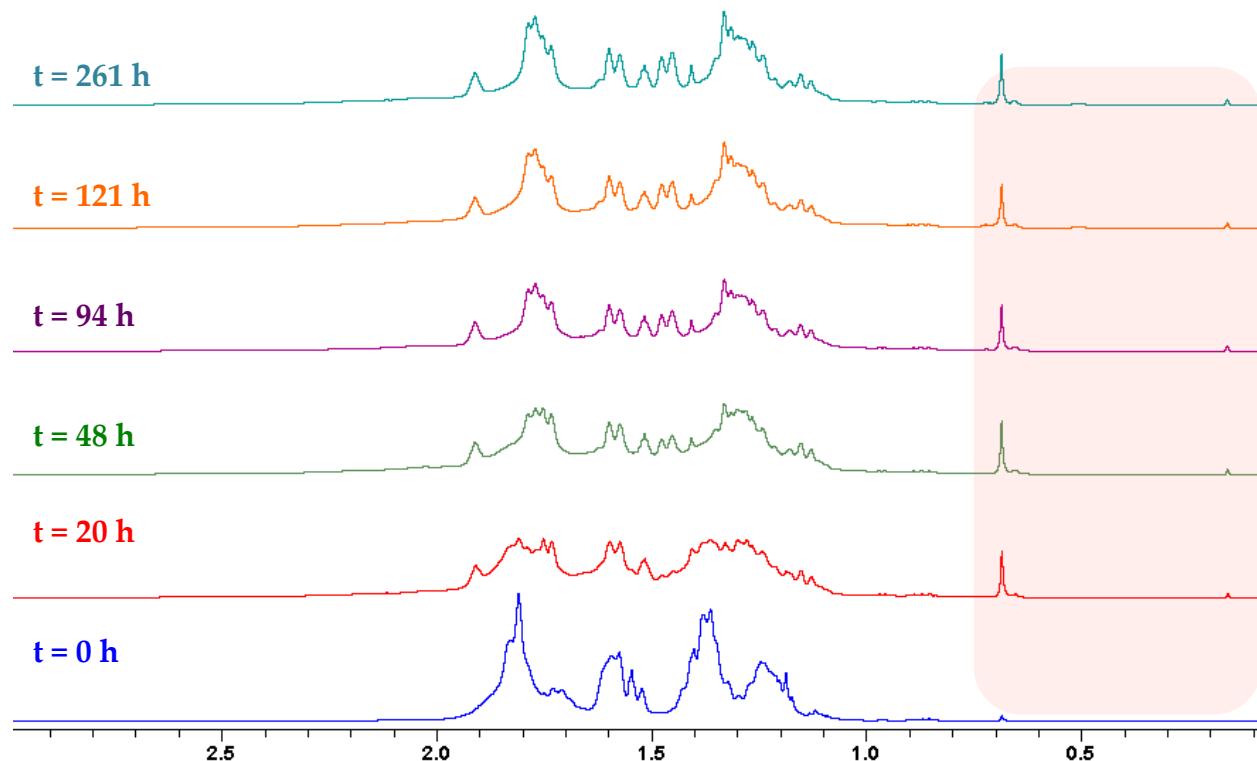


Figure S47 Thermolysis of **2** (100 °C), ^1H NMR (expanded), C_6D_6 , 500 MHz, 298 K showing the absence of molecular hydrides.

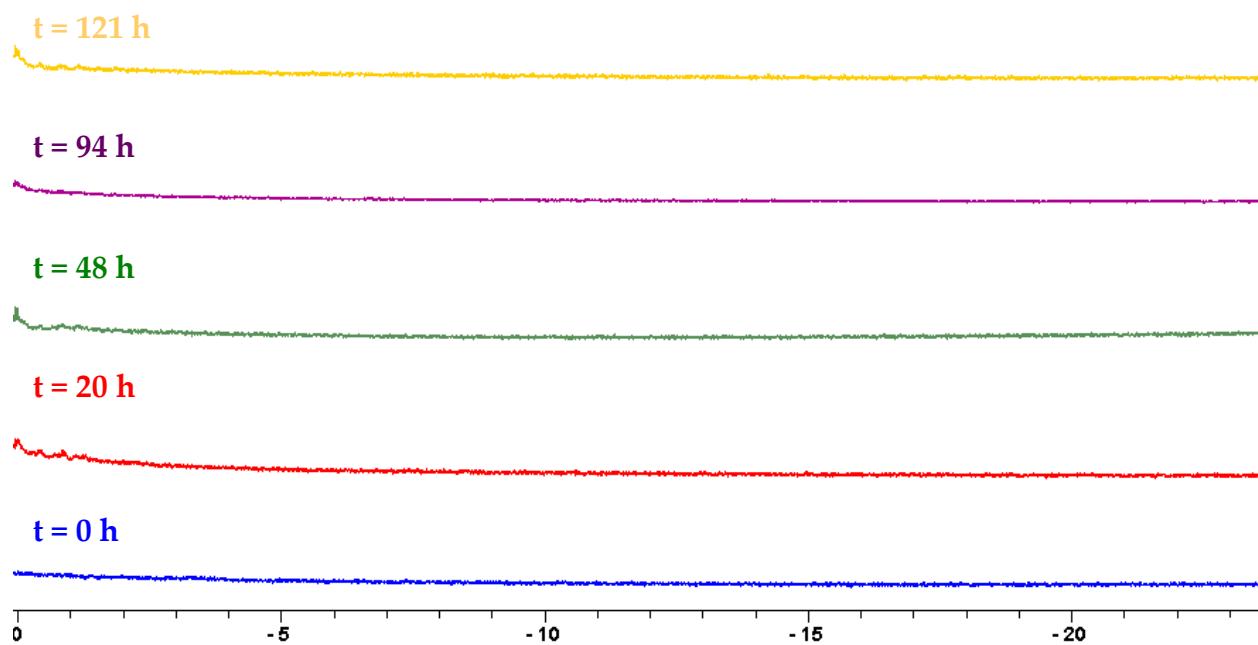


Figure S48. Thermolysis of **2** (100 °C), $^{31}\text{P}\{^1\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K showing decomposition.

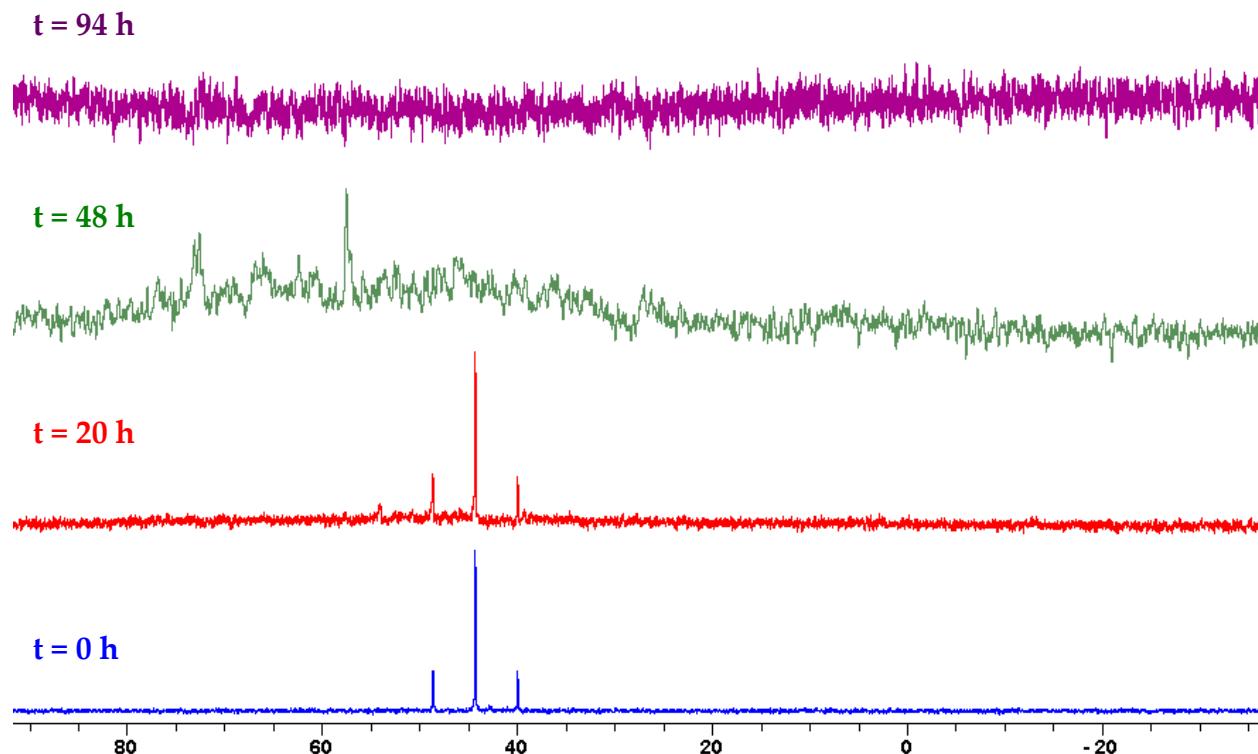


Figure S49. Thermolysis of **2** (100 °C, 48 h), $^{11}\text{B}\{\text{H}\}$ NMR, C_6D_6 , 96 MHz, 298 K.

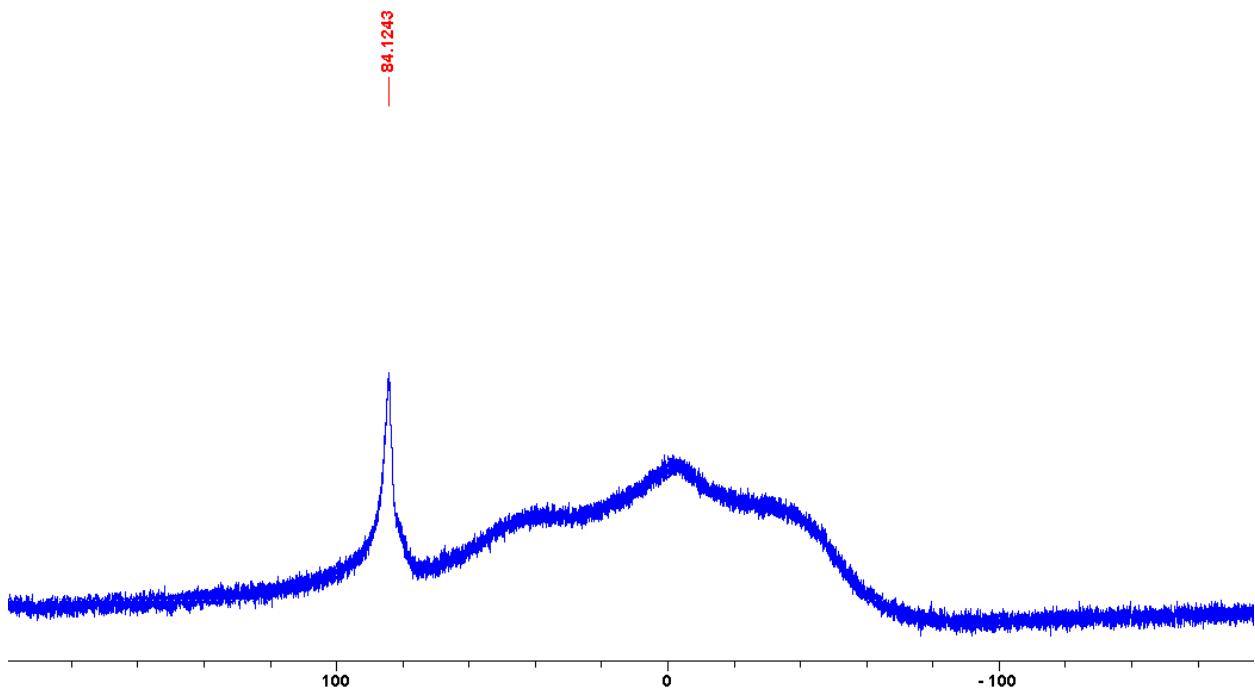


Figure S50. Thermolysis of **2** (100 °C), ^1H - ^{11}B HMQC NMR, C_6D_6 , 500 MHz, 298 K showing cross-peaks for $\delta_{\text{H}} = 0.68$ (B-CH₃) and 1.26 (B-Cy) to an ^{11}B signal at $\delta_{\text{B}} = 84$ ppm.

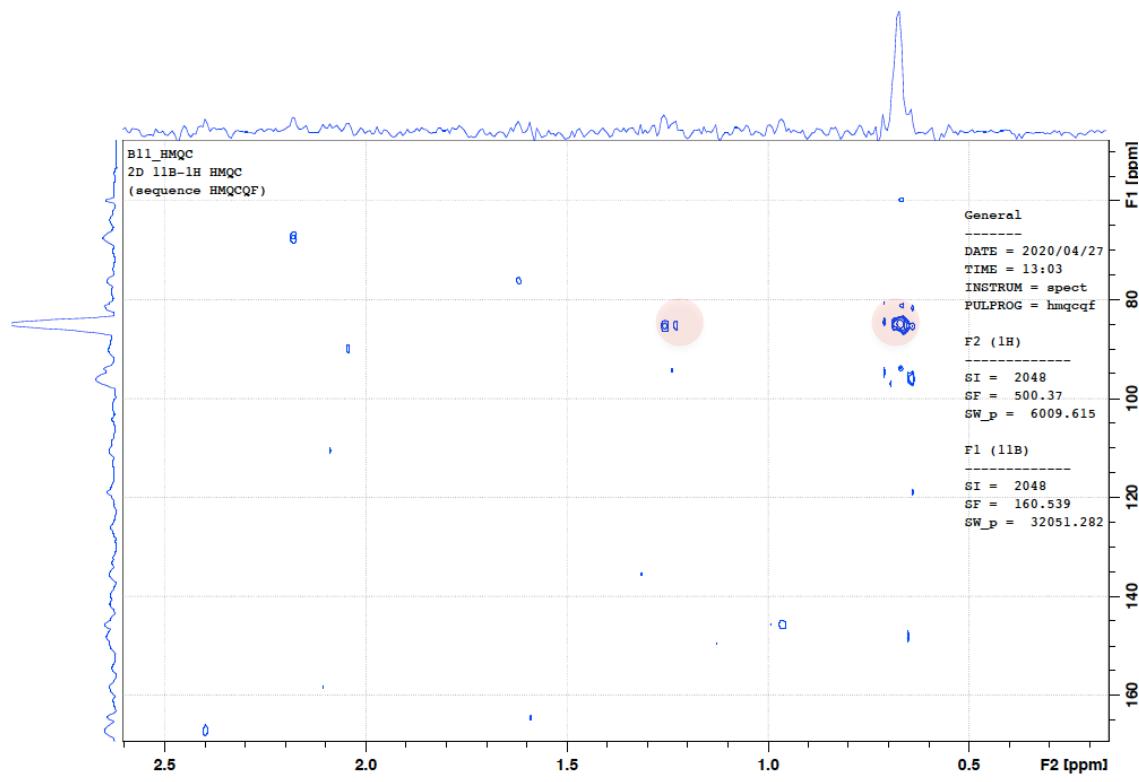


Figure S51. Thermolysis of **2** (100 °C, 48 h), $^{13}\text{C}\{\text{H}\}$ NMR, C_6D_6 , 75 MHz, 298 K. Inset shows broad $\text{B}-\text{CH}_3$ resonance at $\delta_{\text{C}} = 8.39$.

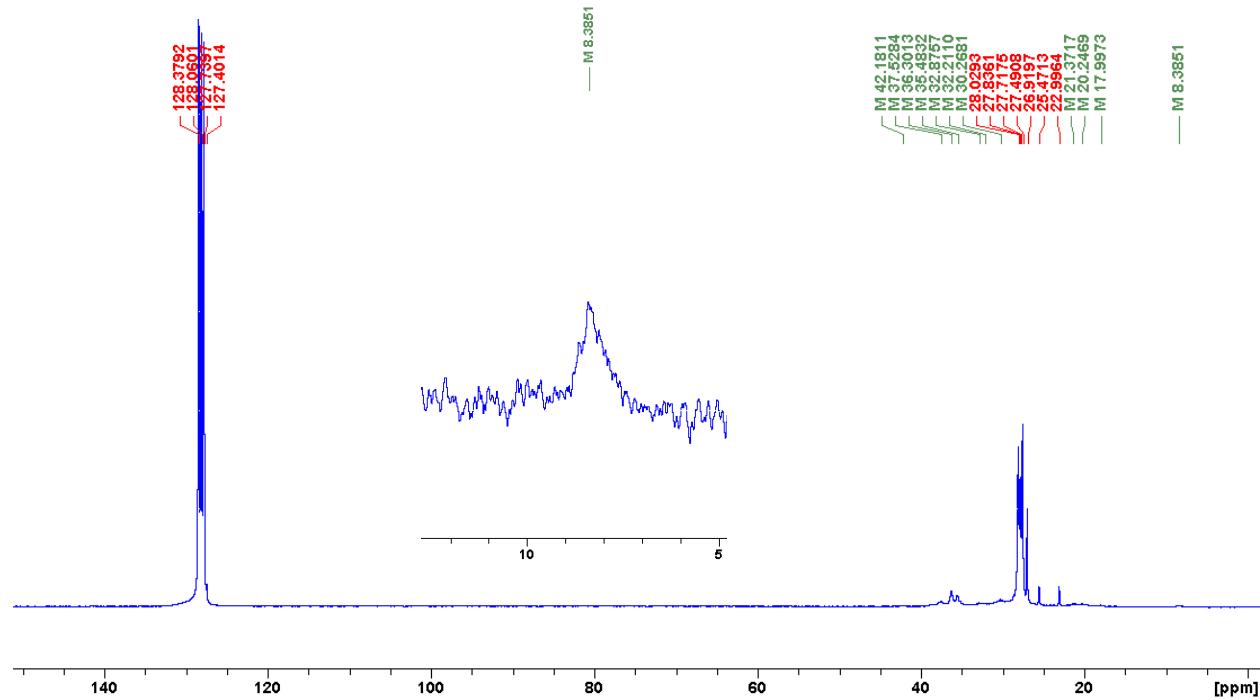


Figure S52. Thermolysis of **2** (100 °C), ^1H - ^{13}C HSQC NMR, C_6D_6 , 500 MHz, 298 K showing cross-peaks for $\delta_{\text{H}} = 5.69$ (cyclohexene: $\delta_{\text{C}} = 127.0$) and 0.68 (B- CH_3 : $\delta_{\text{C}} = 8.39$).

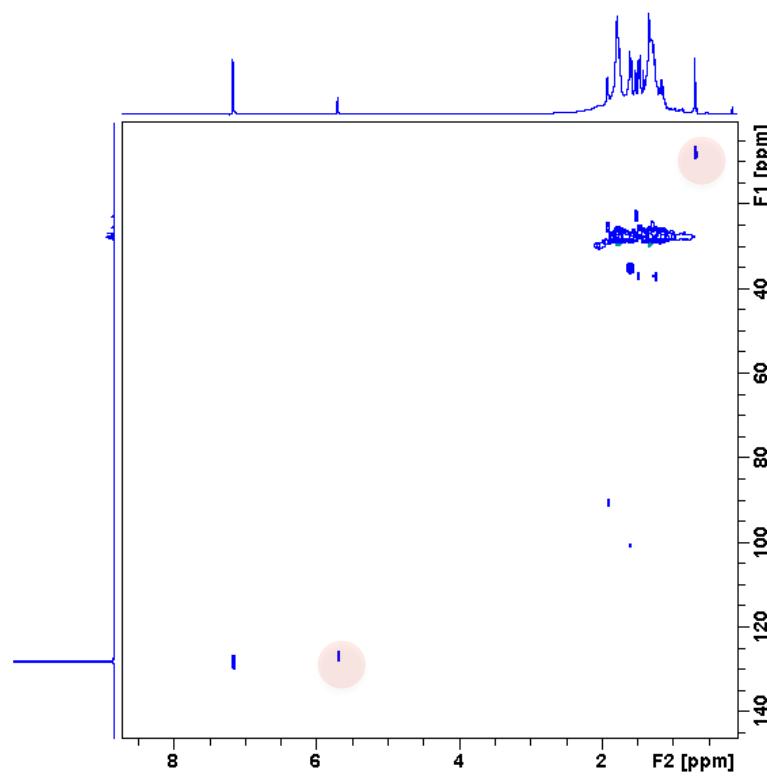


Figure S53. Thermolysis of **6** (100 °C), ^1H NMR, C_6D_6 , 500 MHz, 298 K showing appearance of signal at $\delta_{\text{H}} = 5.69$ (cyclohexene). No signals at $\delta_{\text{H}} = 0.68$ ($\text{B}-\text{CH}_3$), and 0.16 (CH_4) are apparent.

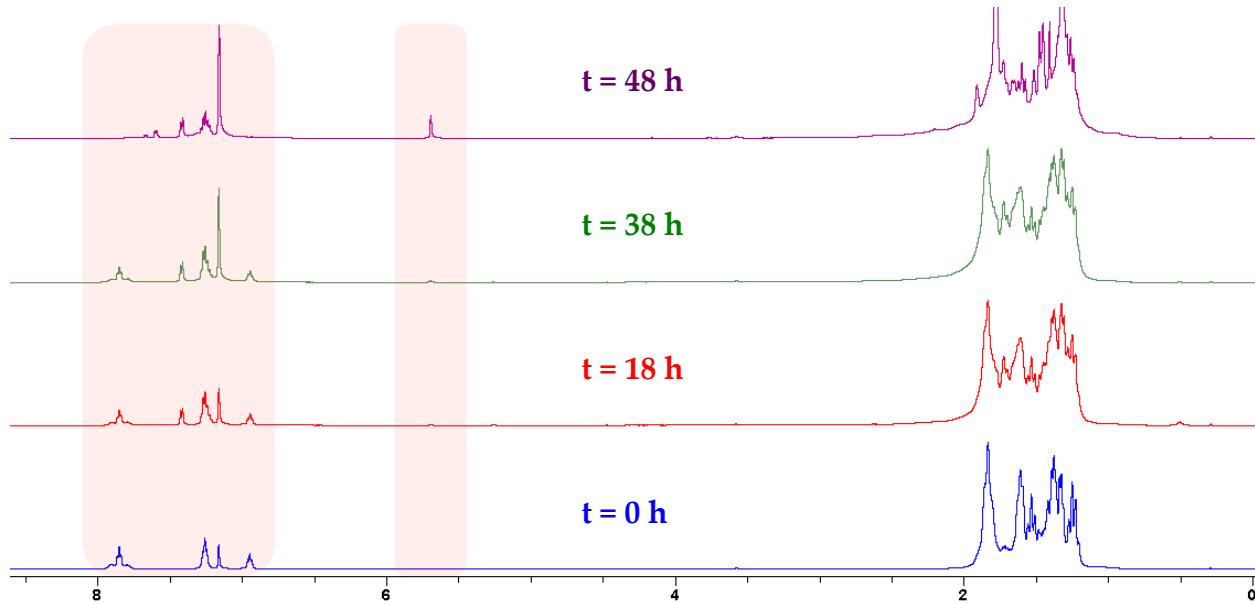


Figure S54. Thermolysis of **6** (100 °C), ^1H NMR, C_6D_6 , 500 MHz, 298 K, showing the absence of molecular hydrides.

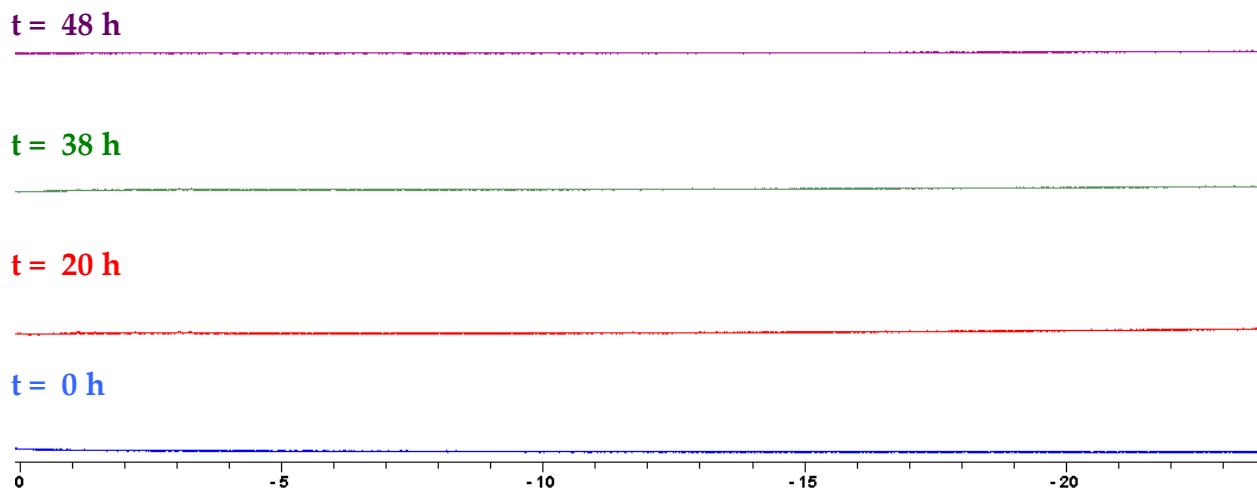


Figure S55. Thermolysis of **6** (100 °C), $^{31}\text{P}\{\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K.

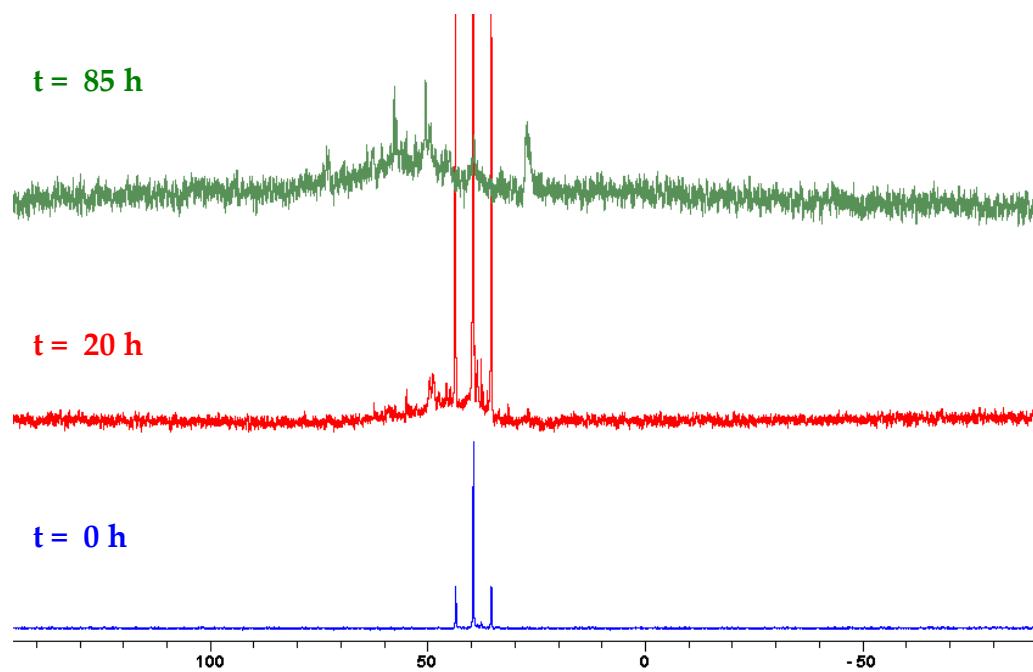


Figure S56. Thermolysis of **6** (100 °C, 48 h), $^{11}\text{B}\{\text{H}\}$ NMR, C_6D_6 , 160.5 MHz, 298 K.

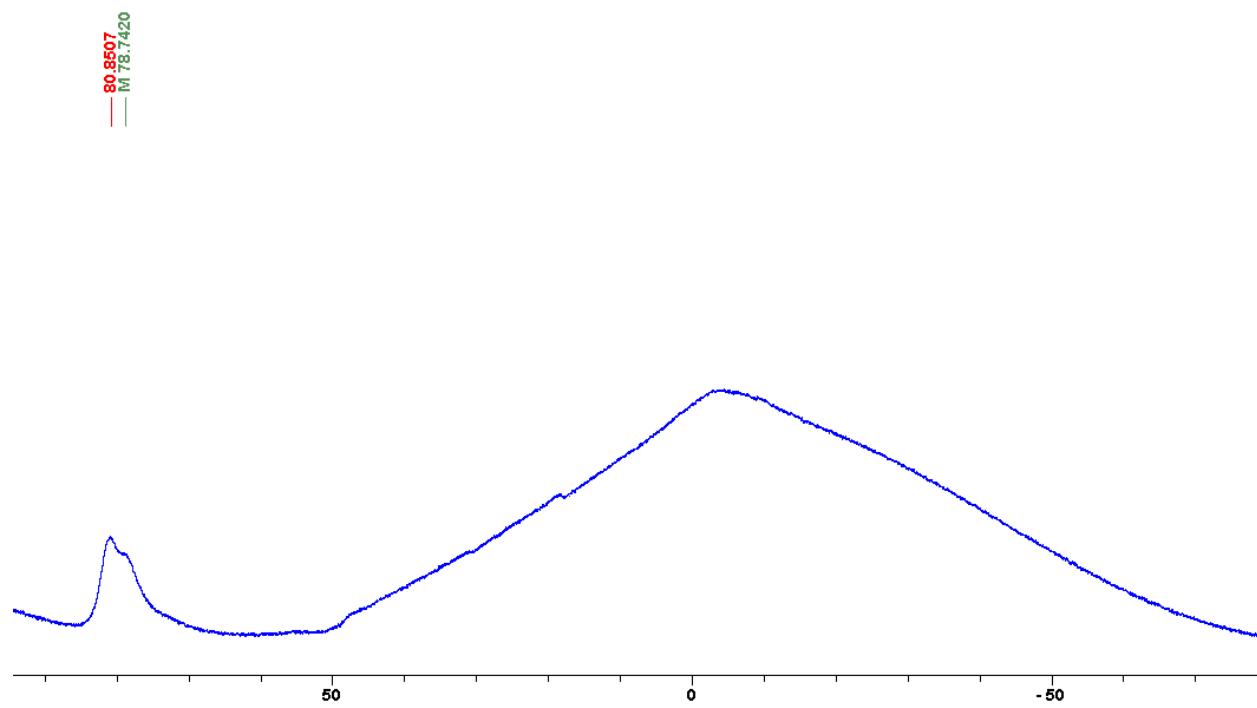


Figure S57. ^1H NMR, C_6D_6 , 500 MHz, 298 K. Cyclohexene (blue), thermolysis (100°C , 48 h) of **6** (red), and thermolysis (100°C , 48 h) of **2** (green) showing cyclohexene formation.

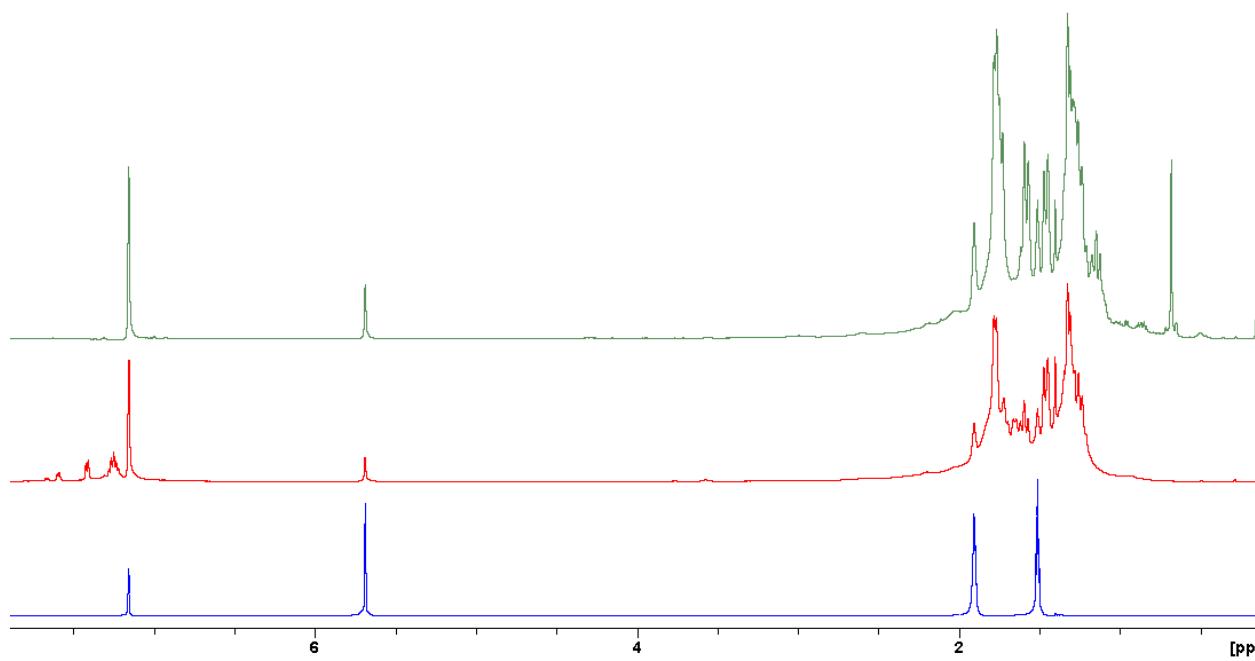


Figure S58. ^1H NMR (expanded), C_6D_6 , 500 MHz, 298 K. Cyclohexene (blue), thermolysis (100°C , 48 h) of **2** (red), and thermolysis (100°C , 48 h) of **6** (green) showing cyclohexene formation.

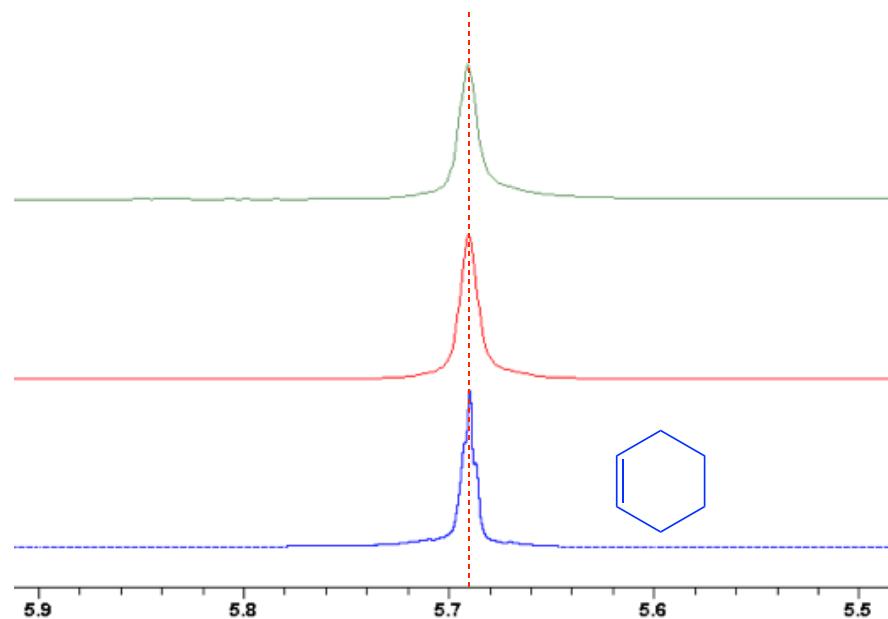


Figure S59. ^1H NMR (expanded), C_6D_6 , 500 MHz, 298 K. Cyclohexene (**blue**), thermolysis (100 $^\circ\text{C}$, 48 h) of **2** (**red**), and thermolysis (100 $^\circ\text{C}$, 48 h) of **6** (**green**) showing cyclohexene formation.

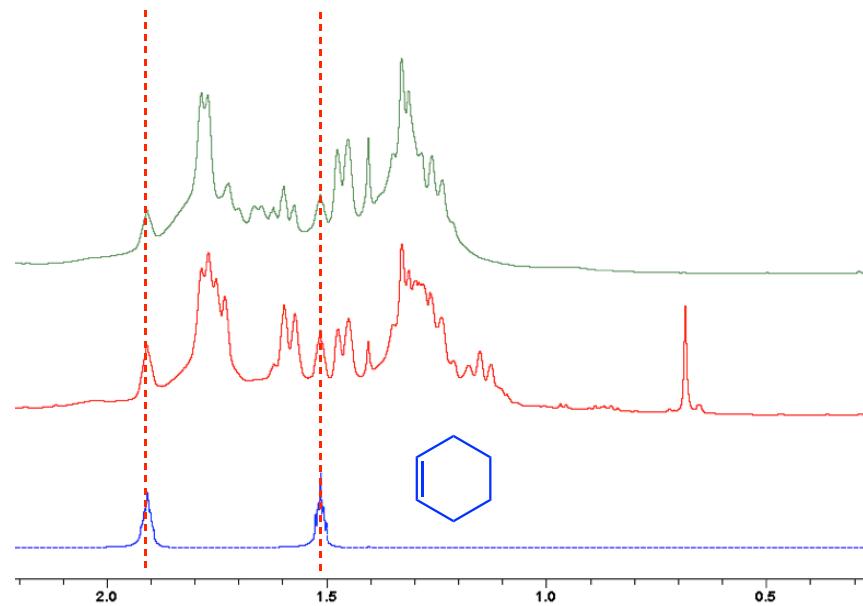


Figure S60. ^{13}C NMR, C_6D_6 , 125 MHz, 298 K. Cyclohexene (**red**) and thermolysis (100 $^\circ\text{C}$, 48 h) of **2** (**blue**) showing cyclohexene formation.

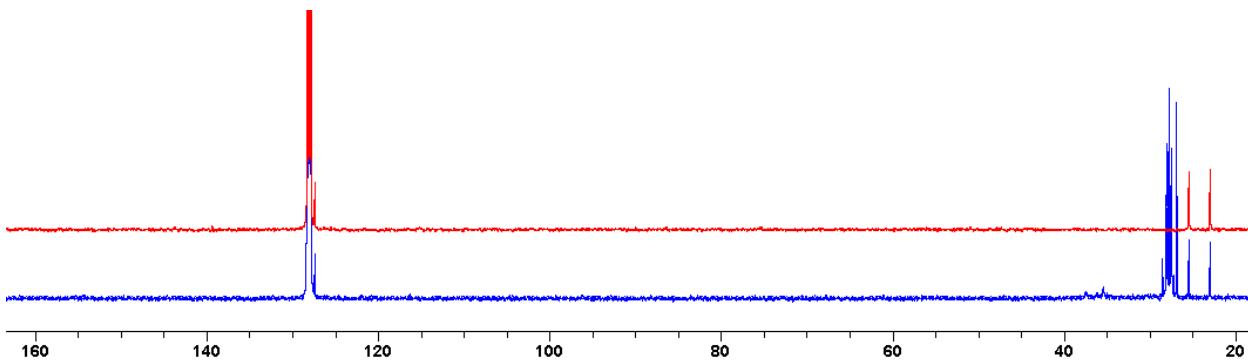


Figure S61. ^{13}C NMR (expanded), C_6D_6 , 125 MHz, 298 K. Cyclohexene (**red**) and thermolysis (100 °C, 48 h) of **2** (**blue**) showing cyclohexene formation.

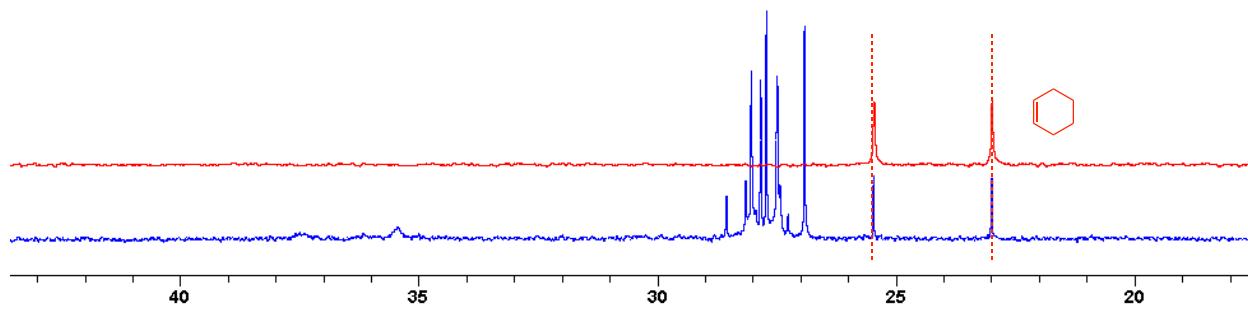


Figure S62. Thermolysis of **7** (100 °C) showing no reaction, $^{31}\text{P}\{^1\text{H}\}$ NMR, C_6D_6 , 203 MHz, 298 K.

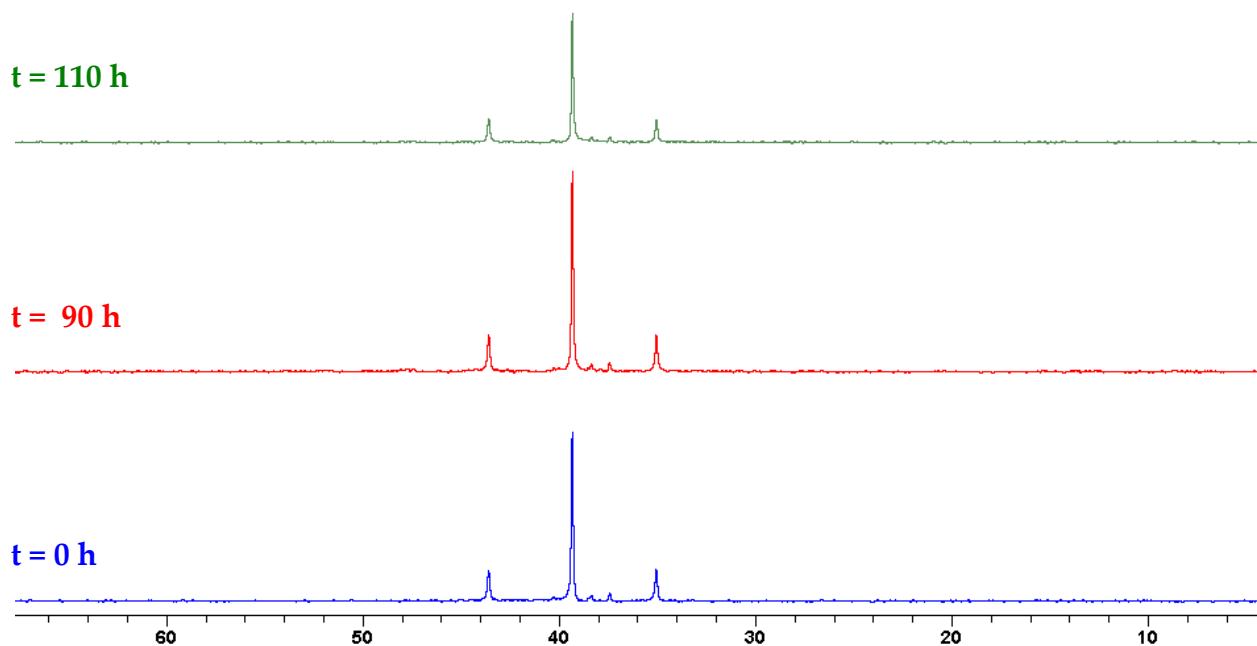
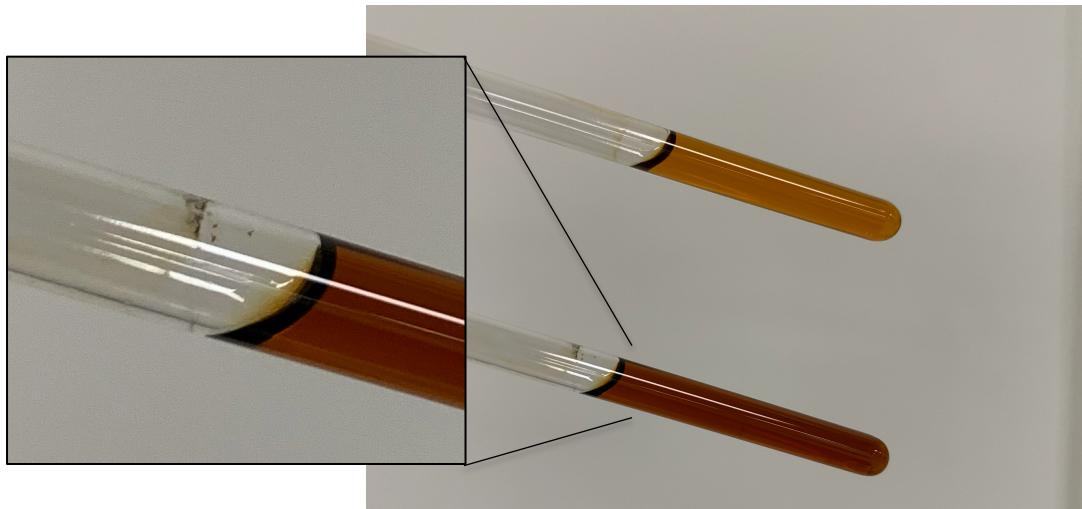


Figure S63. Thermolysis mixtures of **2** (bottom) and **6** (top) following heating (C_6D_6 , 100 °C, 48 h) showing Pt(0) formation.



Crystallographic details:

All crystals were mounted on a mitegen loop. All measurements were made using graphite-monochromated Cu K α radiation ($\lambda = 1.54178 \text{ \AA}$) on a Bruker D8 Venture diffractometer. The structures were solved by direct methods⁵ and refined by full-matrix least-squares procedures on F2 (SHELXL-2013)¹ using the OLEX2 interface.² All hydrogen atoms were placed in calculated positions. Non-hydrogen atoms were refined anisotropically.

CCDC **1987551** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

¹ G.M. Sheldrick, *Acta Cryst.* 2008, **A64**, 112.

² O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard and H.J. Puschmann, *Appl. Cryst.* 2009, **42**, 339.

Table S1. Crystallographic data for **1**.

Empirical formula	C ₁₆ H ₃₀ P ₂ Pt
Formula weight	479.43
Temperature/K	170(2)
Crystal system	Monoclinic
Space group	C2/c
a/Å	9.1592(3)
b/Å	15.1831(5)
c/Å	14.3006(5)
α/°	90
β/°	103.6490(10)
γ/°	90
Volume/Å ³	1932.55(11)
Z	4
ρ _{calc} g/cm ³	1.648
μ/mm ⁻¹	15.031
F(000)	936.0
Crystal size/mm ³	0.22 × 0.17 × 0.12
Radiation	Cu Kα ($\lambda = 1.54178$)
2Θ range for data collection/°	11.524 to 137.266
Index ranges	-11 ≤ h ≤ 11, -18 ≤ k ≤ 17, -17 ≤ l ≤ 17
Reflections collected	21875
Independent reflections	1787 [R _{int} = 0.0488, R _{sigma} = 0.0190]
Data/restraints/parameters	1787/0/88
Goodness-of-fit on F ²	1.171
Final R indexes [I>=2σ (I)]	R ₁ = 0.0172, wR ₂ = 0.0443
Final R indexes [all data]	R ₁ = 0.0182, wR ₂ = 0.0448
Largest diff. peak/hole / e Å ⁻³	0.63/-0.99

$$R_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}; wR_2 = [\sum (w(F_o^2 - F_c^2)^2) / \sum w(F_o^2)^2]^{1/2}$$

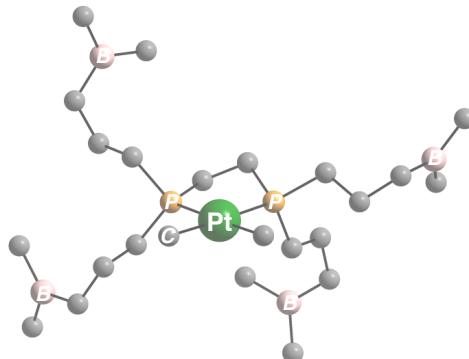
Density Functional Theory:

Geometry optimizations for all complexes were performed with Gaussian 16, Revision C.01³ at the BP86-D3/def2-SVP level of theory.⁴ Vibrational frequencies were calculated to ensure the location of stationary point structures. Single-point calculations were performed at the BP86-D3/def2-TZVP level of theory with the inclusion of PCM solvation (benzene, $\epsilon = 2.2706$).⁵ ¹¹B NMR chemical shifts were calculated using the GIAO method⁶ as implemented in Gaussian 16. Calculated chemical shifts are reported as $\delta(\text{ppm}) = \sigma_{\text{ref}} - \sigma$ referenced to $\text{BF}_3\text{-OEt}_2$ at the BP86-D3/def2-TZVP level of theory (geometry optimization at BP86-D3/def2-SVP) with the inclusion of benzene solvation ($\sigma_{\text{ref}} = 96.8$ ppm).

XYZ Coordinates for 2:

#atoms = 89

P	1.67097300	-0.14657700	0.05664000
P	-1.44873500	-0.25706100	0.00489000
C	0.80369100	-0.58475800	1.65815500
H	0.75621000	-1.69518000	1.67888300
H	1.39382800	-0.26482000	2.54348500
C	2.08642300	1.65265600	0.26573400
H	2.63193600	1.94430600	-0.65839600
H	1.10931400	2.17897400	0.19601900
C	-2.54830300	-1.72076600	0.30177000
H	-2.97585600	-1.98788700	-0.68899200
H	-1.84717500	-2.54947300	0.54673800
C	-0.60551100	0.01978900	1.66399200
H	-0.55240400	1.11888000	1.81447500
H	-1.22625600	-0.38307800	2.49214000
C	3.29842600	-1.01901900	0.24525100
H	3.65930700	-0.89239900	1.29061800
H	3.07504200	-2.09998600	0.10980600



³ Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

⁴ a) A. D. Becke, *Phys. Rev. A* 1988, **38**, 3098; b) J. P. Perdew, *Phys. Rev. B* 1986, **33**, 8822; c) S. Grimme, S. Ehrlich, and L. Goerigk, *J. Comp. Chem.* 2011, **32**, 1456.

⁵ J. Tomasi, B. Mennucci, and R. Cammi, *Chem. Rev.* 2005, **105**, 2999.

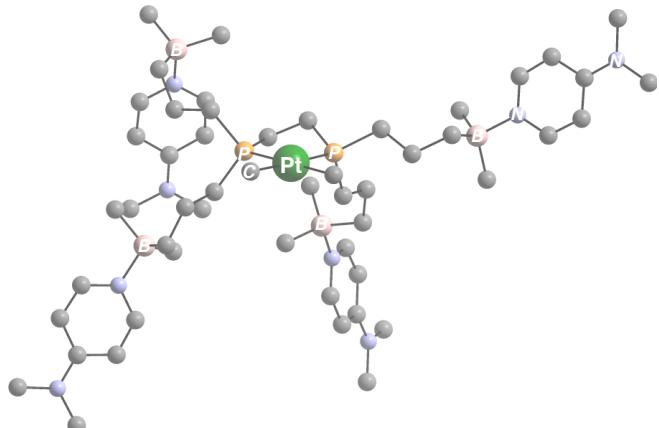
⁶ K. Wolinski, J. F. Hinton, and P. Pulay, *J. Am. Chem. Soc.* 1990, **112**, 8251.

C	4.36545700	-0.56933000	-0.76417400
H	4.57433100	0.51377300	-0.62279100
H	3.95095300	-0.66958200	-1.78820400
C	5.66930800	-1.37108000	-0.61920500
H	5.48356900	-2.45394500	-0.80474400
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C	-3.52285200	1.21232600	-1.28554200
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H	-2.89910200	1.12093300	-2.19877900
C	3.02183300	3.61127400	1.58380000
H	3.65022900	3.97080900	0.73668100
H	3.61746300	3.88889300	2.49317000
C	-2.60097700	1.19809000	-0.05963100
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C	-4.30626500	-2.94300400	1.67008300
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C	-2.17020600	-3.69095200	3.26637300
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H	2.77981900	6.45548400	1.26580300
H	1.49901200	5.95694300	0.14857000
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H	-3.62619600	-6.18631400	3.18136400
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XYZ Coordinates for 3:

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H      1.91557300 -0.58127900  2.00583000
C      1.64390700  0.61578300 -0.77179700
H      1.91743600  0.80955900 -1.83140000
H      0.53571900  0.63251500 -0.75416400
C     -1.18209700 -3.99803900  0.99031600
H     -1.23885500 -4.84780700  0.27838900
H     -0.29308400 -4.19920600  1.62624300
C     -0.03606700 -1.35599100  1.34408600
H     -0.42175100 -0.33471700  1.14270600
H     -0.45355300 -1.66767800  2.31959300
C      3.92764600 -1.13670900 -0.22211400
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C      4.68833200 -0.65704000 -1.46688200
H      4.29761900  0.33724000 -1.77845400
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C      6.21229800 -0.56072300 -1.25635800
H      6.56300000 -1.50389600 -0.76844500
H      6.69840200 -0.55955000 -2.26180700
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H     -2.66161600 -2.78021000 -2.18469900
C      1.52682000  3.04284900  0.10327900
H      1.46358200  3.37468600 -0.96235300
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H     -2.78244400 -1.32714500  0.54258100
H     -1.95392700 -0.66710100 -0.88955200
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H     -3.53500700 -5.00388800  3.34813800
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H	0.19253500	-4.72369300	4.53811500
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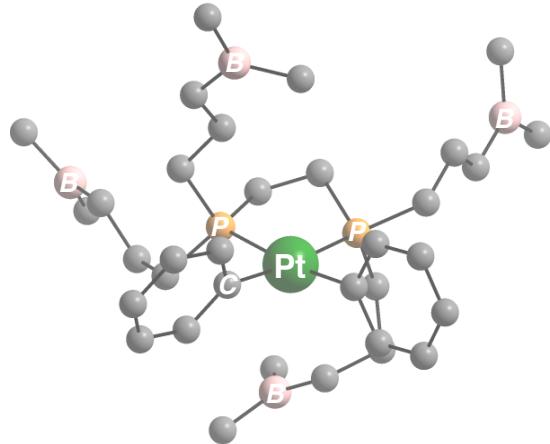
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H	0.96288300	2.98756100	2.96579100
H	-0.83052500	2.93679600	2.95908400
C	-0.75464900	5.35225900	-0.30855500
C	0.11264400	5.56412800	1.82935900
C	-0.90817900	6.72700700	-0.43694100
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C	10.53810900	0.82743100	-1.56845900
H	8.66305000	1.77668100	-2.12401300
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H	12.65722900	-2.30851000	0.11857500
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H	12.95494200	-0.03762700	-2.82322800
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C	-0.24206900	9.79230300	1.66501300
H	-0.80615800	9.55678000	2.59479300
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H	-0.42915700	10.85192500	1.41381800

XYZ Coordinates for 6:

#atoms = 103

C	4.41344300	-2.45474800	0.75929300
C	3.67240700	-2.37037900	-0.58062400
C	2.92782000	-1.05662300	-0.85958600
C	2.26051300	0.22453500	1.73765300
C	1.66799400	1.88960200	3.61244800
C	1.17628200	0.78261200	2.67404200
C	0.71543400	-2.16834800	0.79505600
C	-0.77133200	-1.97084400	1.13997500
C	-0.59490100	-0.86579400	-3.46084500
C	-1.91454100	-1.48047100	-2.96950100
C	-1.83226600	-2.14680700	-1.58287700
C	-3.30308000	-0.54273700	0.45356200
C	-3.97191100	-1.51368400	1.43891200
C	-4.32004900	-2.90687400	0.89825200
H	5.08342700	-1.57355200	0.89796600
H	4.39857800	-2.52253700	-1.41071500
H	3.61714200	-0.18476600	-0.84354600
H	2.96991500	-0.45233300	2.25723700
H	2.85145900	1.06776800	1.31549600
H	2.49820900	-1.07011000	-1.88254800
H	2.18461200	2.67163200	2.99399900
H	1.27306400	-2.61464400	1.64520500
H	0.81603000	-2.87507800	-0.05698000
H	0.72495900	-0.04690400	3.26450400
H	-0.77917800	-0.16859500	-4.31038200
H	-2.70668900	-0.69918800	-2.94372200
H	-0.87896400	-1.40332500	2.08811500
H	-1.28306600	-2.94721900	1.27605300
H	-0.21025200	-0.15146600	-2.66238500
H	-0.96468200	-2.83698800	-1.53989500
H	-2.73645900	-2.75521100	-1.37977300
H	-3.20120000	0.46661000	0.90478300
H	-3.33348900	-1.61310000	2.34410800
H	-3.92484300	-0.38540400	-0.45557400
H	-4.91422900	-2.83056400	-0.04330500
P	1.51299100	-0.56179600	0.23754300
P	-1.60704700	-0.93882400	-0.18119100
H	0.35524500	1.17922900	2.03336500
H	2.46875600	1.52919100	4.29936800



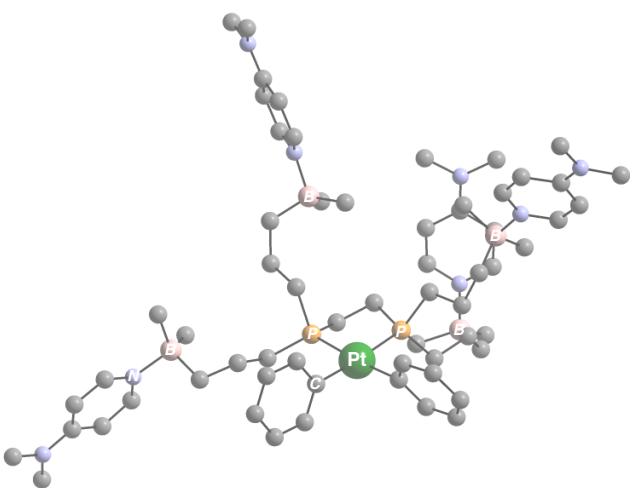
H	2.96268800	-3.22259600	-0.66891000
H	3.69034700	-2.35188200	1.60850500
H	-4.90369700	-1.02490800	1.80251700
H	-3.39330300	-3.44167800	0.56593700
H	-2.26977700	-2.24657100	-3.69468300
C	1.88763800	-1.03061600	-4.50442800
C	0.77820300	-3.29010000	-3.46026600
H	2.87841000	-1.47558900	-4.27157200
H	1.20254300	-3.36195100	-2.42915800
B	0.66211900	-1.74597200	-3.80078100
C	4.97122700	-5.10273300	0.28121700
C	6.17775600	-3.77955100	2.35824500
H	5.63011200	-5.95307400	0.54938200
H	6.09067900	-2.90593700	3.03653300
B	5.19631100	-3.78441600	1.12246300
C	-0.91702500	2.76335000	3.90676800
C	1.04714100	3.66379400	5.58992600
H	-1.31066600	1.76078500	3.63572200
H	2.13984100	3.84355100	5.66028700
B	0.58922500	2.75278900	4.38399100
C	-5.03703700	-3.70571100	3.42805600
C	-5.61307800	-5.27941000	1.25757000
H	-5.41296700	-2.68874800	3.67629400
H	-5.33384600	-5.49573700	0.20580600
B	-5.00072900	-3.95953600	1.86923100
H	-0.93158600	3.34149900	2.95045100
H	-1.62721300	3.26443000	4.59531700
H	0.75193900	3.11370300	6.51727100
H	0.50662900	4.63306000	5.64269300
H	-3.98566900	-3.71507400	3.80332600
H	-5.60621300	-4.45356500	4.01613700
H	-6.72228400	-5.14379000	1.27725900
H	-5.42474300	-6.17789600	1.88403700
H	1.92925200	0.06801900	-4.35326500
H	1.74192800	-1.19018400	-5.60099900
H	1.49647400	-3.83124900	-4.11164100
H	-0.18385000	-3.84296200	-3.44075400
H	7.21078100	-3.75700100	1.93215500
H	6.13501600	-4.71747200	2.95288700
H	5.04375800	-4.92022000	-0.81347800
H	3.91737200	-5.43474900	0.44159700
Pt	-0.16502200	0.84388100	-0.57805600
C	-1.70466900	2.14260500	-1.04368300

C	-2.19533200	2.32550600	-2.35813800
C	-2.35121200	2.85894700	-0.00665800
C	-3.28685100	3.17297200	-2.62352200
H	-1.71052100	1.80103100	-3.19751300
C	-3.44266200	3.70914800	-0.26471300
H	-1.99573400	2.75092900	1.03258700
C	-3.91959900	3.86741000	-1.57722400
H	-3.64414200	3.29525200	-3.65986000
H	-3.92204200	4.25281900	0.56665100
H	-4.77376500	4.53183400	-1.78456000
C	1.20909700	2.38409000	-0.75128500
C	2.24359000	2.36038800	-1.71871900
C	1.21931600	3.45316800	0.17646200
C	3.25241000	3.34171000	-1.74470300
H	2.26538100	1.55497900	-2.47213700
C	2.22961300	4.43234900	0.16389000
H	0.41159300	3.52970100	0.92299000
C	3.25688300	4.37833000	-0.79494500
H	4.04217800	3.29496000	-2.51327200
H	2.20865300	5.25021500	0.90363800
H	4.04870400	5.14436000	-0.80861400

XYZ Coordinates for 7:

#atoms = 179

P	1.99055000	-0.71884800	0.28904300
P	-0.85663500	-1.89473700	0.98883600
C	1.31166300	-0.42339000	2.00372500
H	1.66940000	-1.26451600	2.63637600
H	1.71443900	0.51410100	2.44359800
C	1.62564100	0.87729200	-0.57691800
H	1.95755600	0.74207200	-1.62875600
H	0.51926500	0.92097400	-0.62404900
C	-1.25746600	-3.07511600	2.36862800
H	-1.31092200	-4.08922700	1.92214600
H	-0.35018300	-3.06836800	3.01051700
C	-0.21617600	-0.40743200	1.92731800
H	-0.57017400	0.49843900	1.39267000
H	-0.68588800	-0.39046500	2.92813800
C	3.82196500	-0.73295500	0.52854900
H	4.07885800	0.10676300	1.20687300
H	4.05936700	-1.67405300	1.07166200



C	4.62121200	-0.65712800	-0.78164300
H	4.26848000	0.20990000	-1.38223000
H	4.37998900	-1.55333700	-1.38873900
C	6.14145500	-0.53998000	-0.56404100
H	6.45753500	-1.31347600	0.17934100
H	6.63844400	-0.83895900	-1.51787600
C	-3.42955500	-2.29116600	-0.21493600
H	-3.81819900	-2.91006200	0.62245900
H	-2.86617700	-2.98736500	-0.87042900
C	1.51237900	3.44604000	-0.41560100
H	1.49144100	3.47185200	-1.53286600
H	2.16359600	4.30277500	-0.11741200
C	-2.46579500	-1.24380500	0.35173100
H	-2.94493900	-0.65107400	1.15922500
H	-2.17230900	-0.52010100	-0.44053300
C	2.21211800	2.15284200	0.04246500
H	2.15614000	2.09407900	1.15201100
H	3.29918200	2.18991400	-0.19177800
C	-2.47711400	-3.09619900	4.68477100
H	-1.88442400	-4.02857500	4.83252800
H	-3.50800900	-3.37703600	5.00689400
C	-2.52868000	-2.74721100	3.17905300
H	-3.37940100	-3.26222500	2.68340100
H	-2.76674900	-1.66605000	3.06519100
C	-4.60748100	-1.67683300	-0.99070800
H	-5.24193400	-2.52357500	-1.34578800
H	-4.20954300	-1.20427500	-1.92265200
B	0.00090900	3.72493500	0.19483300
B	-5.55887300	-0.59689800	-0.18152000
B	6.71728600	0.94653300	-0.13704500
B	-1.89559900	-1.94076300	5.72352400
Pt	0.73442400	-2.45767300	-0.63085400
C	6.39193100	2.08452500	-1.26473400
H	6.95851000	3.03252900	-1.11323700
H	6.55310500	1.76058400	-2.31938900
H	5.31588600	2.35764200	-1.20338800
C	6.29936900	1.46794000	1.35919400
H	5.25671500	1.85285600	1.34291200
H	6.32173400	0.69082800	2.15791100
H	6.93090300	2.31847300	1.70739000
C	-0.28231900	-1.71486100	5.62103700
H	0.22286400	-2.65679400	5.92741600
H	0.10712100	-1.47971400	4.60544800

H	0.10249500	-0.92536700	6.30850900
C	-2.35822400	-2.23882700	7.26245900
H	-2.01117100	-1.45749400	7.97646200
H	-3.46129600	-2.33522100	7.39364400
H	-1.92386500	-3.20358300	7.60724700
C	-6.04948000	-1.16101100	1.27136600
H	-6.38681300	-2.22335900	1.27044800
H	-5.19664600	-1.12370300	1.98289100
H	-6.86900100	-0.55976500	1.73359400
C	-4.93622100	0.92027200	-0.06756200
H	-4.24037600	0.98307000	0.79465400
H	-4.34015600	1.24548500	-0.95055600
H	-5.71918100	1.69598400	0.10335300
C	-1.21076700	2.82613000	-0.45016100
H	-1.11257600	2.61245300	-1.53874900
H	-1.26572800	1.83052300	0.03961000
H	-2.21586500	3.28443400	-0.30016400
C	-0.02379800	3.67410700	1.83067800
H	0.00674100	2.61308700	2.16025200
H	0.84291100	4.16575800	2.33003000
H	-0.94948900	4.11318200	2.26999000
C	-0.71456100	5.55323300	-1.52974000
C	0.03558600	6.33803900	0.51709400
C	-0.85290200	6.84159900	-2.03004300
H	-0.95449500	4.67478800	-2.14423100
C	-0.07334200	7.66123800	0.10595600
H	0.39353500	6.08370900	1.52380200
C	-0.52987600	7.96492300	-1.21105300
H	-1.21105500	6.96373100	-3.05970800
H	0.20264500	8.45057600	0.81603000
C	-6.81773400	0.27473100	-2.29377800
C	-7.98334300	-1.23965200	-0.98395300
C	-7.82931200	0.30793800	-3.24509000
H	-5.90163200	0.86902900	-2.41454500
C	-9.04753700	-1.26910900	-1.87789500
H	-7.99142100	-1.84792700	-0.06956900
C	-9.00432500	-0.48215300	-3.06655400
H	-7.69413800	0.94740400	-4.12617200
H	-9.90461200	-1.91278200	-1.64433000
C	-1.99734000	0.51658100	4.73754800
C	-4.01203100	-0.55254000	5.13125600
C	-2.62206300	1.55422500	4.05339900
H	-0.90913800	0.51162900	4.88000700

C	-4.72629000	0.44017200	4.47955500
H	-4.52028700	-1.42635100	5.56216200
C	-4.03470400	1.52868600	3.86356600
H	-1.99662300	2.35645900	3.64189000
H	-5.81570600	0.33896100	4.40959000
C	9.10591800	0.86092600	-1.23197200
C	8.95869300	0.17611600	0.97566000
C	10.45552700	0.53390400	-1.29537000
H	8.57844300	1.27664000	-2.10107200
C	10.30106000	-0.18095300	1.00761900
H	8.31451200	0.04962100	1.85638900
C	11.11291400	-0.01114400	-0.15309700
H	10.98807100	0.70517500	-2.23908800
H	10.70767100	-0.59224800	1.93982900
N	-0.27723200	5.28299600	-0.27429200
N	8.34905300	0.69170100	-0.12040900
N	-6.87361500	-0.48447200	-1.17083900
N	-2.65798700	-0.55294600	5.24299900
N	-10.02540300	-0.48641200	-3.98123600
N	-0.64929800	9.25330800	-1.66196300
N	-4.68840700	2.48301900	3.13644600
N	12.44124900	-0.35162100	-0.16923700
C	-9.91861400	0.31243800	-5.19354400
H	-9.04822400	0.00773300	-5.81701000
H	-10.83382700	0.18086000	-5.79854800
H	-9.81330800	1.39644200	-4.96515500
C	-11.19117600	-1.33117600	-3.76412200
H	-10.91981800	-2.40968200	-3.71656300
H	-11.71980100	-1.06930400	-2.82069000
H	-11.90105400	-1.19474300	-4.59981200
C	-6.13551000	2.41885900	2.98881000
H	-6.65087600	2.49982700	3.97202200
H	-6.47094800	3.25904700	2.35497100
H	-6.45308500	1.47345100	2.49895500
C	-3.92430600	3.51060800	2.44235700
H	-3.39275000	4.18324200	3.15268400
H	-3.17054600	3.06574600	1.75844500
H	-4.61193000	4.12342100	1.83266500
C	13.05996400	-0.92025400	1.01934100
H	14.12640500	-1.12363000	0.81339300
H	13.00582800	-0.22444000	1.88616400
H	12.57982700	-1.87855400	1.31972000
C	13.22115300	-0.17560700	-1.38546700

H	12.81670600	-0.77868300	-2.22919900
H	13.24803500	0.88904000	-1.70857400
H	14.26112400	-0.50102900	-1.20205100
C	-1.10014100	9.50865300	-3.02285100
H	-2.12007400	9.10178900	-3.20271400
H	-1.13424400	10.59924500	-3.19682700
H	-0.41503900	9.06201800	-3.77776400
C	-0.28903100	10.36404200	-0.79195400
H	-0.90567000	10.37919000	0.13411500
H	0.78155900	10.32447500	-0.49013600
H	-0.45720200	11.31583100	-1.32731800
C	2.14239800	-2.82133100	-2.09039000
C	3.11258700	-3.84404700	-1.95545800
C	2.22845600	-1.99786200	-3.23972100
C	4.13851100	-4.01490100	-2.90277500
H	3.07102100	-4.51556200	-1.08183600
C	3.25135100	-2.16283700	-4.19171900
H	1.48709100	-1.19342200	-3.38721000
C	4.21920500	-3.16882600	-4.02389300
H	4.88517500	-4.81526000	-2.76351600
H	3.29733300	-1.49551900	-5.06938000
H	5.02651200	-3.29663700	-4.76346400
C	-0.49290300	-3.88977400	-1.46778300
C	-0.84745700	-5.07978400	-0.78581300
C	-1.09213000	-3.67227100	-2.73343200
C	-1.78015800	-5.98868300	-1.31942300
H	-0.38875200	-5.30150600	0.19299600
C	-2.03252900	-4.57037300	-3.26918100
H	-0.82013700	-2.77347800	-3.31145100
C	-2.38888800	-5.73217600	-2.56063000
H	-2.03819200	-6.90261900	-0.75756300
H	-2.49042500	-4.36309700	-4.25156000
H	-3.12777400	-6.43659300	-2.97660200