# ELECTRONIC SUPPORTING INFORMATION

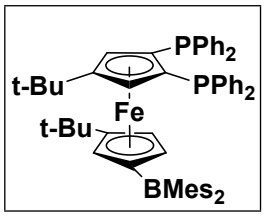
## CONTENT

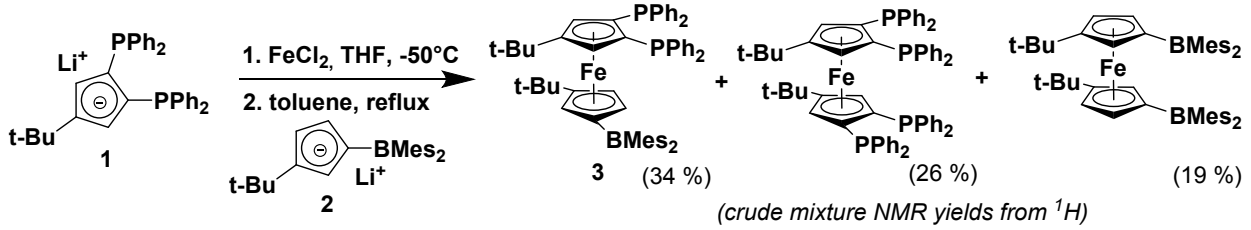
**General methods and synthesis**

All reactions were performed under argon atmosphere using Schlenk techniques or glovebox. Solvents were obtained from a solvent purification system or degassed and distilled from sodium benzophenone treatment under argon atmosphere prior to use. Deuterated solvent used (including $CDCl_3$, benzene-*d6*, toluene-*d8*, THF-*d8* and $CD_2Cl_2$) were dried over 3 Å molecular sieves. The functionalized cyclopentadienides were prepared following the reported procedures.[1,2] The identity and purity of the products were established at the "Pôle Chimie Moléculaire" PACSMUB, using multinuclear NMR, elemental analysis and high-resolution mass spectrometry. Elemental analysis was performed on an Analyzer CHNS/O Thermo Electron Flash EA 1112 Series and ICP-AES iCAP Thermo. Exact masses were obtained from a LTQ-Orbitrap XL (THERMO). $^{1}$H (δ in ppm) spectra (300.13, 500.13 or 600.13 MHz) and $^{11}$B NMR (δ in ppm) spectra (96.3 or 160.5 MHz) and $^{13}$C NMR (δ in ppm) spectra (75.5, 125.8 or 150.9 MHz) and $^{31}$P NMR (δ in ppm) spectra (121.5, 202.5 or 243.0 MHz were recorded at 300 K unless otherwise mentioned on a Bruker 300 Avance, Bruker 500 Avance DRX, or Bruker 600 Avance II spectrometer.

[1] Broussier, R.; Bentabet, E.; Mellet, P.; Blacque, O.; Boyer, P.; Kubicki, M. M.; Gautheron, B. *J. Organomet. Chem.* **2000**, *598*, 365.
[2] Lerayer, E. ; Renaut, P. ; Brandès, S. ; Cattey, H. ; Fleurat-Lessard, P. ; Bouhadir, G. ; Bourissou, D. ; Hierso, J.-C. *Inorg. Chem.*, **2017**, *56*, 1966.

**1,2-bis(diphenylphosphino)-1'-(dimesitylboryl)-3',4-di(tert-butyl)- ferrocene (3).**




A solution of lithium 4-*tert*-butyl-1,2-bis(diphenylphosphino)cyclopentadienide **1** (0.348 g, 0.701 mmol) in 10 mL of THF was added dropwise during 5 min at –50 °C to a suspension of iron dichloride (0.087 g, 0.686 mmol) in 20 mL of THF, suspension previously refluxed independently for a better dispersion. After 1 h stirring at –50 °C, a solution of lithium 1-dimesitylboryl-3-*tert*-butylcyclopentadienide **2** complexed with one equivalent of DME (0.327 g, 0.701 mmol) in 10 mL of THF was added dropwise during 5 min at –50 °C. After 1 h at –50 °C, the reaction mixture was warmed to room temperature. The volatiles were removed under vacuum, 40 mL of toluene was added and the mixture was refluxed during 17 h. After filtration on alumina, 0.5 g of purple-brown crystalline solid containing **3** were isolated (34% NMR yield). Crystallization in a toluene/chloroform mixture gave **3** as a purple crystalline air and moisture-stable solid (0.20 g, 0.109 mmol, 32% yield).

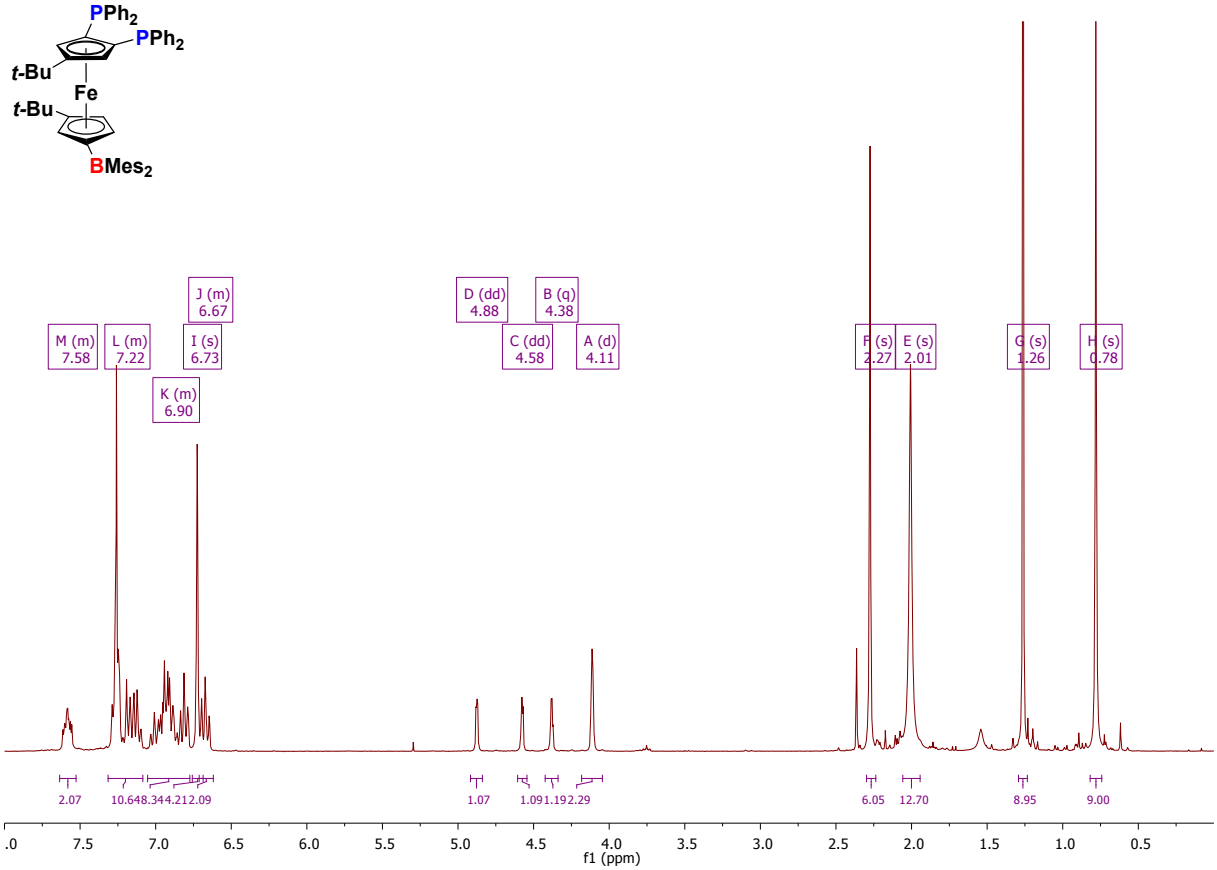
$^{1}H\{^{31}P\}$ NMR (300 MHz, $CDCl_3$): δ 7.64-7.53 (2 H, m, Ph), 7.31-7.08 (8 H, m, Ph), 7.05-6.77 (8 H, m, Ph), 6.73 (4 H, s, *m*-C*H*), 6.71-6.62 (2 H, m, Ph), 4.88 (1 H, dd, *J* 2.6, 1.3, CpB-C*H*), 4.58 (1 H, dd, *J* 2.6, 1.4, CpB-C*H*), 4.38 (1 H, q, *J* 1.8, CpP-C*H*), 4.11 (2 H, m, CpP-C*H* and CpB-C*H*), 2.27 (6 H, s, *p*-C$H_3$), 2.01 (12 H, brs, *o*-C$H_3$), 1.26 (9 H, s, *t-Bu*), and 0.78 (9 H, s, *t-Bu*).

$^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$): δ 139.97 (*o*-*C*$H_3$), 139.15 (dd, *J* 13.6, 3.8, Ph-*C*H), 138.30 (dd, *J* 13.9, 3.8, Ph-*C*H), 137.44 (*p*-*C*$H_3$), 136.17 (d, *J* 23.5, Ph-*C*H), 134.69 (d, *J* 21.8, Ph-*C*H), 134.33 (d, *J* 21.2, Ph-*C*H), 133.21 (d, *J* 20.7, Ph-*C*H), 129.19, 128.39 (d, *J* 8.1, Ph-*C*H), 128.26, 128.26-128.01 (m), 127.70, 127.61 (dd, *J* 7.3, 2.6, Ph-$C_Q$), 109.00 (CpB-$C_Q$), 108.23 (d, *J* 3.1, CpP-$C_Q$), 100.22, 99.93 (CpB-*C*H), 80.53 (CpB-*C*H), 78.61 (m, CpP-*C*H, CpB-*C*H), 73.15 (d, *J* 2.9, CpP-*C*H), 69.70 (CpB-*C*H), 32.62 (C(*C*$H_3$)$_3$), 31.88 (C(*C*$H_3$)$_3$), 30.90 (*C*(CH$_3$)$_3$), 30.74 (*C*(CH$_3$)$_3$), 24.56 (*o*-*C*$H_3$), and 21.16 (*p*-*C*$H_3$). $^{11}B$ signal is hardly detectable (see ref. [22] main text).

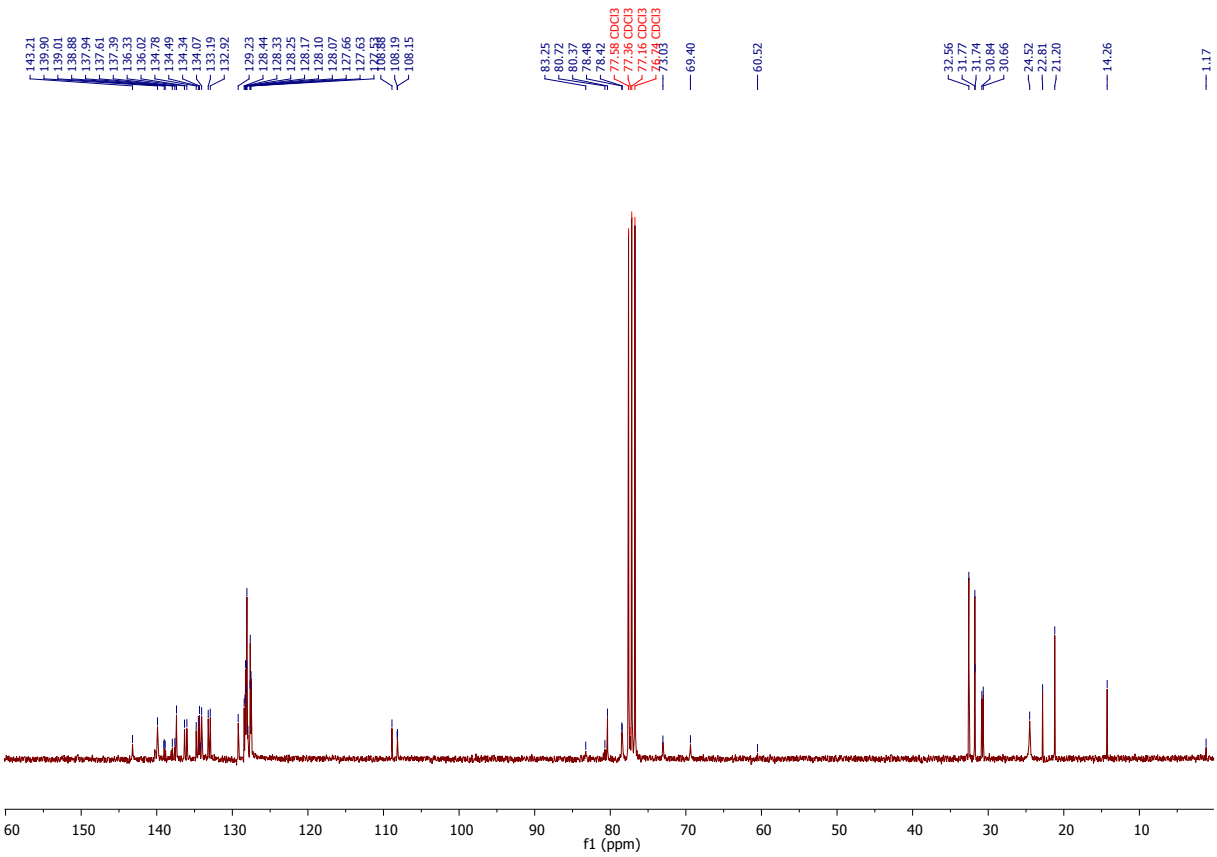
$^{31}P\{^{1}H\}$ NMR (121 MHz, $CDCl_3$): δ –18.3 (broad d, *J* 60.0), and –23.7 (d, *J* 59.8).

Elemental analysis for $C_{60}H_{65}BFeP_2$. Calculated: C (78.78 %), H (7.16%). Obtained: C (78.07%), H (7.00%). ESI-MS: $[M+H]^+$: m/z exp = 915.40505, m/z theo = 915.40767, delta = –2.867 ppm.

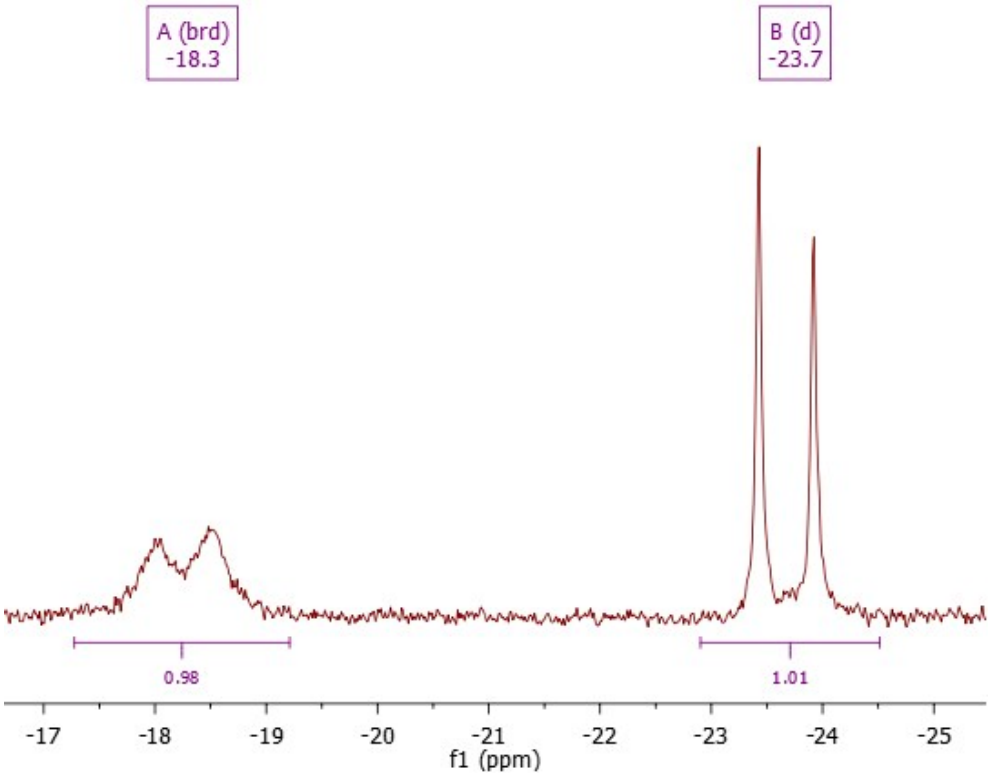
RMN $^{1}H$, $CDCl_3$, 300 MHz



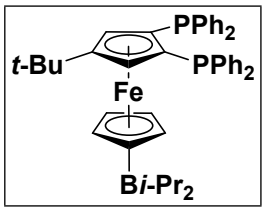

RMN $^{13}C$, $CDCl_3$, 75 MHz



RMN $^{31}P$, $CDCl_3$, 121 MHz ($J_{PP'}$ = 60 Hz)



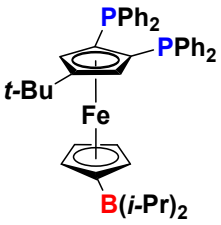
**1,2-bis(diphenylphosphino)-1'-(di-isopopryl)-4-(tert-butyl)-ferrocene (3').**

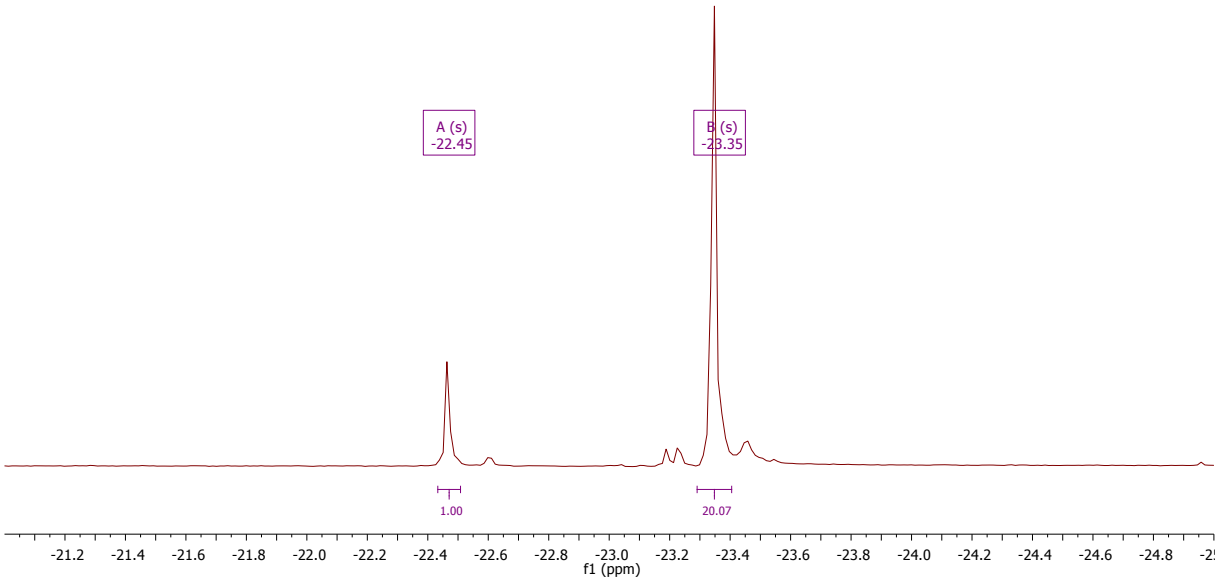



A solution of lithium 4-*tert*-butyl-1,2-bis(diphenylphosphino)cyclopentadienide **1** (0.59 g, 1.18 mmol in 5 mL of THF[1] was added dropwise during 10 min at –50 °C to a suspension of iron dichloride (0.14 g, 1.1 mmol) in 3 mL of THF and the mixture is stirred during 1 h at –50 °C and during 2 h slowly rise up to room temperature. Then, a solution of lithium 1-di(*iso*-propyl)borylcyclopentadienide (0.21 g, 1.2 mmol) in 3 mL of THF was added dropwise during 10 min at –50 °C. During 4 h, the solution slowly rose up to room temperature, then solvent was removed and 5 mL of toluene was added and the mixture refluxed during 10 h. The solution was evaporated in vacuo, giving a mixture containing **3'** in 44% NMR yield. Crystallization in toluene gave 170 mg (0.188 mmol, 17% yield, 82% purity) of **3'** as an orange crystalline solid. The 18 % of impurity was the deborylated product 1,2-bis(diphenylphosphino)-4-(tert-butyl)-ferrocene.[1]

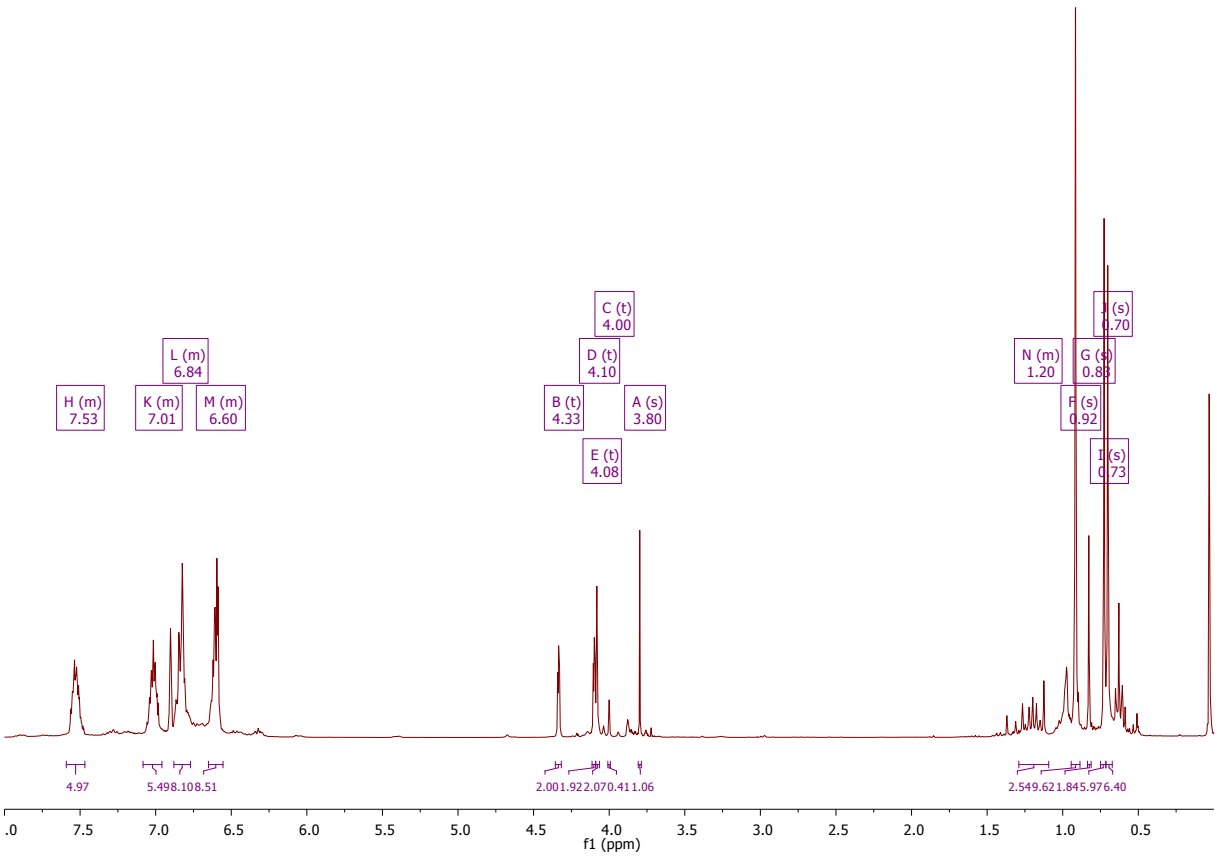
$^{1}$H {$^{31}$P} NMR (500 MHz, C6D6): δ 7.85 - 7.72 (4 H, m, Ph), 7.31 - 7.22 (4 H, m, Ph), 7.14 - 7.01 (6 H, m, Ph), 6.91 - 6.81 (6 H, m, Ph), 4.60 - 4.57 (2 H, m, Cp-CH), 4.38 - 4.35 (2 H, m, Cp-CH), 4.35 - 4.32 (2 H, m, Cp-CH), 1.46 (2 H, hept, J 7.4, i-Pr-CH), 1.18 (9 H, s, t-Bu), and 0.97 (12 H, d, J 7.3, i-Pr-CH3).
$^{13}$C{$^{1}$H} NMR (75 MHz, C6D6): δ 140.12 (t, J 5.6, Ph-CH), 138.68 (t, J 4.1, Ph-CH), 135.96 (t, J 11.8, Ph-CH), 133.34 (t, J 10.1, Ph-CH), 129.41 (Ph-CH), 128.75 - 128.37 (m, Ph-CH), 128.19 - 127.77 (m, Ph-CH), 107.70, 82.36 (d, J 8.6, CpP-CH), 82.25 (d, J 8.9, CpP-CH), 77.66 (CpB-CH), 75.89 (CpB-CH), 71.49 (CpB-CH), 31.97, 31.84, 30.40, 23.65, 23.06, 20.23, and 14.36.
$^{31}$P{$^{1}$H} NMR (202 MHz, $C_6D_6$): δ –23.4 (s).

RMN $^{31}P$, $C_6D_6$, 202 MHz

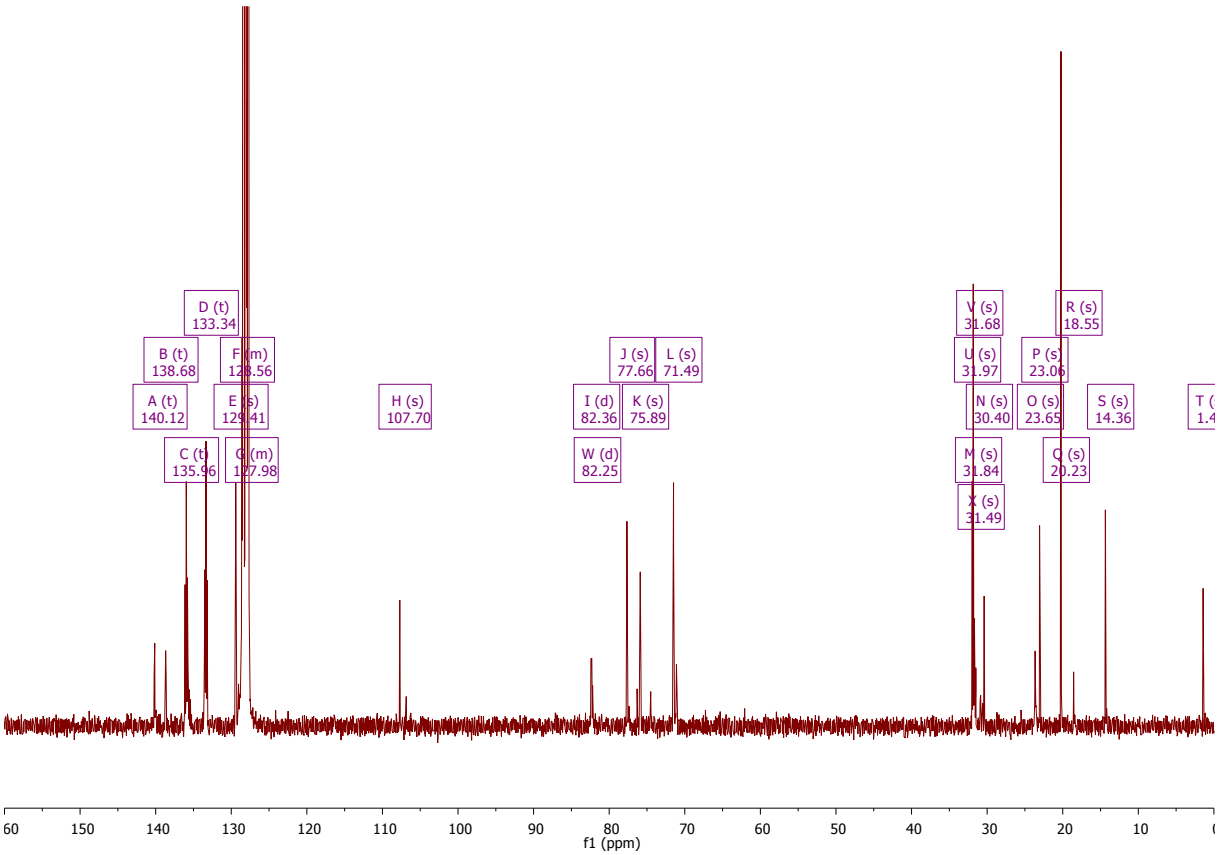


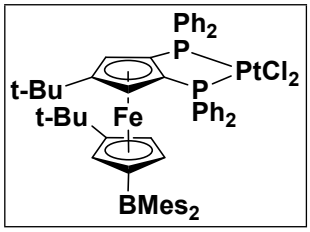

RMN $^{1}H$, $C_6D_6$, 300 MHz



RMN $^{13}C$, $C_6D_6$, 75 MHz



**1,2-bis(diphenylphosphino)-1'-(dimesitylboryl)-3',4-di(tert-butyl)-ferrocene platinum dichloride (4)**




1,2-bis(diphenylphosphino)-1'-(dimesitylboryl)-3,3'-di(*tert*-butyl)-ferrocene **3** (9.5 mg, 0.0104 mmol) and (1,5-cyclooctadiene)platinum dichloride (3.9 mg, 0.0104 mmol) were solubilized in 1 mL of $CD_2Cl_2$ at room temperature, to give quantitatively **4** in a red-orange solution, from which crystals were grown from slow evaporation.

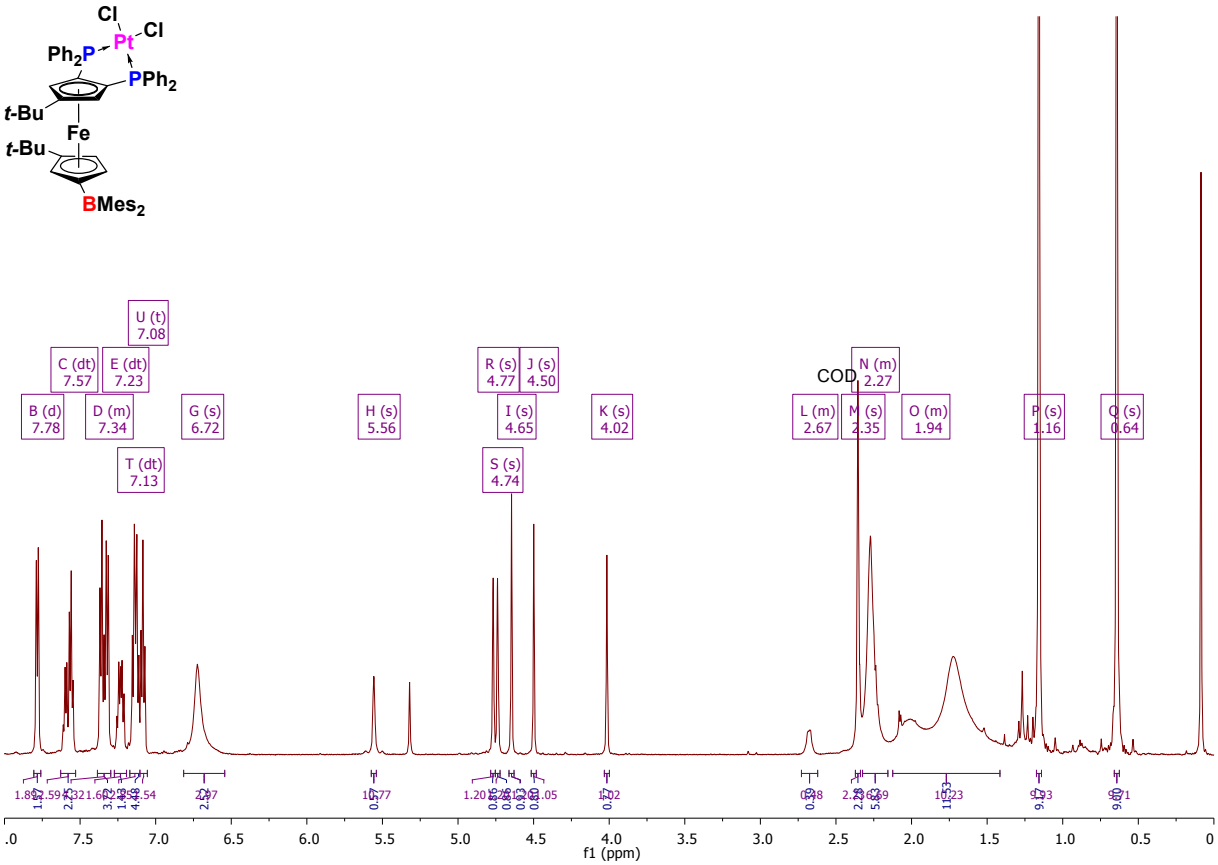
$^1H\{^{31}P\}$ NMR (600 MHz, $CD_2Cl_2$): δ 8.06 (2 H, d, *J* 7.3, Ph), 7.78 (2 H, d, *J* 7.7, Ph), 7.57 (3 H, dt, *J* 14.8, 7.2, Ph), 7.39-7.30 (4 H, m, Ph), 7.23 (2 H, dt, *J* 13.7, 7.5, Ph), 7.13 (3 H, dt, *J* 10.2, 7.7, Ph), 7.08 (2 H, t, *J* 7.6, Ph), 6.72 (4 H, brs, *m*-C*H*), 4.77 (1 H, s, CpB-C*H*), 4.74 (1 H, s, CpB-C*H*), 4.65 (1 H, s, CpP-C*H*), 4.50 (1 H, s, CpP-C*H*), 4.02 (1 H, s, CpB-C*H*), 2.27 (6 H, brs, *p*-C$H_3$), 2.12-1.42 (12 H, m, *o*-C$H_3$), 1.16 (9 H, s, *t-Bu*), and 0.64 (9 H, s, *t-Bu*).

$^{13}C\{^1H\}$ NMR (126 MHz, $CD_2Cl_2$): δ 136.78 (d, *J* 11.9, Ph-*C*H), 135.69 (d, *J* 11.8, Ph-*C*H), 132.91, 132.52 (dd, *J* 38.6, 10.3, Ph-*C*H), 131.45, 130.90 (dd, *J* 6.4, 2.8, Ph-*CQ*), 130.35, 128.90, 128.47 (d, *J* 11.2, Ph-*C*H), 128.12 (d, *J* 12.5, Ph-*C*H), 109.21, 82.24 (CpB-*C*H), 75.27 (CpB-*C*H), 73.19 (CpB-*C*H), 72.11 (dd, *J* 11.8, 3.2, CpP-*C*H), 67.41 (dd, *J* 12.6, 2.7, CpP-*C*H), 32.31 (C(*C*$H_3$)$_3$), 31.73 (C(*C*$H_3$)$_3$), 31.30 (*C*($CH_3$)$_3$), 30.42 (*C*($CH_3$)$_3$), 21.13 (*p*-*C*$H_3$).

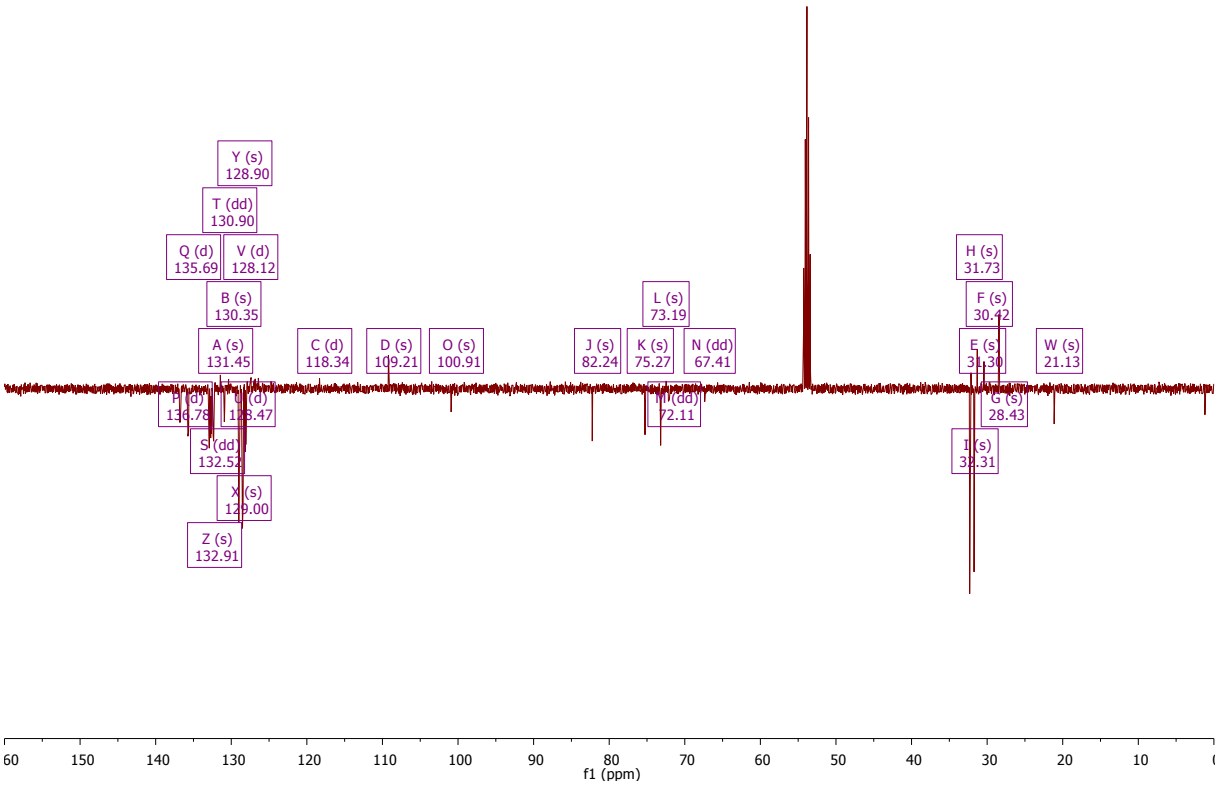
$^{31}P\{^1H\}$ NMR (121 MHz, $CDCl_3$): δ 22.0 (d $J_{PP}$ = 11.5 Hz, $J_{PPt}$ = 3636 Hz), and 21.6 (d, $J_{PP}$ = 11.5 Hz, $J_{PPt}$ = 3636 Hz).

ESI-MS: $[M+Na]^+$: m/z exp = 1202.29120, m/z theo = 1202.29210, delta = –0.747 ppm.

RMN $^{1}H$, $CD_2Cl_2$, 600 MHz



RMN $^{13}C$, $CD_2Cl_2$, 125 MHz




RMN $^{31}P$, $CD_2Cl_2$, 121 MHz

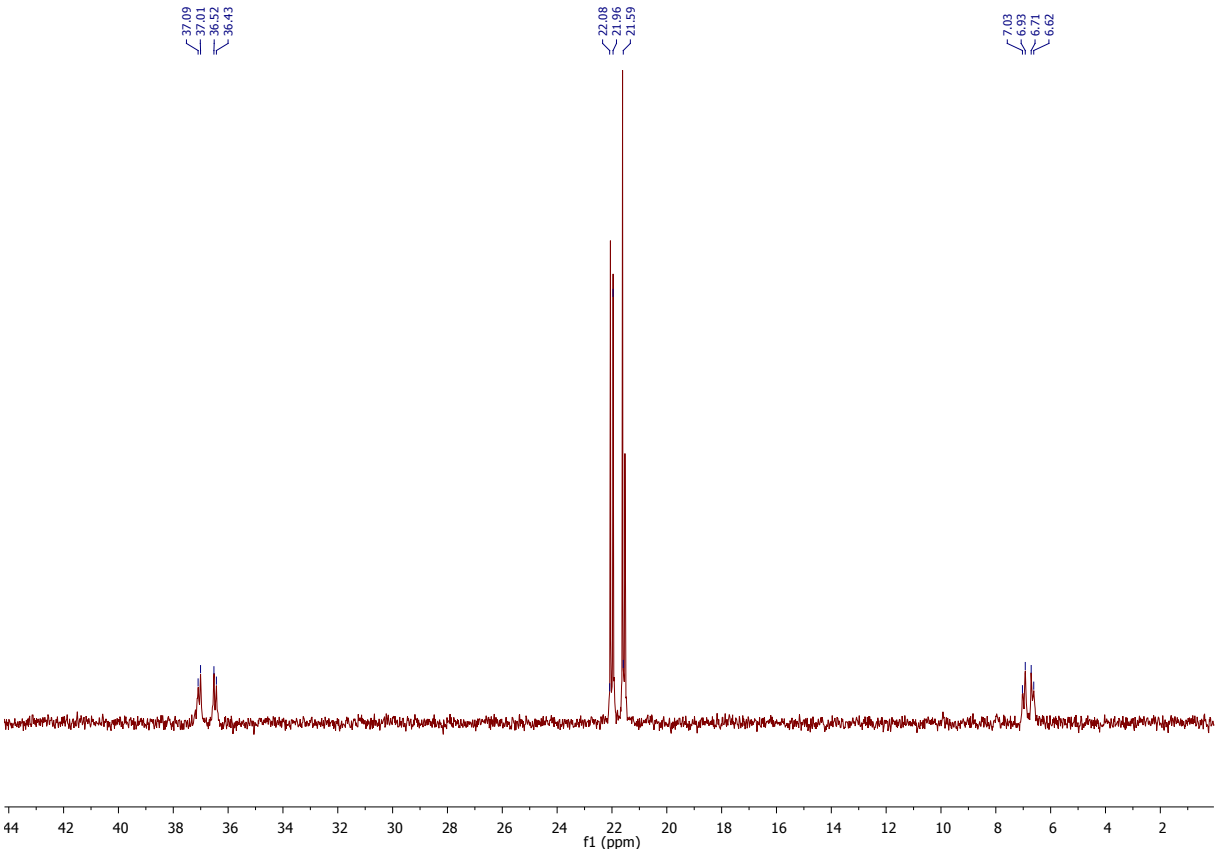


**Figure S1: Complementary views of the solid-state structure of 3 (in mirror images of main text representation since both enantiomers are present in the unit cell)**

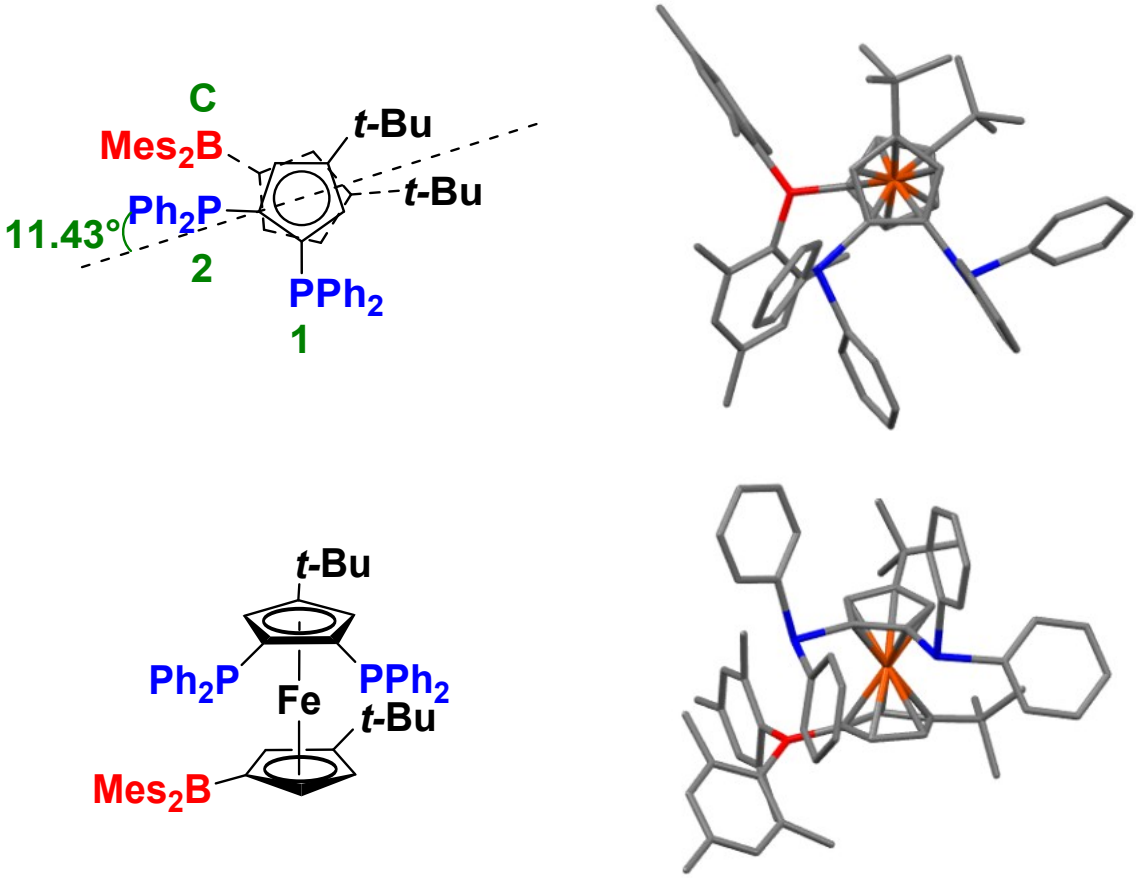
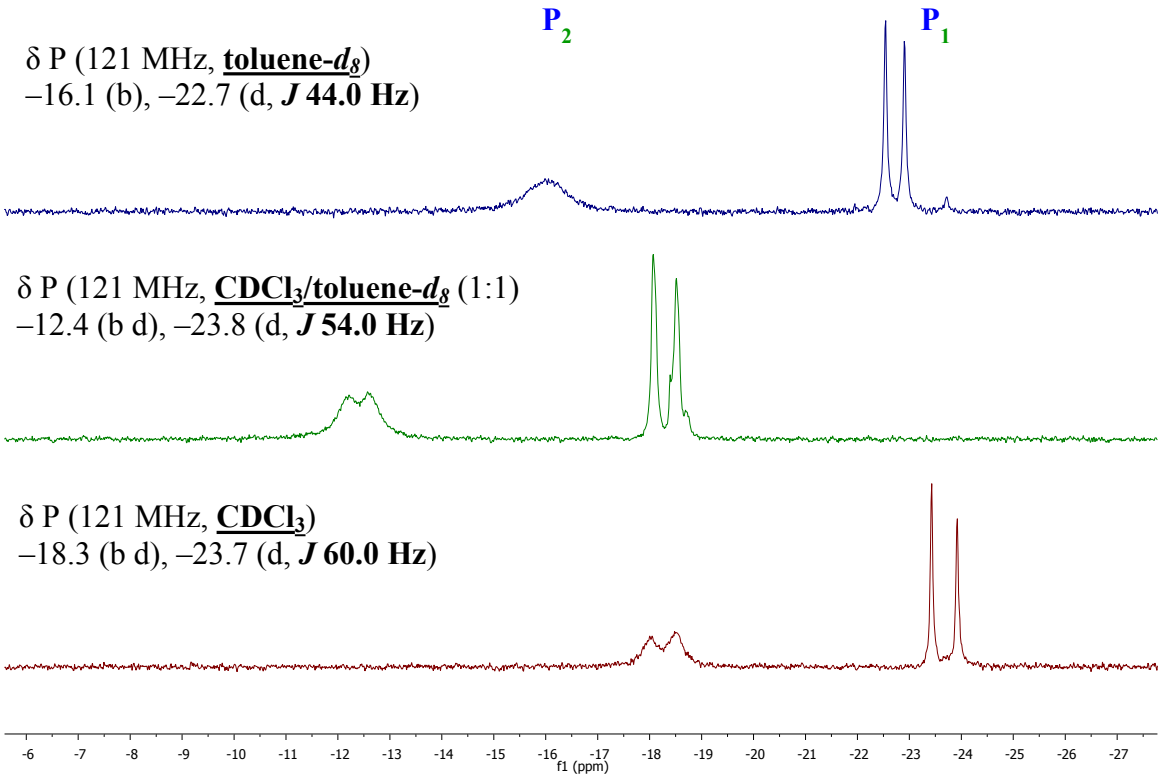


**Figure S2: Solvent dependence of $^{TS}J_{PP'}$ coupling in 3 ($^{31}$P NMR, 121 MHz, 300 K)**




Gradual decrease of solvent polarity correlates weaker coupling constant with $J_{PP'}$ decrease from 60.0 Hz in $CDCl_3$, 54.0 Hz in a 1:1 $CDCl_3$:toluene mixture, down to 44.2 Hz in pure toluene. Solvent dependency is known for "through-space" coupling involving weak hydrogen bonding interaction.[3] Here, intercalation of toluene (from π-stacking with phenyl) presumably does not facilitate phosphorus lone-pair overlap at the origin of TS spin coupling, contrary to more polar chloroform solvent.

[3] Hierso, J.-C. *Chem. Rev.* **2014**, *114*, 4838.

**Figure S3: Variable temperature NMR monitoring of 3 in the range 220-325 K ($CDCl_3$, 243 MHz)**

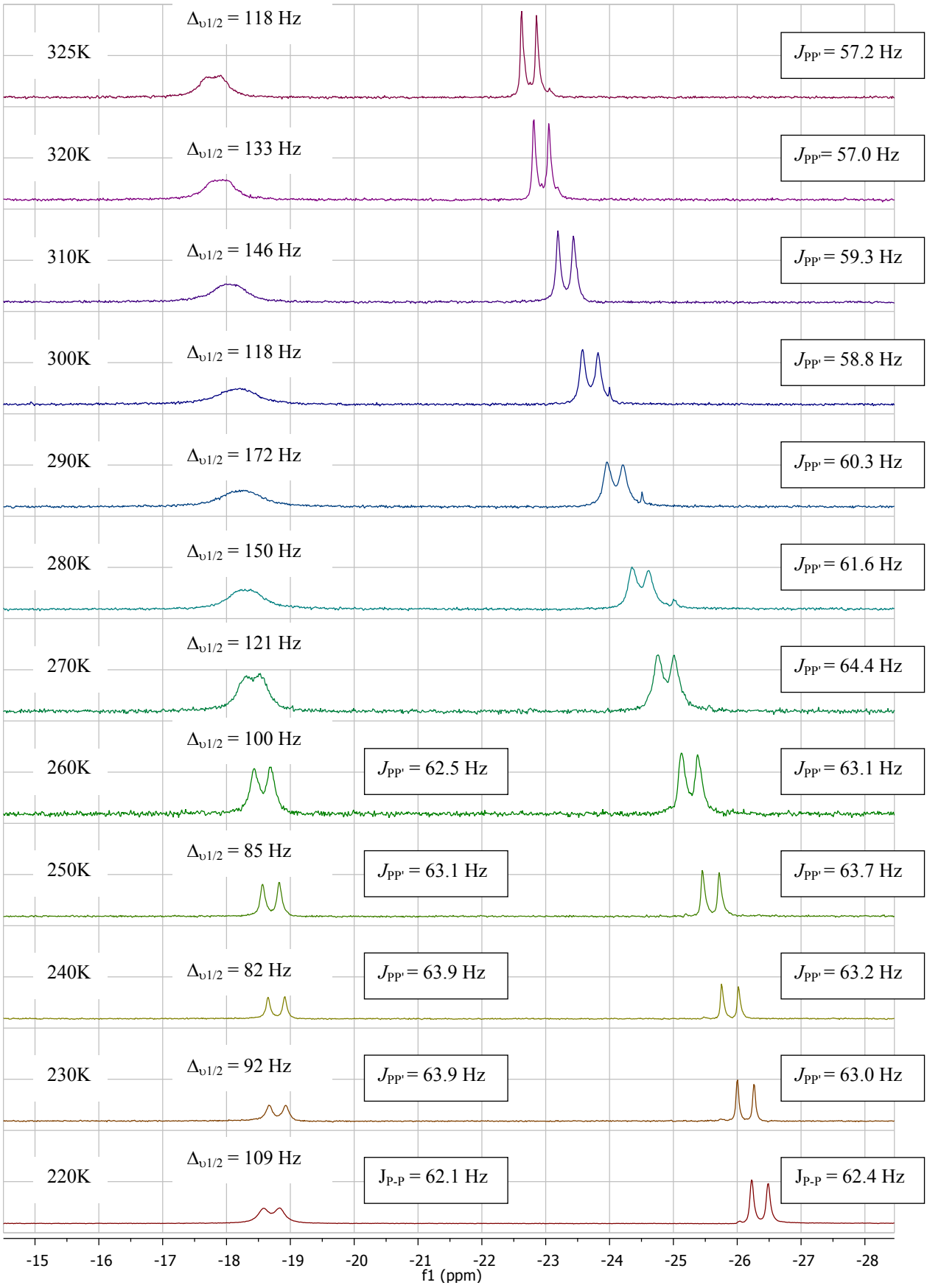


**Figure S4: $^{31}P$ {$^{11}B$,$^{1}H$} NMR monitoring of 3 at variable $^{11}B$ frequency –100 to +100 ppm (300 K, $CDCl_3$)**

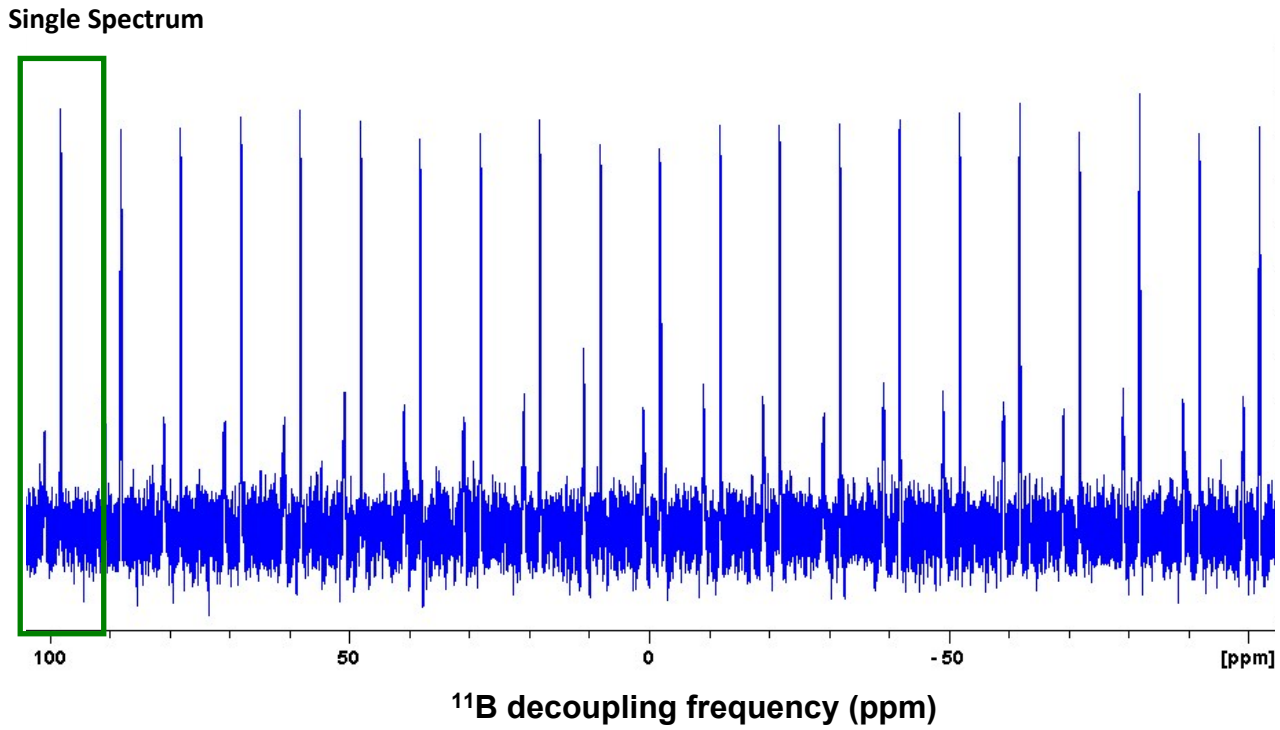
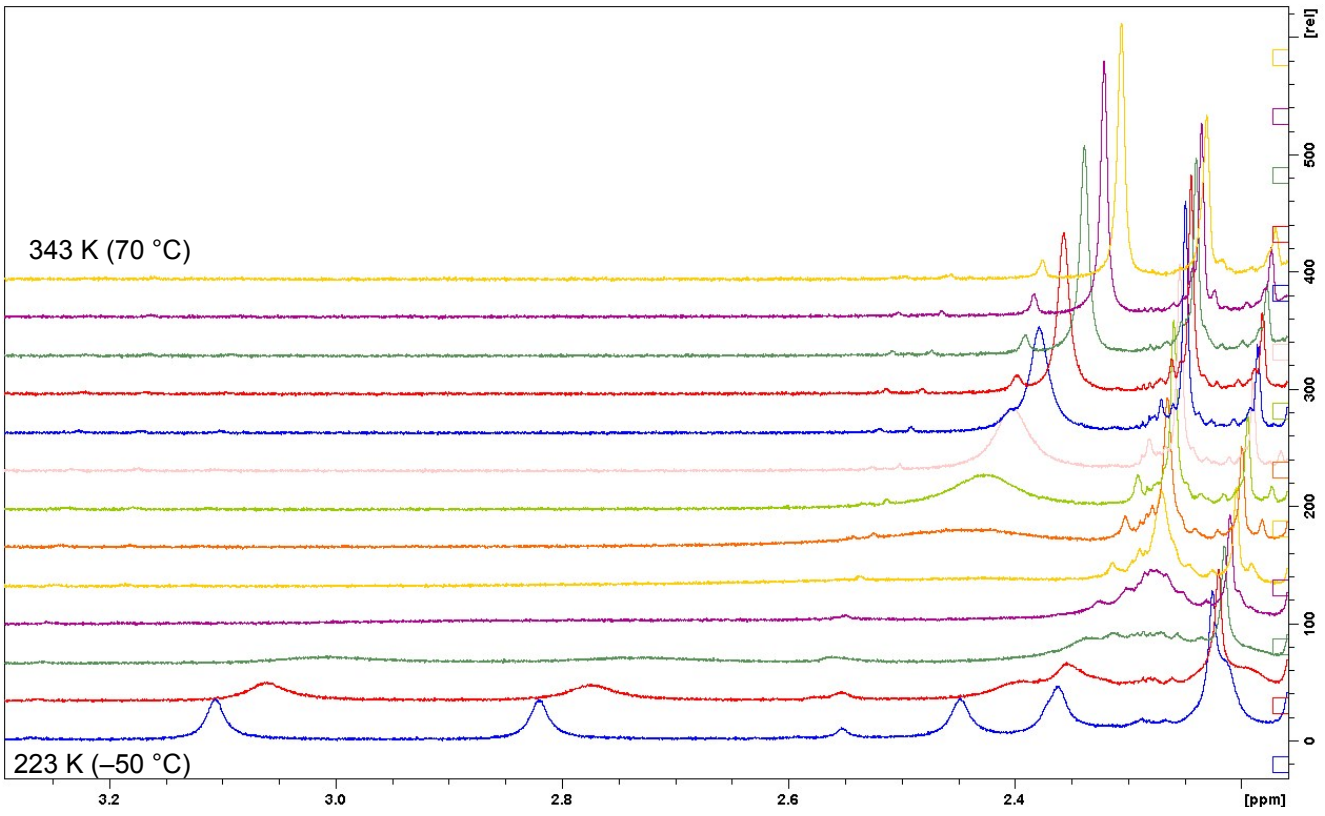


**Figure S5: $^{1}$H NMR variable temperature monitoring of 3 in the methyl (mesityl-B) region between 223-343 K (10 K, toluene-d8, 400 MHz)**

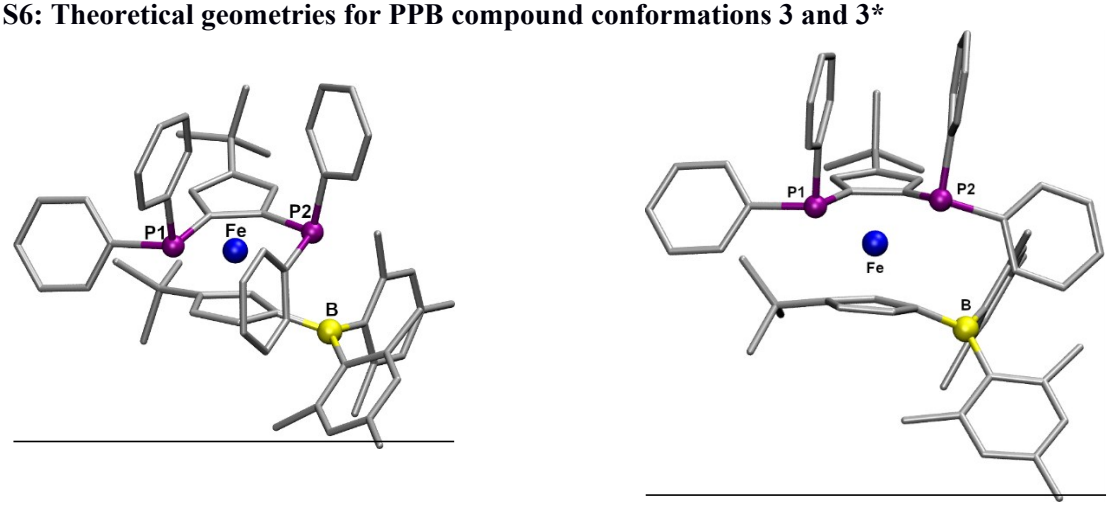


## Computational Details

Quantum mechanics calculations were performed with the Gaussian16 software package.[1] Energy and forces were computed by density functional theory with the global hybrid B3PW91 exchange-correlation functional,[2] with the Pople 6-31+G(d,p) basis sets. Dispersion effects were taken into account using the empirical correction proposed by Grimme with a Becke-Johnson damping.[3] Atoms In Molecules (AIM) analysis were performed with the AIMall software.[4] Topological analyses of the Electron Localization Function (ELF) were performed with the TopChem2 suite.[5]

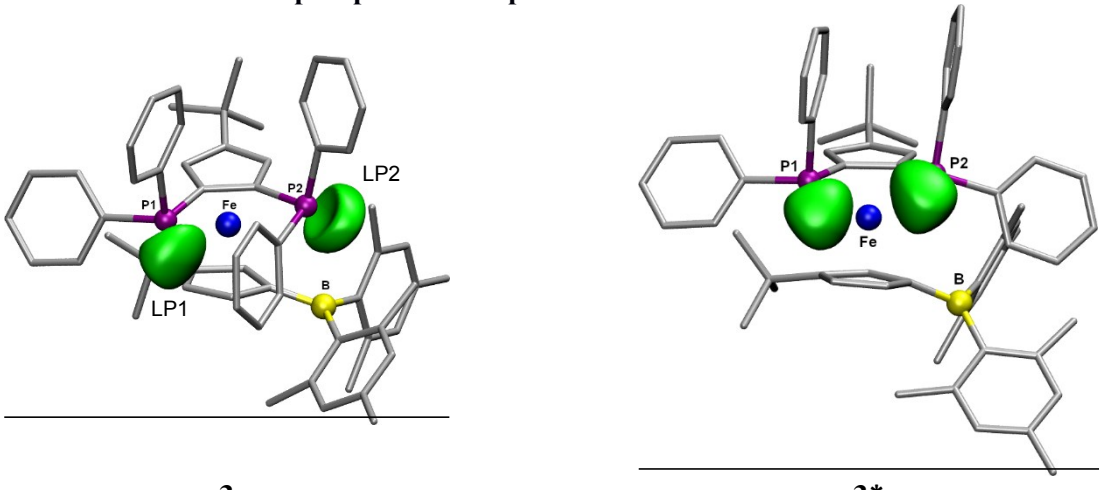
Starting from the X-Ray structure determined for platinum complex **4**, we optimized the geometry of **3***, as a conformer of PPB ligand found in its conformation **3**. In conformer **3*** the two phosphorus lone pairs point towards each other, ready for chelation to transition metals. This conformer was found to be fairly stable but is located in energy 2.6 kcal mol$^{-1}$ higher than conformer **3** (Fig. S6). Phosphorus lone pairs space-occupation were then visualized within the ELF analysis as displayed in Fig. S7.

**Figure S6: Theoretical geometries for PPB compound conformations 3 and 3***




**Conformation 3:** ΔE = 0 kcal/mol **Conformation 3*:** ΔE = 2.6 kcal/mol

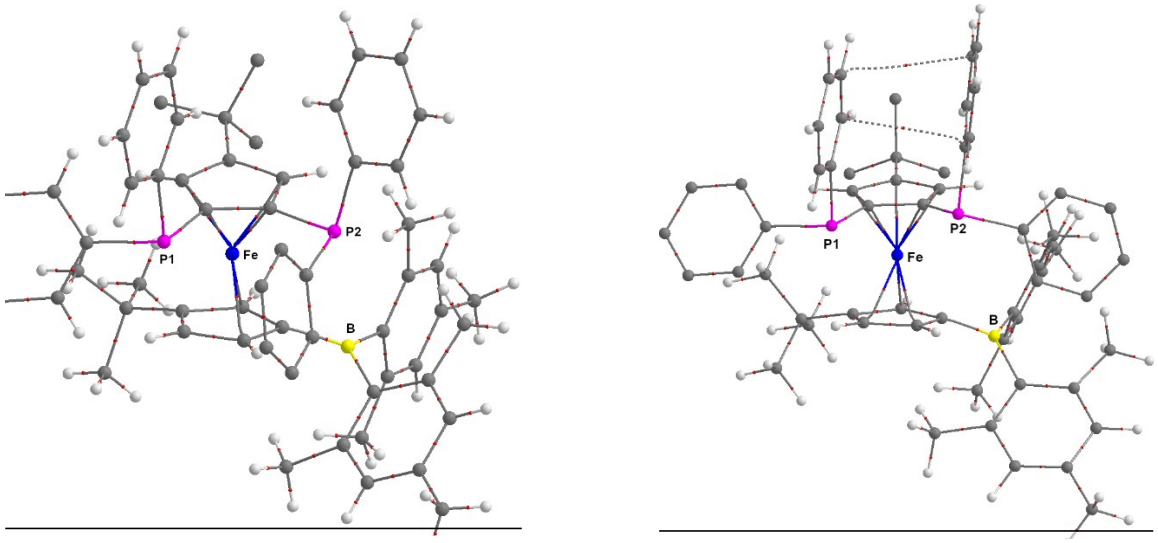
**Figure S7: Visualization of the phosphorus lone pairs basins in conformations 3 and 3***




**3** **3***

While the phosphorus lone pairs are facing each other in **3***, they are avoiding this situation in **3**. The angle between the lone pair of P1 (LP1), P2 and P2 is 81.4° and the angle P1-P2-LP2 is 140.3°.

In the X-ray structure corresponding to optimized conformer **3**, the lone pair of phosphorus P2 is pointing in the direction of the boron atom: the angle LP2–P2–B is only 45.1 °, the question of an interaction between these two atoms is thus pertinent. We thus performed AIM analysis of the electronic structure of **3**. The resulting Bond Critical Points (BCP) and Bond Path are displayed in Fig. S8. No BCP were found between P2 and B in both **3** and **3*** conformations. This rules out a strong interaction between these two atoms, in agreement with the full NMR study.




**Conformation 3** **Conformation 3***

**Figure S8: Main BCP and Bond Path in conformations 3 and 3* within the AIM approach**

## Reference for the theoretical computations


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

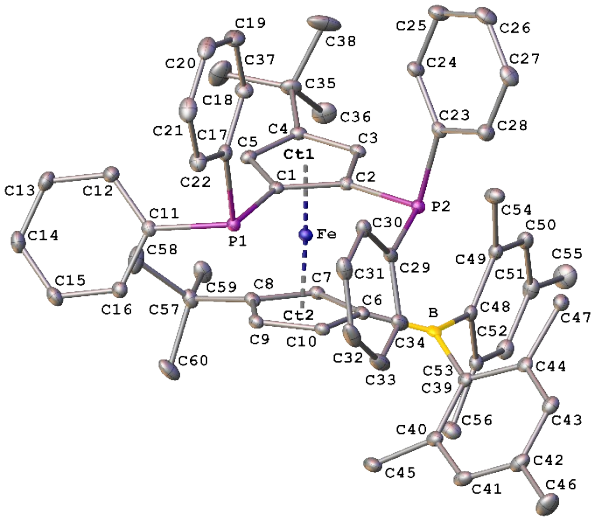
[2] A. D. Becke, "Density-functional thermochemistry. III. The role of exact exchange," *J. Chem. Phys.***1993**, *98,* 5648-52. DOI: 10.1063/1.464913

[3] S. Grimme, S. Ehrlich and L. Goerigk, "Effect of the damping function in dispersion corrected density functional theory," *J. Comp. Chem.* **2011**, *32,* 1456-65. DOI: 10.1002/jcc.21759

[4] AIMAll (Version 19.02.13), Todd A. Keith, TK Gristmill Software, Overland Park KS, USA, 2019 (aim.tkgristmill.com)

[5] a) D. Kozlowski and J. Pilmé "New Insights in Quantum Chemical Topology Studies Using Numerical Grid-based Analyses" *J. Comput. Chem.* **2011**, *32*, 3207–3217, 2011; b) http://www.lct.jussieu.fr/pagesperso/pilme/topchempage.html

# Crystal Data and Experimental




**Experimental.** A single clear light red prism-shaped crystals of C**ompound 3** with dimensions of (0.20×0.15×0.05) mm$^3$ was mounted on a Nonius Kappa Apex II diffractometer. The crystal was kept at $T$ = 115 K during data collection. Data were measured using $\phi$ and $\omega$ scans using MoK$_\alpha$ radiation (λ = 0.71073). Cell parameters were retrieved and refined using SAINT. Data reduction was performed using the SAINT software which corrects for Lorentz polarisation. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the **ShelXS** structure solution program, using the Direct Methods solution method. The model was refined with version 2014/7 of **XL** (Sheldrick, 2008) using Least Squares minimisation.

**Crystal Data.** $C_{60}H_{65}BFeP_2$, $M_r$ = 914.72, monoclinic, P2$_1$/n (No. 14), a = 14.0236(5) Å, b = 19.7055(5) Å, c = 18.3538(6) Å, $\beta$ = 99.8570(10)°, $\alpha$ = $\gamma$ = 90°, $V$ = 4997.1(3) Å$^3$, $T$ = 115 K, $Z$ = 4, $Z'$ = 1, $\mu$(MoK$_\alpha$) = 0.404, 30301 reflections measured, 11419 unique ($R_{int}$ = 0.0374) which were used in all calculations. The final $wR_2$ was 0.1008 (all data) and $R_1$ was 0.0465 (I > 2(I)).

| **Compound** | **3** |
|---|---|
| **N° CCDC** | **1902394** |
| Formula | $C_{60}H_{65}BFeP_2$ |
| $D_{calc.}$/ g cm$^{-3}$ | 1.216 |
| $\mu$/mm$^{-1}$ | 0.404 |
| Formula Weight | 914.72 |
| Colour | clear light red |
| Shape | prism |
| Size/mm$^3$ | 0.20×0.15×0.05 |
| $T$/K | 115 |
| Crystal System | monoclinic |
| Space Group | P2$_1$/n |
| $a$/Å | 14.0236(5) |
| $b$/Å | 19.7055(5) |
| $c$/Å | 18.3538(6) |
| $\alpha$/° | 90 |
| $\beta$/° | 99.857(1) |
| $\gamma$/° | 90 |
| V/Å$^3$ | 4997.1(3) |
| $Z$ | 4 |
| $Z'$ | 1 |
| Wavelength/Å | 0.71073 |
| Radiation type | MoK$_\alpha$ |
| $\Theta_{min}$/° | 2.478 |
| $\Theta_{max}$/° | 27.496 |
| Measured Refl. | 30301 |
| Independent Refl. | 11419 |
| Reflections Used | 9473 |
| $R_{int}$ | 0.0374 |
| Parameters | 583 |
| Restraints | 0 |
| Largest Peak | 0.428 |
| Deepest Hole | -0.381 |
| GooF | 1.093 |
| $wR_2$ (all data) | 0.1008 |
| $wR_2$ | 0.0923 |
| $R_1$ (all data) | 0.0617 |
| $R_1$ | 0.0465 |

A clear light red prism-shaped crystal with dimensions 0.20×0.15×0.05 $mm^3$ was mounted on a mylar loop with oil. X-ray diffraction data were collected using a Nonius Kappa Apex II diffractometer with a Oxford Cryosystems low-temperature device, operating at $T$ = 115 K. Data were measured using $\phi$ and $\omega$ scans using Mo$K_\alpha$ radiation (X-ray tube, 50 kV, 32 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker). The maximum resolution achieved was $\Theta$ = 27.496°.

Cell parameters were retrieved using the **SAINT** (Bruker, V8.34A, 2013) software and refined using **SAINT** (Bruker, V8.34A, 2013) on 44900 reflections. Data reduction was performed using the **SAINT** (Bruker, V8.34A, 2013) software which corrects for Lorentz polarisation. No absorption correction was performed. The absorption coefficient $\mu$ of this material is 0.404 at this wavelength ($\lambda$ = 0.71073).

The structure was solved in the space group $P2_1/n$ (# 14) by Direct Methods using the **ShelXS** structure solution program and refined by Least Squares using version 2014/7 of **XL** (Sheldrick, 2008). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

**Table 1**: Fractional Atomic Coordinates (×$10^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×$10^3$) for **Compound 3**. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{ij}$.

| Atom | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| C1 | 9817.9(14) | 8771(1) | 2569.3(11) | 15.0(4) |
| C2 | 9197.1(14) | 8248.2(10) | 2789.0(11) | 15.6(4) |
| C3 | 8689.7(14) | 7952.6(10) | 2116.6(11) | 17.2(4) |
| C4 | 8989.0(15) | 8258.6(10) | 1493.3(11) | 18.1(4) |
| C5 | 9670.7(14) | 8769.8(10) | 1776.2(11) | 17.8(4) |
| C6 | 7076.4(14) | 9187.9(10) | 2483.5(11) | 16.8(4) |
| C7 | 7061.8(14) | 9382.9(10) | 1723.2(11) | 16.7(4) |
| C8 | 7778.3(14) | 9883.1(10) | 1678.5(12) | 17.6(4) |
| C9 | 8284.2(14) | 9986.1(10) | 2415.1(12) | 17.5(4) |
| C10 | 7874.7(14) | 9562.8(10) | 2904.4(11) | 15.9(4) |
| C11 | 11001.4(14) | 9966.5(10) | 2573.8(11) | 17.5(4) |
| C12 | 11522.3(15) | 9829.9(11) | 2009.4(12) | 22.3(4) |
| C13 | 11823.5(17) | 10351.7(12) | 1593.0(13) | 27.2(5) |
| C14 | 11618.8(17) | 11020.8(12) | 1740.8(13) | 28.5(5) |
| C15 | 11103.7(17) | 11167.2(11) | 2300.8(13) | 26.6(5) |
| C16 | 10800.6(15) | 10644.0(11) | 2716.5(12) | 21.1(4) |
| C17 | 11739.4(15) | 8794.9(10) | 3306.1(12) | 18.9(4) |
| C18 | 11821.0(16) | 8195.1(11) | 2920.2(13) | 24.2(5) |
| C19 | 12693.2(18) | 7837.5(12) | 3026.1(15) | 31.8(5) |
| C20 | 13482.8(17) | 8078.3(13) | 3511.6(15) | 32.5(6) |
| C21 | 13410.6(17) | 8671.7(13) | 3897.2(14) | 32.0(6) |
| C22 | 12541.3(15) | 9021.5(12) | 3803.1(13) | 24.8(5) |
| C23 | 9711.6(15) | 7126.1(10) | 3752.0(12) | 18.2(4) |
| C24 | 10111.2(16) | 6840.0(11) | 3178.9(12) | 22.7(4) |
| C25 | 10607.4(18) | 6226.1(12) | 3279.6(14) | 29.7(5) |
| C26 | 10699.9(18) | 5888.0(11) | 3950.1(14) | 30.0(5) |
| C27 | 10310.0(17) | 6167.7(11) | 4523.9(13) | 27.8(5) |
| C28 | 9819.5(16) | 6782.1(11) | 4428.8(12) | 23.1(4) |
| C29 | 9558.0(16) | 8410.3(10) | 4408.2(11) | 19.0(4) |
| C30 | 10546.4(16) | 8365.2(11) | 4685.9(12) | 22.1(4) |
| C31 | 10961.5(19) | 8780.0(12) | 5270.4(13) | 29.4(5) |
| C32 | 10392(2) | 9238.3(12) | 5572.9(13) | 34.1(6) |
| C33 | 9407(2) | 9278.3(12) | 5309.7(13) | 30.8(5) |
| C34 | 8988.3(17) | 8862.2(11) | 4736.5(12) | 23.4(5) |
| C35 | 8761.4(17) | 7992.4(11) | 705.0(12) | 24.9(5) |
| C36 | 7677.7(19) | 7991.1(14) | 403.1(14) | 36.9(6) |
| C37 | 9289(2) | 8399.5(16) | 192.3(14) | 44.0(7) |

| Atom | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| C38 | 9139(3) | 7257.3(14) | 735.4(16) | 51.4(8) |
| C39 | 6220.8(14) | 8940.2(10) | 3653.1(12) | 18.1(4) |
| C40 | 6258.5(15) | 9598.5(11) | 3973.4(12) | 21.2(4) |
| C41 | 6248.3(15) | 9672.8(12) | 4729.8(13) | 24.8(5) |
| C42 | 6219.9(16) | 9129.5(13) | 5197.3(13) | 26.4(5) |
| C43 | 6163.8(15) | 8484.5(12) | 4883.5(12) | 23.3(5) |
| C44 | 6154.2(14) | 8382.2(11) | 4131.9(12) | 19.2(4) |
| C45 | 6277.1(17) | 10256.7(11) | 3544.3(14) | 26.9(5) |
| C46 | 6272(2) | 9221.2(15) | 6021.3(14) | 38.5(6) |
| C47 | 6131.4(16) | 7659.5(11) | 3859.1(12) | 22.2(4) |
| C48 | 5392.8(15) | 8466.3(10) | 2256.2(11) | 17.8(4) |
| C49 | 5439.5(15) | 7826.7(11) | 1923.0(12) | 20.3(4) |
| C50 | 4643.5(16) | 7564.6(11) | 1436.9(12) | 24.1(5) |
| C51 | 3791.0(16) | 7923.7(12) | 1264.0(13) | 26.0(5) |
| C52 | 3744.4(16) | 8560.8(12) | 1581.7(12) | 24.4(5) |
| C53 | 4513.5(15) | 8831.7(10) | 2071.7(12) | 19.4(4) |
| C54 | 6325.5(16) | 7377.6(12) | 2096.1(14) | 27.1(5) |
| C55 | 2924.1(18) | 7626.9(15) | 760.3(15) | 39.0(6) |
| C56 | 4392.0(17) | 9519.0(11) | 2403.3(14) | 27.1(5) |
| C57 | 7875.2(16) | 10339.6(11) | 1028.0(12) | 21.9(4) |
| C58 | 8923.1(18) | 10410.3(15) | 908.6(15) | 38.5(6) |
| C59 | 7242.7(18) | 10089.5(12) | 316.8(12) | 28.7(5) |
| C60 | 7498(2) | 11039.0(11) | 1216.2(14) | 32.9(6) |
| B | 6258.9(16) | 8825.5(11) | 2799.0(13) | 16.7(4) |
| Fe | 8405.7(2) | 8974.5(2) | 2161.6(2) | 14.21(7) |
| P1 | 10635.6(4) | 9315.4(3) | 3195.9(3) | 15.43(11) |
| P2 | 8937.1(4) | 7884.8(3) | 3648.1(3) | 16.26(11) |

**Table 2**: Anisotropic Displacement Parameters ($\times 10^4$) **Compound 3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| C1 | 12.7(9) | 14.4(9) | 17.2(10) | -0.6(7) | 1.0(7) | 3.0(7) |
| C2 | 12.9(9) | 15.6(9) | 17.3(10) | -0.3(7) | -0.2(7) | 1.2(7) |
| C3 | 16.7(10) | 13.8(9) | 20.1(10) | -2.1(8) | 0.1(8) | 2.0(7) |
| C4 | 17.1(10) | 18.6(10) | 17.9(10) | -1.4(8) | 0.8(8) | 4.4(8) |
| C5 | 15.8(9) | 20.7(10) | 16.9(10) | 0.8(8) | 2.8(8) | 4.1(8) |
| C6 | 14.8(9) | 13.4(9) | 21.6(10) | -0.7(8) | 1.8(8) | 1.7(7) |
| C7 | 15.7(9) | 14.8(9) | 18.4(10) | -0.7(7) | 0.2(8) | 2.3(7) |
| C8 | 15.7(9) | 14.8(9) | 20.8(10) | 1.3(8) | -1.0(8) | 2.5(7) |
| C9 | 15.0(9) | 14.4(9) | 22.2(10) | -1.6(8) | 1.0(8) | 0.5(7) |
| C10 | 14.6(9) | 14.9(9) | 17.5(10) | -2.7(7) | 0.5(8) | 1.1(7) |
| C11 | 14.5(9) | 18.5(10) | 17.9(10) | 1.8(8) | -1.7(8) | -0.9(8) |
| C12 | 20.4(10) | 21.6(10) | 25.6(12) | -0.6(9) | 5.7(9) | 0.1(8) |
| C13 | 24.5(11) | 34.5(13) | 24.3(12) | 3.7(10) | 9.3(9) | -1.6(10) |
| C14 | 29.5(12) | 26.5(12) | 28.8(12) | 7.7(10) | 3.2(10) | -7.1(10) |
| C15 | 29.6(12) | 16.8(10) | 32.3(13) | 1.1(9) | 2.4(10) | -3.5(9) |
| C16 | 19(1) | 20.7(10) | 23.2(11) | -0.1(8) | 2.8(8) | -1.2(8) |
| C17 | 17.1(10) | 18.9(10) | 20.4(10) | 5.3(8) | 2.0(8) | 0.1(8) |
| C18 | 19.6(11) | 23.2(11) | 28.7(12) | 1.6(9) | 1.4(9) | 4.6(9) |
| C19 | 30.3(13) | 26.9(12) | 39.5(14) | 5(1) | 9.2(11) | 10.4(10) |
| C20 | 19.2(11) | 38.0(14) | 40.3(15) | 18.3(11) | 5(1) | 8.9(10) |
| C21 | 17.4(11) | 40.4(14) | 34.9(14) | 13.2(11) | -4.4(10) | -1.3(10) |
| C22 | 19.2(10) | 27.4(11) | 25.9(11) | 4.0(9) | -1.2(9) | -1.3(9) |
| C23 | 17.8(10) | 14.9(9) | 20.2(10) | 0.8(8) | -2.0(8) | -0.5(8) |
| C24 | 28.0(11) | 18.1(10) | 21.6(11) | 1.7(8) | 3.3(9) | 3.2(9) |
| C25 | 36.2(13) | 22.6(11) | 30.2(13) | -2.0(9) | 5.8(10) | 8.2(10) |
| C26 | 35.0(13) | 19.2(11) | 32.4(13) | 0.9(9) | -3.7(10) | 7.3(10) |
| C27 | 29.9(12) | 22.8(11) | 27.1(12) | 6.7(9) | -5.5(10) | 2.0(9) |
| C28 | 25.0(11) | 21.9(11) | 21.9(11) | 1.9(9) | 2.8(9) | 1.5(9) |
| C29 | 26.5(11) | 15.1(9) | 15.5(10) | 0.6(7) | 3.9(8) | -1.3(8) |
| C30 | 26.0(11) | 22(1) | 17.7(10) | 0.7(8) | 2.5(8) | -3.8(9) |

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| C31 | 35.1(13) | 29.7(12) | 21.1(11) | 3.4(9) | -1.7(10) | -11(1) |
| C32 | 59.3(17) | 24.1(12) | 17.4(11) | -4.2(9) | 2.1(11) | -15.4(11) |
| C33 | 51.5(16) | 20.1(11) | 21.4(12) | -2.1(9) | 7.9(11) | 2.5(10) |
| C34 | 32.9(12) | 19.3(10) | 18.1(10) | 2.8(8) | 4.9(9) | 3.0(9) |
| C35 | 30.4(12) | 26.8(11) | 16.1(10) | -5.2(9) | 0.1(9) | 4.6(9) |
| C36 | 35.3(14) | 45.3(15) | 26.8(13) | -11.7(11) | -3.9(11) | -1.7(12) |
| C37 | 48.4(17) | 65(2) | 19.5(13) | -7.0(12) | 9.4(12) | -11.1(15) |
| C38 | 83(2) | 40.0(16) | 27.5(14) | -12.5(12) | 0.1(14) | 29.4(16) |
| C39 | 11.4(9) | 20(1) | 22.9(10) | -2.2(8) | 3.0(8) | -0.8(8) |
| C40 | 15.3(10) | 22.0(11) | 26.5(11) | -4.2(9) | 4.3(8) | -0.7(8) |
| C41 | 18.2(10) | 29.4(12) | 27.0(12) | -11.2(9) | 4.2(9) | -0.7(9) |
| C42 | 17.8(10) | 39.9(13) | 21.9(11) | -5.8(10) | 4.1(9) | -1.0(9) |
| C43 | 16.3(10) | 31.0(12) | 22.3(11) | 3.2(9) | 2.7(8) | 1.9(9) |
| C44 | 10.4(9) | 22.3(10) | 24.9(11) | -0.2(8) | 2.7(8) | 0.7(8) |
| C45 | 25.0(11) | 17.8(10) | 38.9(14) | -5.7(9) | 8.2(10) | 1.3(9) |
| C46 | 38.0(15) | 54.9(17) | 23.8(13) | -9.9(12) | 8.4(11) | -6.2(13) |
| C47 | 21.1(11) | 21(1) | 24.4(11) | 2.6(8) | 3.8(9) | 0.8(8) |
| C48 | 18(1) | 19.1(10) | 16.8(10) | 0.3(8) | 4.0(8) | -2.8(8) |
| C49 | 18.9(10) | 21.7(10) | 20.7(11) | -0.4(8) | 4.8(8) | -3.0(8) |
| C50 | 25.1(11) | 23.7(11) | 24.0(11) | -5.2(9) | 5.7(9) | -6.7(9) |
| C51 | 21.7(11) | 33.9(12) | 21.1(11) | -1.6(9) | -0.3(9) | -8.4(9) |
| C52 | 18.7(11) | 31.6(12) | 21.3(11) | 3.5(9) | -0.9(9) | -0.9(9) |
| C53 | 17.9(10) | 20.2(10) | 19.4(10) | 4.1(8) | 1.6(8) | -1.4(8) |
| C54 | 20.3(11) | 25.3(11) | 35.1(13) | -9.3(10) | 2.7(10) | 0.2(9) |
| C55 | 27.1(13) | 49.4(16) | 36.3(15) | -7.6(12) | -6.5(11) | -7.4(12) |
| C56 | 22.8(11) | 23.0(11) | 33.1(13) | -0.1(9) | -1.7(10) | 3.3(9) |
| C57 | 23.1(11) | 18.9(10) | 21.5(11) | 3.4(8) | -2.4(9) | -2.4(8) |
| C58 | 27.2(13) | 49.9(16) | 37.8(15) | 22.2(12) | 4.3(11) | -4.8(11) |
| C59 | 38.0(14) | 27.5(12) | 18.1(11) | 2.6(9) | -2.6(10) | -5.7(10) |
| C60 | 50.8(16) | 16.4(11) | 27.7(12) | 3.5(9) | -3.8(11) | 1.4(10) |
| B | 14.5(10) | 11.2(10) | 24.0(12) | -0.1(8) | 2.3(9) | 4.2(8) |
| Fe | 13.23(14) | 13.57(13) | 15.08(14) | -0.58(11) | 0.29(10) | 1.10(11) |
| P1 | 14.4(2) | 15.0(2) | 16.2(3) | -0.40(19) | 0.77(19) | -0.74(19) |
| P2 | 16.3(2) | 15.1(2) | 17.2(3) | 0.28(19) | 2.50(19) | 0.40(19) |

**Table 3**: Bond Lengths in Å for **Compound 3**.

| Atom | Atom | Length/Å |
|---|---|---|
| C1 | C2 | 1.450(3) |
| C1 | C5 | 1.435(3) |
| C1 | Fe | 2.0335(19) |
| C1 | P1 | 1.827(2) |
| C2 | C3 | 1.438(3) |
| C2 | Fe | 2.0418(19) |
| C2 | P2 | 1.824(2) |
| C3 | C4 | 1.419(3) |
| C3 | Fe | 2.0573(19) |
| C4 | C5 | 1.424(3) |
| C4 | C35 | 1.521(3) |
| C4 | Fe | 2.123(2) |
| C5 | Fe | 2.059(2) |
| C6 | C7 | 1.444(3) |
| C6 | C10 | 1.449(3) |
| C6 | B | 1.545(3) |
| C6 | Fe | 2.092(2) |
| C7 | C8 | 1.420(3) |
| C7 | Fe | 2.080(2) |
| C8 | C9 | 1.430(3) |
| C8 | C57 | 1.519(3) |
| C8 | Fe | 2.121(2) |
| C9 | C10 | 1.417(3) |
| C9 | Fe | 2.061(2) |
| C10 | Fe | 2.026(2) |
| C11 | C12 | 1.392(3) |
| C11 | C16 | 1.398(3) |
| C11 | P1 | 1.847(2) |
| C12 | C13 | 1.389(3) |
| C13 | C14 | 1.386(3) |
| C14 | C15 | 1.384(3) |
| C15 | C16 | 1.392(3) |
| C17 | C18 | 1.393(3) |
| C17 | C22 | 1.395(3) |
| C17 | P1 | 1.839(2) |
| C18 | C19 | 1.396(3) |
| C19 | C20 | 1.381(4) |
| C20 | C21 | 1.379(4) |
| C21 | C22 | 1.385(3) |
| C23 | C24 | 1.393(3) |
| C23 | C28 | 1.401(3) |
| C23 | P2 | 1.838(2) |
| C24 | C25 | 1.392(3) |
| C25 | C26 | 1.386(3) |
| C26 | C27 | 1.382(3) |
| C27 | C28 | 1.389(3) |
| C29 | C30 | 1.395(3) |
| C29 | C34 | 1.400(3) |
| C29 | P2 | 1.833(2) |
| C30 | C31 | 1.394(3) |
| C31 | C32 | 1.383(4) |
| C32 | C33 | 1.385(4) |
| C33 | C34 | 1.383(3) |
| C35 | C36 | 1.526(3) |
| C35 | C37 | 1.521(4) |
| C35 | C38 | 1.540(3) |
| C39 | C40 | 1.421(3) |
| C39 | C44 | 1.420(3) |
| C39 | B | 1.594(3) |
| C40 | C41 | 1.398(3) |
| C40 | C45 | 1.520(3) |
| C41 | C42 | 1.377(3) |
| C42 | C43 | 1.392(3) |
| C42 | C46 | 1.512(3) |
| C43 | C44 | 1.392(3) |
| C44 | C47 | 1.508(3) |
| C48 | C49 | 1.407(3) |
| C48 | C53 | 1.418(3) |
| C48 | B | 1.598(3) |
| C49 | C50 | 1.403(3) |
| C49 | C54 | 1.514(3) |
| C50 | C51 | 1.379(3) |
| C51 | C52 | 1.391(3) |
| C51 | C55 | 1.513(3) |
| C52 | C53 | 1.387(3) |
| C53 | C56 | 1.506(3) |
| C57 | C58 | 1.529(3) |
| C57 | C59 | 1.529(3) |
| C57 | C60 | 1.537(3) |

**Table 4**: Bond Angles in ° for **Compound 3**.

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| C2 | C1 | Fe | 69.46(11) |
| C2 | C1 | P1 | 125.76(15) |
| C5 | C1 | C2 | 106.98(17) |
| C5 | C1 | Fe | 70.43(11) |
| C5 | C1 | P1 | 127.26(15) |
| P1 | C1 | Fe | 125.64(10) |
| C1 | C2 | Fe | 68.85(11) |
| C1 | C2 | P2 | 137.52(15) |
| C3 | C2 | C1 | 106.36(17) |
| C3 | C2 | Fe | 70.04(11) |
| C3 | C2 | P2 | 116.10(15) |
| P2 | C2 | Fe | 126.36(10) |
| C2 | C3 | Fe | 68.89(11) |
| C4 | C3 | C2 | 110.40(18) |
| C4 | C3 | Fe | 72.68(11) |
| C3 | C4 | C5 | 106.23(18) |
| C3 | C4 | C35 | 125.28(19) |
| C3 | C4 | Fe | 67.68(11) |
| C5 | C4 | C35 | 127.55(19) |
| C5 | C4 | Fe | 67.69(11) |
| C35 | C4 | Fe | 137.74(15) |
| C1 | C5 | Fe | 68.53(11) |
| C4 | C5 | C1 | 110.00(18) |
| C4 | C5 | Fe | 72.53(12) |
| C7 | C6 | C10 | 105.15(17) |
| C7 | C6 | B | 126.62(18) |
| C7 | C6 | Fe | 69.30(11) |
| C10 | C6 | B | 126.23(19) |
| C10 | C6 | Fe | 66.96(11) |
| B | C6 | Fe | 140.10(14) |

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| C6 | C7 | Fe | 70.21(11) |
| C8 | C7 | C6 | 110.33(18) |
| C8 | C7 | Fe | 71.80(11) |
| C7 | C8 | C9 | 106.58(18) |
| C7 | C8 | C57 | 128.00(18) |
| C7 | C8 | Fe | 68.70(11) |
| C9 | C8 | C57 | 124.22(18) |
| C9 | C8 | Fe | 67.75(11) |
| C57 | C8 | Fe | 137.88(15) |
| C8 | C9 | Fe | 72.30(11) |
| C10 | C9 | C8 | 109.05(17) |
| C10 | C9 | Fe | 68.40(11) |
| C6 | C10 | Fe | 71.88(11) |
| C9 | C10 | C6 | 108.80(18) |
| C9 | C10 | Fe | 71.03(12) |
| C12 | C11 | C16 | 118.17(19) |
| C12 | C11 | P1 | 124.20(16) |
| C16 | C11 | P1 | 117.46(16) |
| C13 | C12 | C11 | 120.9(2) |
| C14 | C13 | C12 | 120.2(2) |
| C15 | C14 | C13 | 119.7(2) |
| C14 | C15 | C16 | 120.0(2) |
| C15 | C16 | C11 | 121.0(2) |
| C18 | C17 | C22 | 118.5(2) |
| C18 | C17 | P1 | 123.94(16) |
| C22 | C17 | P1 | 117.55(17) |
| C17 | C18 | C19 | 120.3(2) |
| C20 | C19 | C18 | 120.2(2) |
| C21 | C20 | C19 | 120.1(2) |
| C20 | C21 | C22 | 119.9(2) |
| C21 | C22 | C17 | 121.1(2) |
| C24 | C23 | C28 | 118.53(19) |
| C24 | C23 | P2 | 123.89(16) |
| C28 | C23 | P2 | 117.25(16) |
| C25 | C24 | C23 | 120.5(2) |
| C26 | C25 | C24 | 120.3(2) |
| C27 | C26 | C25 | 119.7(2) |
| C26 | C27 | C28 | 120.3(2) |
| C27 | C28 | C23 | 120.6(2) |
| C30 | C29 | C34 | 119.2(2) |
| C30 | C29 | P2 | 123.69(16) |
| C34 | C29 | P2 | 117.08(17) |
| C31 | C30 | C29 | 120.1(2) |
| C32 | C31 | C30 | 119.9(2) |
| C31 | C32 | C33 | 120.4(2) |
| C34 | C33 | C32 | 120.0(2) |
| C33 | C34 | C29 | 120.4(2) |
| C4 | C35 | C36 | 112.32(19) |
| C4 | C35 | C37 | 111.19(19) |
| C4 | C35 | C38 | 105.98(19) |
| C36 | C35 | C38 | 109.0(2) |
| C37 | C35 | C36 | 109.6(2) |
| C37 | C35 | C38 | 108.5(2) |
| C40 | C39 | B | 122.07(18) |
| C44 | C39 | C40 | 116.89(19) |
| C44 | C39 | B | 121.04(18) |
| C39 | C40 | C45 | 124.6(2) |
| C41 | C40 | C39 | 120.0(2) |
| C41 | C40 | C45 | 115.40(19) |
| C42 | C41 | C40 | 122.9(2) |
| C41 | C42 | C43 | 117.2(2) |
| C41 | C42 | C46 | 121.9(2) |
| C43 | C42 | C46 | 120.8(2) |

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| C44 | C43 | C42 | 122.2(2) |
| C39 | C44 | C47 | 121.69(19) |
| C43 | C44 | C39 | 120.7(2) |
| C43 | C44 | C47 | 117.51(19) |
| C49 | C48 | C53 | 117.01(19) |
| C49 | C48 | B | 125.50(18) |
| C53 | C48 | B | 117.45(18) |
| C48 | C49 | C54 | 121.99(19) |
| C50 | C49 | C48 | 121.0(2) |
| C50 | C49 | C54 | 116.96(19) |
| C51 | C50 | C49 | 121.4(2) |
| C50 | C51 | C52 | 117.9(2) |
| C50 | C51 | C55 | 121.1(2) |
| C52 | C51 | C55 | 121.0(2) |
| C53 | C52 | C51 | 122.1(2) |
| C48 | C53 | C56 | 120.92(19) |
| C52 | C53 | C48 | 120.5(2) |
| C52 | C53 | C56 | 118.60(19) |
| C8 | C57 | C58 | 112.58(18) |
| C8 | C57 | C59 | 111.30(18) |
| C8 | C57 | C60 | 105.89(18) |
| C58 | C57 | C59 | 109.8(2) |
| C58 | C57 | C60 | 109.1(2) |
| C59 | C57 | C60 | 108.01(18) |
| C6 | B | C39 | 117.07(18) |
| C6 | B | C48 | 120.30(19) |
| C39 | B | C48 | 121.74(18) |
| C1 | Fe | C2 | 41.68(8) |
| C1 | Fe | C3 | 68.82(8) |
| C1 | Fe | C4 | 68.55(8) |
| C1 | Fe | C5 | 41.04(8) |
| C1 | Fe | C6 | 142.59(8) |
| C1 | Fe | C7 | 168.33(8) |
| C1 | Fe | C8 | 128.94(8) |
| C1 | Fe | C9 | 102.75(8) |
| C2 | Fe | C3 | 41.07(8) |
| C2 | Fe | C4 | 68.53(8) |
| C2 | Fe | C5 | 68.86(8) |
| C2 | Fe | C6 | 113.96(8) |
| C2 | Fe | C7 | 149.12(8) |
| C2 | Fe | C8 | 166.92(8) |
| C2 | Fe | C9 | 127.50(8) |
| C3 | Fe | C4 | 39.64(8) |
| C3 | Fe | C5 | 67.07(8) |
| C3 | Fe | C6 | 113.33(8) |
| C3 | Fe | C7 | 122.14(8) |
| C3 | Fe | C8 | 151.51(8) |
| C3 | Fe | C9 | 168.54(8) |
| C5 | Fe | C4 | 39.78(8) |
| C5 | Fe | C6 | 176.37(8) |
| C5 | Fe | C7 | 136.03(8) |
| C5 | Fe | C8 | 109.99(8) |
| C5 | Fe | C9 | 112.12(8) |
| C6 | Fe | C4 | 138.30(8) |
| C6 | Fe | C8 | 67.82(8) |
| C7 | Fe | C4 | 116.54(8) |
| C7 | Fe | C6 | 40.49(8) |
| C7 | Fe | C8 | 39.49(8) |
| C8 | Fe | C4 | 119.52(8) |
| C9 | Fe | C4 | 145.92(8) |
| C9 | Fe | C6 | 68.27(8) |
| C9 | Fe | C7 | 66.96(8) |
| C9 | Fe | C8 | 39.95(8) |

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| C10 | Fe | C1 | 108.19(8) |
| C10 | Fe | C2 | 104.39(8) |
| C10 | Fe | C3 | 133.09(8) |
| C10 | Fe | C4 | 172.45(8) |
| C10 | Fe | C5 | 141.34(8) |
| C10 | Fe | C6 | 41.16(8) |
| C10 | Fe | C7 | 68.03(8) |
| C10 | Fe | C8 | 67.93(8) |
| C10 | Fe | C9 | 40.57(8) |
| C1 | P1 | C11 | 103.27(9) |
| C1 | P1 | C17 | 99.65(9) |
| C17 | P1 | C11 | 97.92(9) |
| C2 | P2 | C23 | 101.94(9) |
| C2 | P2 | C29 | 107.27(9) |
| C29 | P2 | C23 | 100.67(9) |

**Table 5**: Torsion Angles in ° for **Compound 3**.

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| C1 | C2 | C3 | C4 | 1.5(2) |
| C1 | C2 | C3 | Fe | -59.56(13) |
| C1 | C2 | P2 | C23 | -97.1(2) |
| C1 | C2 | P2 | C29 | 8.2(2) |
| C2 | C1 | C5 | C4 | -0.7(2) |
| C2 | C1 | C5 | Fe | 60.15(13) |
| C2 | C1 | P1 | C11 | -168.75(17) |
| C2 | C1 | P1 | C17 | 90.66(18) |
| C2 | C3 | C4 | C5 | -1.9(2) |
| C2 | C3 | C4 | C35 | 167.64(19) |
| C2 | C3 | C4 | Fe | -58.76(14) |
| C3 | C2 | P2 | C23 | 81.18(16) |
| C3 | C2 | P2 | C29 | -173.51(15) |
| C3 | C4 | C5 | C1 | 1.6(2) |
| C3 | C4 | C5 | Fe | -56.84(13) |
| C3 | C4 | C35 | C36 | 63.2(3) |
| C3 | C4 | C35 | C37 | -173.6(2) |
| C3 | C4 | C35 | C38 | -55.8(3) |
| C5 | C1 | C2 | C3 | -0.4(2) |
| C5 | C1 | C2 | Fe | -60.77(13) |
| C5 | C1 | C2 | P2 | 177.98(17) |
| C5 | C1 | P1 | C11 | 11.94(19) |
| C5 | C1 | P1 | C17 | -88.64(18) |
| C5 | C4 | C35 | C36 | -129.5(2) |
| C5 | C4 | C35 | C37 | -6.3(3) |
| C5 | C4 | C35 | C38 | 111.5(3) |
| C6 | C7 | C8 | C9 | 2.6(2) |
| C6 | C7 | C8 | C57 | -165.24(19) |
| C6 | C7 | C8 | Fe | 59.87(14) |
| C7 | C6 | C10 | C9 | 2.7(2) |
| C7 | C6 | C10 | Fe | -59.13(13) |
| C7 | C6 | B | C39 | -154.29(19) |
| C7 | C6 | B | C48 | 15.1(3) |
| C7 | C8 | C9 | C10 | -0.8(2) |
| C7 | C8 | C9 | Fe | 57.91(13) |
| C7 | C8 | C57 | C58 | -138.2(2) |
| C7 | C8 | C57 | C59 | -14.4(3) |
| C7 | C8 | C57 | C60 | 102.7(2) |
| C8 | C9 | C10 | C6 | -1.2(2) |
| C8 | C9 | C10 | Fe | 61.14(14) |
| C9 | C8 | C57 | C58 | 56.0(3) |
| C9 | C8 | C57 | C59 | 179.75(19) |
| C9 | C8 | C57 | C60 | -63.1(3) |
| C10 | C6 | C7 | C8 | -3.2(2) |
| C10 | C6 | C7 | Fe | 57.60(13) |

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| C10 | C6 | B | C39 | 7.2(3) |
| C10 | C6 | B | C48 | 176.57(18) |
| C11 | C12 | C13 | C14 | 0.8(3) |
| C12 | C11 | C16 | C15 | 0.7(3) |
| C12 | C11 | P1 | C1 | -63.58(19) |
| C12 | C11 | P1 | C17 | 38.3(2) |
| C12 | C13 | C14 | C15 | -0.7(4) |
| C13 | C14 | C15 | C16 | 0.5(4) |
| C14 | C15 | C16 | C11 | -0.5(3) |
| C16 | C11 | C12 | C13 | -0.8(3) |
| C16 | C11 | P1 | C1 | 121.24(17) |
| C16 | C11 | P1 | C17 | -136.84(17) |
| C17 | C18 | C19 | C20 | -0.3(4) |
| C18 | C17 | C22 | C21 | 1.9(3) |
| C18 | C17 | P1 | C1 | 5.0(2) |
| C18 | C17 | P1 | C11 | -99.99(19) |
| C18 | C19 | C20 | C21 | 0.4(4) |
| C19 | C20 | C21 | C22 | 0.7(4) |
| C20 | C21 | C22 | C17 | -1.9(4) |
| C22 | C17 | C18 | C19 | -0.8(3) |
| C22 | C17 | P1 | C1 | -175.50(17) |
| C22 | C17 | P1 | C11 | 79.50(18) |
| C23 | C24 | C25 | C26 | 0.7(4) |
| C24 | C23 | C28 | C27 | -0.3(3) |
| C24 | C23 | P2 | C2 | -17.4(2) |
| C24 | C23 | P2 | C29 | -127.80(19) |
| C24 | C25 | C26 | C27 | -1.0(4) |
| C25 | C26 | C27 | C28 | 0.6(4) |
| C26 | C27 | C28 | C23 | 0.1(3) |
| C28 | C23 | C24 | C25 | -0.1(3) |
| C28 | C23 | P2 | C2 | 169.29(16) |
| C28 | C23 | P2 | C29 | 58.89(18) |
| C29 | C30 | C31 | C32 | -0.2(3) |
| C30 | C29 | C34 | C33 | 2.6(3) |
| C30 | C29 | P2 | C2 | -78.60(19) |
| C30 | C29 | P2 | C23 | 27.6(2) |
| C30 | C31 | C32 | C33 | 1.4(4) |
| C31 | C32 | C33 | C34 | -0.5(4) |
| C32 | C33 | C34 | C29 | -1.5(3) |
| C34 | C29 | C30 | C31 | -1.7(3) |
| C34 | C29 | P2 | C2 | 103.63(17) |
| C34 | C29 | P2 | C23 | -150.16(16) |
| C35 | C4 | C5 | C1 | -167.62(19) |
| C35 | C4 | C5 | Fe | 133.9(2) |
| C39 | C40 | C41 | C42 | 1.2(3) |
| C40 | C39 | C44 | C43 | -2.4(3) |
| C40 | C39 | C44 | C47 | -178.64(18) |
| C40 | C39 | B | C6 | 49.9(3) |
| C40 | C39 | B | C48 | -119.3(2) |
| C40 | C41 | C42 | C43 | -2.4(3) |
| C40 | C41 | C42 | C46 | 176.1(2) |
| C41 | C42 | C43 | C44 | 1.2(3) |
| C42 | C43 | C44 | C39 | 1.2(3) |
| C42 | C43 | C44 | C47 | 177.6(2) |
| C44 | C39 | C40 | C41 | 1.2(3) |
| C44 | C39 | C40 | C45 | -176.62(19) |

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| C44 | C39 | B | C6 | -129.6(2) |
| C44 | C39 | B | C48 | 61.1(3) |
| C45 | C40 | C41 | C42 | 179.2(2) |
| C46 | C42 | C43 | C44 | -177.3(2) |
| C48 | C49 | C50 | C51 | 0.4(3) |
| C49 | C48 | C53 | C52 | -0.2(3) |
| C49 | C48 | C53 | C56 | 179.67(19) |
| C49 | C48 | B | C6 | 79.0(3) |
| C49 | C48 | B | C39 | -112.1(2) |
| C49 | C50 | C51 | C52 | 0.6(3) |
| C49 | C50 | C51 | C55 | -177.8(2) |
| C50 | C51 | C52 | C53 | -1.4(3) |
| C51 | C52 | C53 | C48 | 1.2(3) |
| C51 | C52 | C53 | C56 | -178.6(2) |
| C53 | C48 | C49 | C50 | -0.6(3) |
| C53 | C48 | C49 | C54 | -177.8(2) |
| C53 | C48 | B | C6 | -98.6(2) |
| C53 | C48 | B | C39 | 70.3(3) |
| C54 | C49 | C50 | C51 | 177.7(2) |
| C55 | C51 | C52 | C53 | 177.0(2) |
| C57 | C8 | C9 | C10 | 167.56(19) |
| C57 | C8 | C9 | Fe | -133.7(2) |
| B | C6 | C7 | C8 | 161.35(18) |
| B | C6 | C7 | Fe | -137.8(2) |
| B | C6 | C10 | C9 | -162.00(18) |
| B | C6 | C10 | Fe | 136.20(19) |
| B | C39 | C40 | C41 | -178.33(19) |
| B | C39 | C40 | C45 | 3.8(3) |
| B | C39 | C44 | C43 | 177.18(18) |
| B | C39 | C44 | C47 | 0.9(3) |
| B | C48 | C49 | C50 | -178.2(2) |
| B | C48 | C49 | C54 | 4.6(3) |
| B | C48 | C53 | C52 | 177.57(19) |
| B | C48 | C53 | C56 | -2.6(3) |
| Fe | C1 | C2 | C3 | 60.34(13) |
| Fe | C1 | C2 | P2 | -121.3(2) |
| Fe | C1 | C5 | C4 | -60.89(14) |
| Fe | C1 | P1 | C11 | -79.64(14) |
| Fe | C1 | P1 | C17 | 179.77(12) |
| Fe | C2 | C3 | C4 | 61.04(14) |
| Fe | C2 | P2 | C23 | 164.79(12) |
| Fe | C2 | P2 | C29 | -89.90(14) |
| Fe | C3 | C4 | C5 | 56.84(13) |
| Fe | C3 | C4 | C35 | -133.6(2) |
| Fe | C4 | C5 | C1 | 58.47(14) |
| Fe | C4 | C35 | C36 | -31.8(3) |
| Fe | C4 | C35 | C37 | 91.4(3) |
| Fe | C4 | C35 | C38 | -150.8(2) |
| Fe | C6 | C7 | C8 | -60.83(14) |
| Fe | C6 | C10 | C9 | 61.79(14) |
| Fe | C6 | B | C39 | 104.0(2) |
| Fe | C6 | B | C48 | -86.6(3) |
| Fe | C7 | C8 | C9 | -57.31(13) |
| Fe | C7 | C8 | C57 | 134.9(2) |
| Fe | C8 | C9 | C10 | -58.74(14) |
| Fe | C8 | C57 | C58 | -38.0(3) |
| Fe | C8 | C57 | C59 | 85.8(3) |
| Fe | C8 | C57 | C60 | -157.10(18) |
| Fe | C9 | C10 | C6 | -62.33(13) |
| P1 | C1 | C2 | C3 | -179.86(14 |

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| P1 | C1 | C2 | Fe | 119.81(15) |
| P1 | C1 | C2 | P2 | -1.4(3) |
| P1 | C1 | C5 | C4 | 178.67(14) |
| P1 | C1 | C5 | Fe | -120.44(16) |
| P1 | C11 | C12 | C13 | -175.98(17) |
| P1 | C11 | C16 | C15 | 176.17(17) |
| P1 | C17 | C18 | C19 | 178.69(18) |
| P1 | C17 | C22 | C21 | -177.58(18) |
| P2 | C2 | C3 | C4 | -177.33(14) |
| P2 | C2 | C3 | Fe | 121.63(13) |
| P2 | C23 | C24 | C25 | -173.32(18) |
| P2 | C23 | C28 | C27 | 173.36(17) |
| P2 | C29 | C30 | C31 | -179.44(17) |
| P2 | C29 | C34 | C33 | -179.56(17) |

**Table 6**: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **Compound 3**. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{ij}$.

| Atom | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| H3 | 8221 | 7602 | 2093 | 21 |
| H5 | 9982 | 9066 | 1483 | 21 |
| H7 | 6634 | 9202 | 1312 | 20 |
| H9 | 8810 | 10290 | 2554 | 21 |
| H10 | 8088 | 9530 | 3423 | 19 |
| H12 | 11674 | 9374 | 1908 | 27 |
| H13 | 12171 | 10250 | 1206 | 33 |
| H14 | 11831 | 11377 | 1459 | 34 |
| H15 | 10957 | 11625 | 2401 | 32 |
| H16 | 10452 | 10749 | 3103 | 25 |
| H18 | 11281 | 8029 | 2584 | 29 |
| H19 | 12744 | 7427 | 2763 | 38 |
| H20 | 14076 | 7835 | 3580 | 39 |
| H21 | 13956 | 8840 | 4227 | 38 |
| H22 | 12491 | 9422 | 4082 | 30 |
| H24 | 10045 | 7066 | 2716 | 27 |
| H25 | 10884 | 6038 | 2887 | 36 |
| H26 | 11030 | 5466 | 4015 | 36 |
| H27 | 10378 | 5939 | 4985 | 33 |
| H28 | 9554 | 6971 | 4827 | 28 |
| H30 | 10937 | 8051 | 4476 | 26 |
| H31 | 11634 | 8748 | 5460 | 35 |
| H32 | 10679 | 9528 | 5964 | 41 |
| H33 | 9020 | 9592 | 5523 | 37 |
| H34 | 8310 | 8883 | 4565 | 28 |
| H36A | 7566 | 7816 | -104 | 55 |
| H36B | 7345 | 7701 | 714 | 55 |
| H36C | 7426 | 8455 | 406 | 55 |
| H37A | 9130 | 8218 | -311 | 66 |
| H37B | 9088 | 8876 | 194 | 66 |
| H37C | 9989 | 8367 | 364 | 66 |
| H38A | 9010 | 7059 | 238 | 77 |
| H38B | 9837 | 7255 | 920 | 77 |
| H38C | 8809 | 6990 | 1068 | 77 |
| H41 | 6261 | 10118 | 4930 | 30 |
| H43 | 6131 | 8101 | 5193 | 28 |
| H45A | 6248 | 10154 | 3018 | 40 |
| H45B | 6876 | 10504 | 3730 | 40 |
| H45C | 5719 | 10536 | 3608 | 40 |
| H46A | 5922 | 8851 | 6216 | 58 |
| H46B | 5978 | 9656 | 6117 | 58 |
| H46C | 6951 | 9216 | 6265 | 58 |
| H47A | 5654 | 7618 | 3404 | 33 |
| H47B | 5953 | 7357 | 4237 | 33 |
| H47C | 6772 | 7534 | 3758 | 33 |
| H50 | 4693 | 7130 | 1222 | 29 |
| H52 | 3167 | 8819 | 1459 | 29 |
| H54A | 6151 | 6952 | 2315 | 41 |
| H54B | 6826 | 7611 | 2446 | 41 |
| H54C | 6573 | 7280 | 1639 | 41 |
| H55A | 2355 | 7911 | 777 | 59 |
| H55B | 2802 | 7167 | 925 | 59 |
| H55C | 3054 | 7610 | 253 | 59 |
| H56A | 4513 | 9484 | 2944 | 41 |
| H56B | 3731 | 9682 | 2235 | 41 |
| H56C | 4853 | 9838 | 2247 | 41 |
| H58A | 8947 | 10708 | 485 | 58 |
| H58B | 9315 | 10606 | 1352 | 58 |
| H58C | 9178 | 9962 | 812 | 58 |

| Atom | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| H59A | 7320 | 10393 | -92 | 43 |
| H59B | 7440 | 9629 | 206 | 43 |
| H59C | 6563 | 10086 | 381 | 43 |
| H60A | 7543 | 11357 | 813 | 49 |
| H60B | 6821 | 10999 | 1281 | 49 |
| H60C | 7888 | 11207 | 1675 | 49 |

**Citations**

*APEX2 suite for crystallographic software, SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA. (2013)

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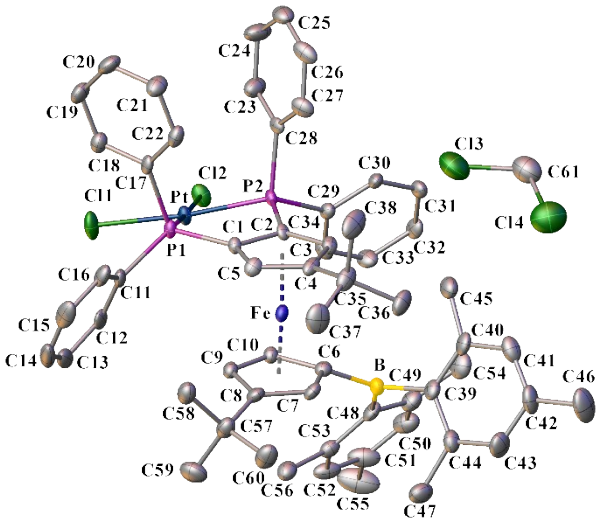
# Crystal Data and Experimental




**Experimental.** A single clear orange prism-shaped crystals of Compound 4 (0.15×0.13×0.05 mm$^3$) was obtained by recrystallization, was selected and mounted on a mylar loop with oil on an Bruker D8 Venture triumph Mo diffractometer. The crystal was kept at a steady $T$ = 100.0 K during data collection. The structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program using the intrinsic phasing methods solution method and by using **Olex2** (Dolomanov et al., 2009) as the graphical interface. The model was refined with version 2018/3 of **ShelXL** (Sheldrick, 2015) using Least Squares minimisation.

**Crystal Data.** $C_{61}H_{67}BCl_4FeP_2Pt$, $M_r$ = 1265.63, monoclinic, $P2_1/n$ (No. 14), a = 12.3692(11) Å, b = 32.732(3) Å, c = 16.6670(14) Å, $\beta$ = 103.454(3)°, $\alpha$ = $\gamma$ = 90°, $V$ = 6562.7(10) Å$^3$, $T$ = 100.0 K, $Z$ = 4, $Z'$ = 1, $\mu$(MoK$_\alpha$) = 2.595, 57058 reflections measured, 12046 unique ($R_{int}$ = 0.0468) which were used in all calculations. The final $wR_2$ was 0.0894 (all data) and $R_1$ was 0.0417 (I > 2(I)).

| | |
|---|---|
| **Compound** | **4** |
| **N° CCDC** | **1902395** |
| Formula | $C_{61}H_{67}BCl_4FeP_2Pt$ |
| $D_{calc.}$/ g cm$^{-3}$ | 1.281 |
| $\mu$/mm$^{-1}$ | 2.595 |
| Formula Weight | 1265.63 |
| Colour | clear orange |
| Shape | prism |
| Size/mm$^3$ | 0.15×0.13×0.05 |
| $T$/K | 100.0 |
| Crystal System | monoclinic |
| Space Group | $P2_1/n$ |
| $a$/Å | 12.3692(11) |
| $b$/Å | 32.732(3) |
| $c$/Å | 16.6670(14) |
| $\alpha$/° | 90 |
| $\beta$/° | 103.454(3) |
| $\gamma$/° | 90 |
| V/Å$^3$ | 6562.7(10) |
| $Z$ | 4 |
| $Z'$ | 1 |
| Wavelength/Å | 0.71073 |
| Radiation type | MoK$_\alpha$ |
| $\Theta_{min}$/° | 2.788 |
| $\Theta_{max}$/° | 25.462 |
| Measured Refl. | 57058 |
| Independent Refl. | 12046 |
| Reflections with I > 2(I) | 9746 |
| $R_{int}$ | 0.0468 |
| Parameters | 643 |
| Restraints | 0 |
| Largest Peak | 1.843 |
| Deepest Hole | -1.277 |
| GooF | 1.027 |
| $wR_2$ (all data) | 0.0894 |
| $wR_2$ | 0.0847 |
| $R_1$ (all data) | 0.0573 |
| $R_1$ | 0.0417 |

A clear orange prism-shaped crystal with dimensions 0.15×0.13×0.05 mm$^3$ was mounted on a mylar loop with oil. Data were collected using an Bruker D8 Venture triumph Mo diffractometer equipped with an Oxford Cryosystems low-temperature device operating at $T$ = 100.0 K. Data were measured using $\phi$ and $\omega$ scans' using Mo$K_\alpha$ radiation. The total number of runs and images was based on the strategy calculation from the program APEX2 (Bruker). The maximum resolution that was achieved was $\Theta$ = 25.462° (0.83 Å). The diffraction pattern was indexed The total number of runs and images was based on the strategy calculation from the program APEX2 (Bruker) and the unit cell was refined using **SAINT** (Bruker, V8.38A, after 2013) on 9788 reflections, 17% of the observed reflections.

A clear orange prism-shaped crystal with dimensions 0.15×0.13×0.05 mm$^3$ as mounted on a mylar loop with oil. X-ray diffraction data were collected using a Bruker D8 Venture triumph Mo diffractometer equipped with an Oxford Cryosystems low-temperature device, operating at $T$ = 100.0 K. Data were measured using $\phi$ and $\omega$ scans using Mo$K_\alpha$ radiation (X-ray tube, 50 kV, 30 mA). The total number of runs and images was based on the strategy calculation from the program **APEX2** (Bruker).The maximum resolution achieved was $\Theta$ = 25.462°.

Cell parameters were retrieved using the **SAINT** (Bruker, V8.34A, 2014) software and refined using **SAINT** (Bruker, V8.34A, 2014) on 9788 reflections, 18 % of the observed reflections. Data reduction was performed using the **SAINT** (Bruker, V8.34A, 2014) software which corrects for Lorentz polarisation. The final completeness is 98.10 out to 25.462 in $\Theta$. The absorption coefficient $\mu$ of this material is 2.644 at this wavelength ($\lambda$ = 0.71073) and the minimum and maximum transmissions are 0.6852 and 0.7452.

The structure was solved in the space group P2$_1$/n (# 14) by intrinsic phasing methods using the **ShelXT** (Sheldrick, 2015) structure solution program and refined by Least Squares using version 2014/7 of **ShelXL** (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. During the structure refinement, the atoms of $CH_2Cl_2$ solvent molecules were observed but these molecules are badly disordered and any attempt to modelise these solvent molecules failed. The Squeeze routine in Platon (Spek, A.L. (2003), J. Appl. Cryst. 36, 7-13) was used and the hkl intensity were modified accordingly for a total of 270 solvent electrons per unit cell, ie about 1.6 dichloromethane molecule par asymetric (or formula) unit, which gives in total 2.6 dichloromethane molecules.

**Table 7**: Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for **Compound 4**. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{ij}$.

| Atom | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| Pt | 10243.9(2) | 7561.6(2) | 92.8(2) | 16.73(6) |
| Fe | 8040.1(5) | 6560.8(2) | -587.3(4) | 15.49(15) |
| Cl2 | 11195.7(10) | 7747.6(4) | 1424.5(7) | 24.8(3) |
| Cl1 | 11862.2(11) | 7715.0(4) | -367.1(8) | 31.2(3) |
| Cl3 | 4305.7(15) | 7188.7(6) | 391.6(12) | 60.3(5) |
| Cl4 | 2610.6(17) | 6568.7(6) | 412.4(12) | 67.2(5) |
| P1 | 9281.7(10) | 7419.2(4) | -1175.0(7) | 15.8(2) |
| P2 | 8630.9(10) | 7472.4(4) | 463.9(7) | 14.5(2) |
| C1 | 8079(4) | 7132.6(14) | -1076(3) | 14.5(10) |
| C2 | 7780(4) | 7148.6(14) | -293(3) | 14.8(10) |
| C29 | 8586(4) | 7294.9(14) | 1480(3) | 18.0(10) |
| C34 | 9439(4) | 7061.9(15) | 1946(3) | 23.5(11) |
| C33 | 9392(5) | 6936.6(15) | 2726(3) | 26.7(12) |
| C32 | 8495(4) | 7041.0(15) | 3050(3) | 24.8(12) |
| C31 | 7631(4) | 7271.9(15) | 2589(3) | 23.0(11) |
| C30 | 7677(4) | 7397.6(14) | 1808(3) | 19.9(10) |
| C23 | 7874(4) | 7957.4(14) | 343(3) | 16.9(10) |
| C28 | 6758(4) | 7986.5(16) | -52(3) | 26.4(12) |
| C27 | 6240(5) | 8358.8(17) | -131(3) | 30.1(13) |

| Atom | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| C26 | 6804(5) | 8705.3(17) | 177(3) | 31.5(13) |
| C25 | 7915(5) | 8680.2(17) | 572(4) | 42.4(16) |
| C24 | 8441(5) | 8306.9(16) | 655(4) | 32.4(13) |
| C8 | 8712(4) | 6029.9(14) | -1012(3) | 22.7(11) |
| C9 | 9557(4) | 6302.0(14) | -591(3) | 18.1(10) |
| C10 | 9447(4) | 6352.8(14) | 220(3) | 17.6(10) |
| C6 | 8518(4) | 6118.5(14) | 340(3) | 18.7(10) |
| B | 8316(5) | 5902.5(17) | 1129(4) | 21.6(12) |
| C48 | 9361(4) | 5787.6(15) | 1828(3) | 22.5(11) |
| C49 | 9325(5) | 5812.6(16) | 2667(3) | 29.7(13) |
| C50 | 10259(5) | 5714.9(17) | 3275(3) | 36.6(14) |
| C52 | 11256(5) | 5528.1(15) | 2292(3) | 30.1(13) |
| C53 | 10351(4) | 5631.1(14) | 1655(3) | 22.7(11) |
| C56 | 10509(4) | 5534.4(16) | 797(3) | 27.4(12) |
| C54 | 8305(5) | 5945.0(18) | 2940(3) | 37.1(14) |
| C39 | 7118(4) | 5726.9(15) | 1126(3) | 22.6(11) |
| C40 | 6228(4) | 5972.1(16) | 1226(3) | 25.9(12) |
| C41 | 5199(4) | 5799.1(18) | 1210(3) | 30.4(13) |
| C43 | 5871(5) | 5145.3(18) | 990(4) | 37.7(14) |
| C44 | 6928(4) | 5304.6(16) | 1015(3) | 26.8(12) |
| C47 | 7849(5) | 5018.1(16) | 915(4) | 36.7(14) |
| C45 | 6376(5) | 6419.0(16) | 1421(3) | 31.8(13) |
| C7 | 8050(4) | 5936.1(14) | -452(3) | 19.4(10) |
| C57 | 8695(5) | 5823.8(15) | -1835(3) | 27.3(12) |
| C58 | 8554(5) | 6127.2(16) | -2538(3) | 30.5(13) |
| C59 | 9825(5) | 5609.0(18) | -1727(4) | 40.0(15) |
| C60 | 7794(5) | 5497.2(17) | -2026(3) | 37.2(14) |
| C5 | 7244(4) | 6893.4(14) | -1608(3) | 19.1(10) |
| C4 | 6438(4) | 6768.2(15) | -1175(3) | 21.3(11) |
| C3 | 6767(4) | 6922.7(14) | -362(3) | 18.0(10) |
| C35 | 5339(4) | 6558.5(16) | -1555(3) | 29.0(12) |
| C36 | 4959(4) | 6281.2(17) | -932(3) | 33.3(13) |
| C38 | 4508(4) | 6902.7(19) | -1822(4) | 43.2(16) |
| C37 | 5416(5) | 6305.1(19) | -2308(4) | 41.3(15) |
| C22 | 7680(4) | 8000.2(15) | -1947(3) | 24.1(11) |
| C21 | 7380(5) | 8382.0(16) | -2296(3) | 29.9(12) |
| C20 | 8192(5) | 8658.1(16) | -2376(3) | 34.4(14) |
| C19 | 9304(5) | 8558.2(16) | -2116(3) | 30.3(13) |
| C18 | 9610(4) | 8181.2(15) | -1764(3) | 24.8(11) |
| C11 | 9921(4) | 7161.1(14) | -1908(3) | 19.8(11) |
| C12 | 10907(4) | 6942.6(15) | -1654(3) | 25.1(12) |
| C13 | 11331(5) | 6727.0(16) | -2226(4) | 36.6(15) |
| C14 | 10807(6) | 6738.6(18) | -3042(4) | 43.0(17) |
| C15 | 9845(6) | 6958.6(18) | -3300(3) | 39.8(16) |
| C16 | 9393(5) | 7170.7(15) | -2737(3) | 26.7(12) |
| C61 | 3292(6) | 6998(2) | 900(4) | 50.3(17) |
| C17 | 8790(4) | 7899.0(14) | -1686(3) | 17.4(10) |
| C51 | 11239(5) | 5576.4(17) | 3106(4) | 39.4(15) |
| C42 | 4996(5) | 5386.5(19) | 1094(3) | 36.1(14) |
| C55 | 12251(6) | 5473(2) | 3777(4) | 61(2) |
| C46 | 3882(5) | 5201(2) | 1116(4) | 54.1(19) |

**Table 8**: Anisotropic Displacement Parameters ($\times 10^4$) **Compound 4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \ldots + 2hka^* \times b^* \times U_{12}]$

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Pt | 14.34(10) | 25.08(10) | 11.19(9) | -2.61(8) | 3.86(7) | -3.60(8) |
| Fe | 13.2(3) | 19.3(4) | 13.8(3) | 3.1(3) | 2.8(3) | -2.6(3) |
| Cl2 | 19.7(6) | 38.5(7) | 14.3(6) | -6.3(5) | 0.1(5) | -1.6(5) |
| Cl1 | 21.8(7) | 50.0(8) | 24.7(7) | -9.6(6) | 11.1(6) | -16.2(6) |
| Cl3 | 52.6(11) | 66.3(12) | 64.5(12) | -3.6(9) | 18.6(9) | 17.1(9) |
| Cl4 | 67.2(13) | 66.3(12) | 59.3(12) | -1.7(9) | -3.2(10) | 1.2(10) |

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| P1 | 15.7(6) | 21.4(6) | 11.2(6) | -1.3(5) | 4.8(5) | -4.9(5) |
| P2 | 13.4(6) | 20.3(7) | 11.4(6) | 1.8(5) | 5.9(5) | 1.7(5) |
| C1 | 12(2) | 20(2) | 11(2) | 2.2(18) | 2.2(19) | 0.4(19) |
| C2 | 8(2) | 22(3) | 14(2) | 3.1(18) | 2.1(19) | 2.4(18) |
| C29 | 24(3) | 18(2) | 14(2) | 0.9(18) | 7(2) | 0(2) |
| C34 | 25(3) | 29(3) | 19(3) | 0(2) | 9(2) | 7(2) |
| C33 | 33(3) | 26(3) | 20(3) | 9(2) | 5(2) | 11(2) |
| C32 | 37(3) | 27(3) | 12(3) | 0(2) | 11(2) | -3(2) |
| C31 | 30(3) | 23(3) | 20(3) | 0(2) | 13(2) | 3(2) |
| C30 | 24(3) | 15(2) | 24(3) | 4(2) | 12(2) | 1(2) |
| C23 | 23(3) | 21(3) | 9(2) | 2.3(18) | 7(2) | 5(2) |
| C28 | 31(3) | 32(3) | 14(3) | -5(2) | 2(2) | 7(2) |
| C27 | 32(3) | 44(4) | 13(3) | -2(2) | 2(2) | 15(3) |
| C26 | 37(3) | 27(3) | 32(3) | 10(2) | 12(3) | 14(3) |
| C25 | 42(4) | 20(3) | 64(4) | 1(3) | 11(3) | 3(3) |
| C24 | 24(3) | 26(3) | 47(4) | 6(3) | 6(3) | 1(2) |
| C8 | 29(3) | 14(2) | 26(3) | 3(2) | 9(2) | 0(2) |
| C9 | 18(3) | 19(3) | 18(3) | 4.2(19) | 6(2) | 0(2) |
| C10 | 16(2) | 20(3) | 17(3) | 3.2(19) | 5(2) | 1(2) |
| C6 | 18(3) | 18(2) | 20(3) | 3.1(19) | 3(2) | 3(2) |
| B | 24(3) | 21(3) | 23(3) | 1(2) | 13(3) | 0(2) |
| C48 | 28(3) | 20(3) | 19(3) | 7(2) | 3(2) | -4(2) |
| C49 | 36(3) | 27(3) | 25(3) | 7(2) | 5(3) | -2(2) |
| C50 | 55(4) | 30(3) | 23(3) | 1(2) | 4(3) | 4(3) |
| C52 | 27(3) | 19(3) | 36(3) | -2(2) | -9(3) | 1(2) |
| C53 | 23(3) | 18(3) | 24(3) | 2(2) | 1(2) | -3(2) |
| C56 | 26(3) | 26(3) | 30(3) | 8(2) | 6(2) | 3(2) |
| C54 | 45(4) | 47(4) | 19(3) | 6(2) | 8(3) | -1(3) |
| C39 | 24(3) | 27(3) | 17(3) | 9(2) | 6(2) | 0(2) |
| C40 | 30(3) | 31(3) | 18(3) | 8(2) | 10(2) | -5(2) |
| C41 | 18(3) | 50(4) | 22(3) | 0(2) | 4(2) | 2(2) |
| C43 | 32(3) | 36(3) | 47(4) | -6(3) | 14(3) | -15(3) |
| C44 | 20(3) | 36(3) | 26(3) | 5(2) | 8(2) | 0(2) |
| C47 | 35(4) | 25(3) | 50(4) | 0(3) | 9(3) | -3(2) |
| C45 | 36(3) | 34(3) | 29(3) | 9(2) | 17(3) | 5(3) |
| C7 | 22(3) | 15(2) | 20(3) | 5.1(19) | 3(2) | -4(2) |
| C57 | 36(3) | 24(3) | 24(3) | -3(2) | 10(2) | -7(2) |
| C58 | 38(3) | 29(3) | 28(3) | -2(2) | 14(3) | -6(2) |
| C59 | 48(4) | 37(3) | 36(3) | -8(3) | 11(3) | 9(3) |
| C60 | 53(4) | 32(3) | 30(3) | -9(2) | 14(3) | -13(3) |
| C5 | 17(3) | 23(3) | 14(2) | 3.3(19) | -3(2) | -2(2) |
| C4 | 12(2) | 21(3) | 29(3) | 10(2) | 0(2) | 0(2) |
| C3 | 12(2) | 23(3) | 19(3) | 5(2) | 3(2) | 2.0(19) |
| C35 | 19(3) | 35(3) | 29(3) | 9(2) | -3(2) | -7(2) |
| C36 | 23(3) | 37(3) | 38(3) | 10(3) | 3(3) | -11(2) |
| C38 | 17(3) | 50(4) | 57(4) | 17(3) | -5(3) | -10(3) |
| C37 | 30(3) | 55(4) | 35(3) | -7(3) | -1(3) | -18(3) |
| C22 | 28(3) | 26(3) | 19(3) | 1(2) | 7(2) | -9(2) |
| C21 | 24(3) | 29(3) | 35(3) | 9(2) | 2(2) | 2(2) |
| C20 | 46(4) | 18(3) | 40(3) | 5(2) | 13(3) | -3(3) |
| C19 | 33(3) | 23(3) | 37(3) | 3(2) | 12(3) | -9(2) |
| C18 | 27(3) | 26(3) | 24(3) | 0(2) | 9(2) | -6(2) |
| C11 | 21(3) | 20(3) | 23(3) | -1(2) | 13(2) | -6(2) |
| C12 | 21(3) | 22(3) | 36(3) | -3(2) | 15(2) | -12(2) |
| C13 | 33(3) | 22(3) | 64(4) | -6(3) | 32(3) | -9(2) |
| C14 | 62(5) | 30(3) | 52(4) | -17(3) | 46(4) | -18(3) |
| C15 | 67(5) | 37(3) | 21(3) | -11(2) | 23(3) | -21(3) |
| C16 | 41(3) | 24(3) | 18(3) | 1(2) | 12(2) | -10(2) |
| C61 | 53(4) | 57(4) | 39(4) | 0(3) | 8(3) | 13(3) |
| C17 | 22(3) | 21(3) | 10(2) | -0.6(18) | 8(2) | -5(2) |
| C51 | 47(4) | 31(3) | 30(3) | -9(2) | -12(3) | 10(3) |
| C42 | 23(3) | 55(4) | 33(3) | -4(3) | 13(3) | -12(3) |
| C55 | 68(5) | 63(5) | 35(4) | -17(3) | -26(4) | 28(4) |

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| C46 | 29(4) | 77(5) | 60(5) | -18(4) | 17(3) | -21(3) |

**Table 9**: Bond Lengths in Å for **Compound 4**.

| Atom | Atom | Length/Å |
|---|---|---|
| Pt | Cl2 | 2.3383(12) |
| Pt | Cl1 | 2.3581(12) |
| Pt | P1 | 2.2199(12) |
| Pt | P2 | 2.2411(12) |
| Fe | C1 | 2.046(4) |
| Fe | C2 | 2.030(5) |
| Fe | C8 | 2.118(5) |
| Fe | C9 | 2.060(5) |
| Fe | C10 | 2.052(5) |
| Fe | C6 | 2.100(5) |
| Fe | C7 | 2.057(5) |
| Fe | C5 | 2.066(5) |
| Fe | C4 | 2.108(5) |
| Fe | C3 | 2.073(5) |
| Cl3 | C61 | 1.782(7) |
| Cl4 | C61 | 1.739(7) |
| P1 | C1 | 1.799(5) |
| P1 | C11 | 1.811(5) |
| P1 | C17 | 1.822(5) |
| P2 | C2 | 1.790(5) |
| P2 | C29 | 1.803(5) |
| P2 | C23 | 1.830(5) |
| C1 | C2 | 1.438(6) |
| C1 | C5 | 1.428(6) |
| C2 | C3 | 1.437(6) |
| C29 | C34 | 1.384(7) |
| C29 | C30 | 1.401(6) |
| C34 | C33 | 1.377(7) |
| C33 | C32 | 1.384(7) |
| C32 | C31 | 1.386(7) |
| C31 | C30 | 1.379(7) |
| C23 | C28 | 1.387(7) |
| C23 | C24 | 1.379(7) |
| C28 | C27 | 1.369(7) |
| C27 | C26 | 1.368(8) |
| C26 | C25 | 1.382(8) |
| C25 | C24 | 1.376(7) |
| C8 | C9 | 1.427(7) |
| C8 | C7 | 1.412(7) |
| C8 | C57 | 1.524(7) |
| C9 | C10 | 1.399(6) |
| C10 | C6 | 1.434(6) |
| C6 | B | 1.563(7) |
| C6 | C7 | 1.442(7) |
| B | C48 | 1.571(8) |
| B | C39 | 1.589(7) |
| C48 | C49 | 1.412(7) |
| C48 | C53 | 1.417(7) |
| C49 | C50 | 1.386(8) |
| C49 | C54 | 1.502(8) |
| C50 | C51 | 1.382(8) |
| C52 | C53 | 1.393(7) |
| C52 | C51 | 1.371(8) |
| C53 | C56 | 1.520(7) |
| C39 | C40 | 1.403(7) |
| C39 | C44 | 1.407(7) |
| C40 | C41 | 1.387(7) |
| C40 | C45 | 1.501(7) |
| C41 | C42 | 1.379(8) |
| C43 | C44 | 1.400(7) |
| C43 | C42 | 1.382(8) |
| C44 | C47 | 1.514(7) |
| C57 | C58 | 1.515(7) |
| C57 | C59 | 1.537(8) |
| C57 | C60 | 1.523(7) |
| C5 | C4 | 1.420(7) |
| C4 | C3 | 1.414(7) |
| C4 | C35 | 1.523(7) |
| C35 | C36 | 1.534(7) |
| C35 | C38 | 1.521(8) |
| C35 | C37 | 1.526(8) |
| C22 | C21 | 1.391(7) |
| C22 | C17 | 1.381(7) |
| C21 | C20 | 1.380(7) |
| C20 | C19 | 1.381(8) |
| C19 | C18 | 1.381(7) |
| C18 | C17 | 1.400(7) |
| C11 | C12 | 1.392(7) |
| C11 | C16 | 1.384(7) |
| C12 | C13 | 1.385(7) |
| C13 | C14 | 1.364(9) |
| C14 | C15 | 1.371(9) |
| C15 | C16 | 1.385(7) |
| C51 | C55 | 1.511(8) |
| C42 | C46 | 1.514(8) |

**Table 10**: Bond Angles in ° for **Compound 4**.

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| Cl2 | Pt | Cl1 | 88.57(4) |
| P1 | Pt | Cl2 | 176.56(5) |
| P1 | Pt | Cl1 | 92.46(4) |
| P1 | Pt | P2 | 85.46(4) |
| P2 | Pt | Cl2 | 93.20(4) |
| P2 | Pt | Cl1 | 174.26(5) |
| C1 | Fe | C8 | 124.76(18) |
| C1 | Fe | C9 | 105.63(18) |
| C1 | Fe | C10 | 118.01(18) |
| C1 | Fe | C6 | 153.51(18) |
| C1 | Fe | C7 | 162.35(18) |
| C1 | Fe | C5 | 40.64(18) |

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| C1 | Fe | C4 | 68.11(18) |
| C1 | Fe | C3 | 68.82(18) |
| C2 | Fe | C1 | 41.33(17) |
| C2 | Fe | C8 | 162.79(18) |
| C2 | Fe | C9 | 125.89(18) |
| C2 | Fe | C10 | 108.28(18) |
| C2 | Fe | C6 | 120.57(18) |
| C2 | Fe | C7 | 155.90(18) |
| C2 | Fe | C5 | 68.15(18) |
| C2 | Fe | C4 | 67.82(18) |
| C2 | Fe | C3 | 40.97(17) |
| C9 | Fe | C8 | 39.92(19) |
| C9 | Fe | C6 | 67.55(18) |
| C9 | Fe | C5 | 118.33(19) |
| C9 | Fe | C4 | 152.82(19) |
| C9 | Fe | C3 | 165.05(19) |
| C10 | Fe | C8 | 66.93(19) |
| C10 | Fe | C9 | 39.78(18) |
| C10 | Fe | C6 | 40.38(18) |
| C10 | Fe | C7 | 67.40(19) |
| C10 | Fe | C5 | 152.07(18) |
| C10 | Fe | C4 | 166.74(19) |
| C10 | Fe | C3 | 129.40(18) |
| C6 | Fe | C8 | 67.38(18) |
| C6 | Fe | C4 | 129.57(18) |
| C7 | Fe | C8 | 39.50(18) |
| C7 | Fe | C9 | 67.01(19) |
| C7 | Fe | C6 | 40.56(18) |
| C7 | Fe | C5 | 127.14(19) |
| C7 | Fe | C4 | 110.61(19) |
| C7 | Fe | C3 | 122.23(19) |
| C5 | Fe | C8 | 107.83(19) |
| C5 | Fe | C6 | 165.44(19) |
| C5 | Fe | C4 | 39.77(18) |
| C5 | Fe | C3 | 67.13(19) |
| C4 | Fe | C8 | 120.6(2) |
| C3 | Fe | C8 | 154.55(19) |
| C3 | Fe | C6 | 110.86(18) |
| C3 | Fe | C4 | 39.52(19) |
| C1 | P1 | Pt | 107.09(15) |
| C1 | P1 | C11 | 108.6(2) |
| C1 | P1 | C17 | 107.4(2) |
| C11 | P1 | Pt | 121.23(17) |
| C11 | P1 | C17 | 103.7(2) |
| C17 | P1 | Pt | 108.10(15) |
| C2 | P2 | Pt | 107.34(15) |
| C2 | P2 | C29 | 109.2(2) |
| C2 | P2 | C23 | 103.5(2) |
| C29 | P2 | Pt | 121.67(17) |
| C29 | P2 | C23 | 104.9(2) |
| C23 | P2 | Pt | 108.79(16) |
| P1 | C1 | Fe | 127.6(2) |
| C2 | C1 | Fe | 68.7(3) |
| C2 | C1 | P1 | 117.2(3) |
| C5 | C1 | Fe | 70.4(3) |
| C5 | C1 | P1 | 136.3(4) |
| C5 | C1 | C2 | 106.4(4) |
| P2 | C2 | Fe | 129.2(2) |
| C1 | C2 | Fe | 69.9(3) |
| C1 | C2 | P2 | 115.3(3) |
| C3 | C2 | Fe | 71.2(3) |
| C3 | C2 | P2 | 136.1(4) |
| C3 | C2 | C1 | 108.1(4) |

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| C34 | C29 | P2 | 121.2(4) |
| C34 | C29 | C30 | 119.3(4) |
| C30 | C29 | P2 | 119.5(4) |
| C33 | C34 | C29 | 119.9(5) |
| C34 | C33 | C32 | 120.6(5) |
| C33 | C32 | C31 | 120.2(4) |
| C30 | C31 | C32 | 119.3(5) |
| C31 | C30 | C29 | 120.7(5) |
| C28 | C23 | P2 | 122.6(4) |
| C24 | C23 | P2 | 118.4(4) |
| C24 | C23 | C28 | 119.0(5) |
| C27 | C28 | C23 | 119.9(5) |
| C26 | C27 | C28 | 121.0(5) |
| C27 | C26 | C25 | 119.6(5) |
| C24 | C25 | C26 | 119.7(5) |
| C25 | C24 | C23 | 120.8(5) |
| C9 | C8 | Fe | 67.8(3) |
| C9 | C8 | C57 | 125.1(4) |
| C7 | C8 | Fe | 67.9(3) |
| C7 | C8 | C9 | 106.3(4) |
| C7 | C8 | C57 | 127.6(4) |
| C57 | C8 | Fe | 137.7(4) |
| C8 | C9 | Fe | 72.2(3) |
| C10 | C9 | Fe | 69.8(3) |
| C10 | C9 | C8 | 108.9(4) |
| C9 | C10 | Fe | 70.4(3) |
| C9 | C10 | C6 | 109.4(4) |
| C6 | C10 | Fe | 71.6(3) |
| C10 | C6 | Fe | 68.0(3) |
| C10 | C6 | B | 130.5(4) |
| C10 | C6 | C7 | 104.9(4) |
| B | C6 | Fe | 149.1(4) |
| C7 | C6 | Fe | 68.1(3) |
| C7 | C6 | B | 118.3(4) |
| C6 | B | C48 | 117.8(4) |
| C6 | B | C39 | 119.5(4) |
| C48 | B | C39 | 121.5(4) |
| C49 | C48 | B | 120.7(5) |
| C49 | C48 | C53 | 116.7(5) |
| C53 | C48 | B | 122.5(4) |
| C48 | C49 | C54 | 122.7(5) |
| C50 | C49 | C48 | 119.9(5) |
| C50 | C49 | C54 | 117.5(5) |
| C51 | C50 | C49 | 123.2(5) |
| C51 | C52 | C53 | 122.1(5) |
| C48 | C53 | C56 | 124.9(4) |
| C52 | C53 | C48 | 120.8(5) |
| C52 | C53 | C56 | 114.2(5) |
| C40 | C39 | B | 123.3(4) |
| C40 | C39 | C44 | 117.8(5) |
| C44 | C39 | B | 118.8(4) |
| C39 | C40 | C45 | 121.6(5) |
| C41 | C40 | C39 | 120.4(5) |
| C41 | C40 | C45 | 117.8(5) |
| C42 | C41 | C40 | 122.6(5) |
| C42 | C43 | C44 | 122.5(5) |
| C39 | C44 | C47 | 121.1(5) |
| C43 | C44 | C39 | 119.7(5) |
| C43 | C44 | C47 | 119.2(5) |
| C8 | C7 | Fe | 72.6(3) |
| C8 | C7 | C6 | 110.1(4) |
| C6 | C7 | Fe | 71.3(3) |
| C8 | C57 | C59 | 106.0(4) |

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| C58 | C57 | C8 | 112.4(4) |
| C58 | C57 | C59 | 109.2(4) |
| C58 | C57 | C60 | 110.5(5) |
| C60 | C57 | C8 | 110.8(4) |
| C60 | C57 | C59 | 107.7(5) |
| C1 | C5 | Fe | 68.9(3) |
| C4 | C5 | Fe | 71.7(3) |
| C4 | C5 | C1 | 109.5(4) |
| C5 | C4 | Fe | 68.5(3) |
| C5 | C4 | C35 | 125.6(5) |
| C3 | C4 | Fe | 68.9(3) |
| C3 | C4 | C5 | 107.7(4) |
| C3 | C4 | C35 | 126.1(4) |
| C35 | C4 | Fe | 134.4(4) |
| C2 | C3 | Fe | 67.9(3) |
| C4 | C3 | Fe | 71.6(3) |
| C4 | C3 | C2 | 108.2(4) |
| C4 | C35 | C36 | 111.7(4) |
| C4 | C35 | C37 | 111.5(4) |
| C38 | C35 | C4 | 105.4(4) |
| C38 | C35 | C36 | 110.1(5) |
| C38 | C35 | C37 | 109.2(5) |
| C37 | C35 | C36 | 108.9(5) |

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| C17 | C22 | C21 | 119.7(5) |
| C20 | C21 | C22 | 120.0(5) |
| C21 | C20 | C19 | 120.5(5) |
| C18 | C19 | C20 | 120.0(5) |
| C19 | C18 | C17 | 119.7(5) |
| C12 | C11 | P1 | 121.5(4) |
| C16 | C11 | P1 | 119.0(4) |
| C16 | C11 | C12 | 119.5(5) |
| C13 | C12 | C11 | 119.8(5) |
| C14 | C13 | C12 | 120.3(6) |
| C13 | C14 | C15 | 120.2(5) |
| C14 | C15 | C16 | 120.6(6) |
| C11 | C16 | C15 | 119.6(6) |
| Cl4 | C61 | Cl3 | 112.3(4) |
| C22 | C17 | P1 | 123.6(4) |
| C22 | C17 | C18 | 120.1(5) |
| C18 | C17 | P1 | 116.2(4) |
| C50 | C51 | C55 | 122.5(6) |
| C52 | C51 | C50 | 117.1(5) |
| C52 | C51 | C55 | 120.4(6) |
| C41 | C42 | C43 | 117.0(5) |
| C41 | C42 | C46 | 121.8(6) |
| C43 | C42 | C46 | 121.1(6) |

**Table 11**: Torsion Angles in ° for **Compound 4**.

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| Pt | P1 | C1 | Fe | -65.9(3) |
| Pt | P1 | C1 | C2 | 17.2(4) |
| Pt | P1 | C1 | C5 | -167.1(5) |
| Pt | P1 | C11 | C12 | 18.6(5) |
| Pt | P1 | C11 | C16 | -163.7(3) |
| Pt | P1 | C17 | C22 | -116.3(4) |
| Pt | P1 | C17 | C18 | 60.0(4) |
| Pt | P2 | C2 | Fe | 63.3(3) |
| Pt | P2 | C2 | C1 | -20.8(4) |
| Pt | P2 | C2 | C3 | 167.5(4) |
| Pt | P2 | C29 | C34 | -25.5(5) |
| Pt | P2 | C29 | C30 | 153.8(3) |
| Pt | P2 | C23 | C28 | 132.4(4) |
| Pt | P2 | C23 | C24 | -47.4(4) |
| Fe | C1 | C2 | P2 | 124.8(3) |
| Fe | C1 | C2 | C3 | -61.2(3) |
| Fe | C1 | C5 | C4 | 60.4(3) |
| Fe | C2 | C3 | C4 | -60.4(3) |
| Fe | C8 | C9 | C10 | 60.5(3) |
| Fe | C8 | C7 | C6 | -61.8(3) |
| Fe | C8 | C57 | C58 | 29.0(7) |
| Fe | C8 | C57 | C59 | 148.1(5) |
| Fe | C8 | C57 | C60 | -95.3(6) |
| Fe | C9 | C10 | C6 | 61.3(3) |
| Fe | C10 | C6 | B | -150.8(5) |
| Fe | C10 | C6 | C7 | 58.4(3) |
| Fe | C6 | B | C48 | -140.9(6) |
| Fe | C6 | B | C39 | 51.5(9) |
| Fe | C6 | C7 | C8 | 62.6(3) |
| Fe | C5 | C4 | C3 | 57.9(3) |
| Fe | C5 | C4 | C35 | -130.0(5) |
| Fe | C4 | C3 | C2 | 58.2(3) |
| Fe | C4 | C35 | C36 | 57.1(7) |
| Fe | C4 | C35 | C38 | 176.7(4) |

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| Fe | C4 | C35 | C37 | -65.0(6) |
| P1 | C1 | C2 | Fe | -122.4(3) |
| P1 | C1 | C2 | P2 | 2.4(5) |
| P1 | C1 | C2 | C3 | 176.4(3) |
| P1 | C1 | C5 | Fe | 124.4(5) |
| P1 | C1 | C5 | C4 | -175.2(4) |
| P1 | C11 | C12 | C13 | 175.7(4) |
| P1 | C11 | C16 | C15 | -177.0(4) |
| P2 | C2 | C3 | Fe | -127.4(5) |
| P2 | C2 | C3 | C4 | 172.1(4) |
| P2 | C29 | C34 | C33 | 178.8(4) |
| P2 | C29 | C30 | C31 | -178.9(4) |
| P2 | C23 | C28 | C27 | -179.4(4) |
| P2 | C23 | C24 | C25 | 179.2(5) |
| C1 | P1 | C11 | C12 | -106.0(4) |
| C1 | P1 | C11 | C16 | 71.8(4) |
| C1 | P1 | C17 | C22 | -1.1(5) |
| C1 | P1 | C17 | C18 | 175.2(3) |
| C1 | C2 | C3 | Fe | 60.5(3) |
| C1 | C2 | C3 | C4 | 0.0(5) |
| C1 | C5 | C4 | Fe | -58.7(3) |
| C1 | C5 | C4 | C3 | -0.8(5) |
| C1 | C5 | C4 | C35 | 171.3(4) |
| C2 | P2 | C29 | C34 | 100.3(4) |
| C2 | P2 | C29 | C30 | -80.3(4) |
| C2 | P2 | C23 | C28 | 18.5(4) |
| C2 | P2 | C23 | C24 | -161.3(4) |
| C2 | C1 | C5 | Fe | -59.6(3) |
| C2 | C1 | C5 | C4 | 0.8(5) |
| C29 | P2 | C2 | Fe | -70.5(3) |
| C29 | P2 | C2 | C1 | -154.5(3) |
| C29 | P2 | C2 | C3 | 33.8(5) |
| C29 | P2 | C23 | C28 | -96.0(4) |
| C29 | P2 | C23 | C24 | 84.3(4) |
| C29 | C34 | C33 | C32 | 0.1(8) |
| C34 | C29 | C30 | C31 | 0.5(7) |
| C34 | C33 | C32 | C31 | 0.3(8) |
| C33 | C32 | C31 | C30 | -0.3(8) |
| C32 | C31 | C30 | C29 | -0.1(7) |
| C30 | C29 | C34 | C33 | -0.5(7) |
| C23 | P2 | C2 | Fe | 178.2(3) |
| C23 | P2 | C2 | C1 | 94.2(4) |
| C23 | P2 | C2 | C3 | -77.5(5) |
| C23 | P2 | C29 | C34 | -149.3(4) |
| C23 | P2 | C29 | C30 | 30.1(4) |
| C23 | C28 | C27 | C26 | -0.2(8) |
| C28 | C23 | C24 | C25 | -0.6(8) |
| C28 | C27 | C26 | C25 | 0.1(8) |
| C27 | C26 | C25 | C24 | -0.3(9) |
| C26 | C25 | C24 | C23 | 0.5(9) |
| C24 | C23 | C28 | C27 | 0.4(7) |
| C8 | C9 | C10 | Fe | -62.0(3) |
| C8 | C9 | C10 | C6 | -0.7(5) |
| C9 | C8 | C7 | Fe | 57.1(3) |
| C9 | C8 | C7 | C6 | -4.7(5) |
| C9 | C8 | C57 | C58 | -66.0(7) |
| C9 | C8 | C57 | C59 | 53.2(6) |
| C9 | C8 | C57 | C60 | 169.8(5) |
| C9 | C10 | C6 | Fe | -60.5(3) |
| C9 | C10 | C6 | B | 148.7(5) |
| C9 | C10 | C6 | C7 | -2.1(5) |
| C10 | C6 | B | C48 | -22.9(8) |
| C10 | C6 | B | C39 | 169.5(5) |

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| C10 | C6 | C7 | Fe | -58.4(3) |
| C10 | C6 | C7 | C8 | 4.2(5) |
| C6 | B | C48 | C49 | 144.2(5) |
| C6 | B | C48 | C53 | -39.9(7) |
| C6 | B | C39 | C40 | -78.4(6) |
| C6 | B | C39 | C44 | 101.3(6) |
| B | C6 | C7 | Fe | 146.5(4) |
| B | C6 | C7 | C8 | -150.9(4) |
| B | C48 | C49 | C50 | -179.2(5) |
| B | C48 | C49 | C54 | 0.4(8) |
| B | C48 | C53 | C52 | -179.2(5) |
| B | C48 | C53 | C56 | -3.4(7) |
| B | C39 | C40 | C41 | 179.5(5) |
| B | C39 | C40 | C45 | -5.7(7) |
| B | C39 | C44 | C43 | -178.5(5) |
| B | C39 | C44 | C47 | 1.2(7) |
| C48 | B | C39 | C40 | 114.5(6) |
| C48 | B | C39 | C44 | -65.8(7) |
| C48 | C49 | C50 | C51 | -2.5(9) |
| C49 | C48 | C53 | C52 | -3.1(7) |
| C49 | C48 | C53 | C56 | 172.7(5) |
| C49 | C50 | C51 | C52 | -1.4(9) |
| C49 | C50 | C51 | C55 | 179.7(6) |
| C53 | C48 | C49 | C50 | 4.7(7) |
| C53 | C48 | C49 | C54 | -175.7(5) |
| C53 | C52 | C51 | C50 | 3.0(8) |
| C53 | C52 | C51 | C55 | -178.0(5) |
| C54 | C49 | C50 | C51 | 177.8(5) |
| C39 | B | C48 | C49 | -48.4(7) |
| C39 | B | C48 | C53 | 127.5(5) |
| C39 | C40 | C41 | C42 | -0.3(8) |
| C40 | C39 | C44 | C43 | 1.2(7) |
| C40 | C39 | C44 | C47 | -179.1(5) |
| C40 | C41 | C42 | C43 | -0.2(8) |
| C40 | C41 | C42 | C46 | 177.3(5) |
| C44 | C39 | C40 | C41 | -0.2(7) |
| C44 | C39 | C40 | C45 | 174.6(5) |
| C44 | C43 | C42 | C41 | 1.2(9) |
| C44 | C43 | C42 | C46 | -176.3(6) |
| C45 | C40 | C41 | C42 | -175.4(5) |
| C7 | C8 | C9 | Fe | -57.2(3) |
| C7 | C8 | C9 | C10 | 3.3(5) |
| C7 | C8 | C57 | C58 | 127.1(5) |
| C7 | C8 | C57 | C59 | -113.7(6) |
| C7 | C8 | C57 | C60 | 2.8(7) |
| C7 | C6 | B | C48 | 124.8(5) |
| C7 | C6 | B | C39 | -42.9(7) |
| C57 | C8 | C9 | Fe | 133.6(5) |
| C57 | C8 | C9 | C10 | -165.9(5) |
| C57 | C8 | C7 | Fe | -134.0(5) |
| C57 | C8 | C7 | C6 | 164.2(5) |
| C5 | C1 | C2 | Fe | 60.7(3) |
| C5 | C1 | C2 | P2 | -174.4(3) |
| C5 | C1 | C2 | C3 | -0.5(5) |
| C5 | C4 | C3 | Fe | -57.7(3) |
| C5 | C4 | C3 | C2 | 0.5(5) |
| C5 | C4 | C35 | C36 | 151.2(5) |
| C5 | C4 | C35 | C38 | -89.2(6) |
| C5 | C4 | C35 | C37 | 29.2(7) |
| C3 | C4 | C35 | C36 | -38.2(7) |
| C3 | C4 | C35 | C38 | 81.4(6) |
| C3 | C4 | C35 | C37 | -160.2(5) |
| C35 | C4 | C3 | Fe | 130.3(5) |

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| C35 | C4 | C3 | C2 | -171.5(4) |
| C22 | C21 | C20 | C19 | 0.3(8) |
| C21 | C22 | C17 | P1 | 176.8(4) |
| C21 | C22 | C17 | C18 | 0.6(7) |
| C21 | C20 | C19 | C18 | -0.7(8) |
| C20 | C19 | C18 | C17 | 1.1(8) |
| C19 | C18 | C17 | P1 | -177.5(4) |
| C19 | C18 | C17 | C22 | -1.1(7) |
| C11 | P1 | C1 | Fe | 66.6(3) |
| C11 | P1 | C1 | C2 | 149.8(4) |
| C11 | P1 | C1 | C5 | -34.6(6) |
| C11 | P1 | C17 | C22 | 113.8(4) |
| C11 | P1 | C17 | C18 | -69.9(4) |
| C11 | C12 | C13 | C14 | 2.2(7) |
| C12 | C11 | C16 | C15 | 0.8(7) |
| C12 | C13 | C14 | C15 | -1.1(8) |
| C13 | C14 | C15 | C16 | -0.1(8) |
| C14 | C15 | C16 | C11 | 0.3(8) |
| C16 | C11 | C12 | C13 | -2.0(7) |
| C17 | P1 | C1 | Fe | 178.2(3) |
| C17 | P1 | C1 | C2 | -98.7(4) |
| C17 | P1 | C1 | C5 | 77.0(5) |
| C17 | P1 | C11 | C12 | 140.0(4) |
| C17 | P1 | C11 | C16 | -42.2(4) |
| C17 | C22 | C21 | C20 | -0.2(8) |
| C51 | C52 | C53 | C48 | -0.7(8) |
| C51 | C52 | C53 | C56 | -176.9(5) |
| C42 | C43 | C44 | C39 | -1.8(9) |
| C42 | C43 | C44 | C47 | 178.6(5) |

**Table 12**: Hydrogen Fractional Atomic Coordinates (×10$^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×10$^3$) for **Compound 4**. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{ij}$.

| Atom | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| H34 | 10056.45 | 6988.44 | 1727.41 | 28 |
| H33 | 9979.3 | 6777.19 | 3043.91 | 32 |
| H32 | 8472.75 | 6954.18 | 3589.34 | 30 |
| H31 | 7013.03 | 7342.69 | 2808.99 | 28 |
| H30 | 7086.67 | 7555.55 | 1489.12 | 24 |
| H28 | 6354.27 | 7748.34 | -267.73 | 32 |
| H27 | 5475.9 | 8376.61 | -403.91 | 36 |
| H26 | 6433.64 | 8961.73 | 118.76 | 38 |
| H25 | 8314.17 | 8919.62 | 785.62 | 51 |
| H24 | 9203.92 | 8289.76 | 930.94 | 39 |
| H9 | 10105.2 | 6428.19 | -822.99 | 22 |
| H10 | 9914.73 | 6517.14 | 627.39 | 21 |
| H50 | 10225.36 | 5744.68 | 3835.25 | 44 |
| H52 | 11905.51 | 5420.82 | 2158.33 | 36 |
| H56A | 9780.73 | 5512.08 | 411.47 | 41 |
| H56B | 10909.62 | 5275.32 | 810.96 | 41 |
| H56C | 10937.5 | 5753.51 | 616.77 | 41 |
| H54A | 7708.82 | 5745.54 | 2751.8 | 56 |
| H54B | 8064.91 | 6213.26 | 2702.95 | 56 |
| H54C | 8474.8 | 5962.63 | 3543.25 | 56 |
| H41 | 4611.64 | 5971.75 | 1281.95 | 36 |
| H43 | 5749.19 | 4860.83 | 898.4 | 45 |
| H47A | 8464.33 | 5034.05 | 1405.17 | 55 |
| H47B | 8114.08 | 5097.09 | 426.69 | 55 |
| H47C | 7564.75 | 4737.63 | 847.99 | 55 |
| H45A | 7076.76 | 6513.33 | 1307.37 | 48 |
| H45B | 6390.04 | 6463.42 | 2005.28 | 48 |
| H45C | 5756.15 | 6572.26 | 1079.17 | 48 |
| H7 | 7391.49 | 5775.94 | -578.15 | 23 |
| H58A | 9086.7 | 6351.31 | -2380.01 | 46 |
| H58B | 7796 | 6236.62 | -2660.91 | 46 |
| H58C | 8688.85 | 5989.97 | -3028.29 | 46 |
| H59A | 9969.26 | 5443.05 | -1223.79 | 60 |
| H59B | 10412.19 | 5814.2 | -1684.37 | 60 |
| H59C | 9812.96 | 5432.6 | -2204.09 | 60 |
| H60A | 7931 | 5292.18 | -1585.49 | 56 |
| H60B | 7806.31 | 5365.58 | -2552.05 | 56 |
| H60C | 7066.19 | 5623.78 | -2063.83 | 56 |
| H5 | 7229.35 | 6828.2 | -2165.76 | 23 |
| H3 | 6383.62 | 6883.8 | 64.1 | 22 |
| H36A | 4871.77 | 6443.99 | -457.33 | 50 |
| H36B | 5515.8 | 6067.53 | -745.2 | 50 |
| H36C | 4246.16 | 6154.79 | -1194.23 | 50 |
| H38A | 4400.65 | 7049.62 | -1334.33 | 65 |
| H38B | 3796.1 | 6788.5 | -2123.25 | 65 |
| H38C | 4790.16 | 7091.61 | -2181.46 | 65 |
| H37A | 5979.51 | 6091.58 | -2143.28 | 62 |
| H37B | 5624.34 | 6482.39 | -2721.5 | 62 |
| H37C | 4693.84 | 6178.56 | -2543.22 | 62 |
| H22 | 7123.11 | 7810.03 | -1889.12 | 29 |
| H21 | 6617.7 | 8452.61 | -2478.11 | 36 |
| H20 | 7984.71 | 8918.92 | -2611.91 | 41 |
| H19 | 9857.21 | 8748.73 | -2179.56 | 36 |
| H18 | 10373.93 | 8113.48 | -1576.43 | 30 |
| H12 | 11287.53 | 6941.45 | -1088.42 | 30 |
| H13 | 11989.7 | 6570.32 | -2050.16 | 44 |
| H14 | 11108.87 | 6593.71 | -3433.32 | 52 |

| Atom | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| H15 | 9486.2 | 6965.64 | -3869.13 | 48 |
| H16 | 8725.13 | 7321.7 | -2918.59 | 32 |
| H61A | 3659.62 | 6926.96 | 1476.45 | 60 |
| H61B | 2738.58 | 7214.4 | 915.43 | 60 |
| H55A | 12016.45 | 5355.17 | 4249.69 | 92 |
| H55B | 12681.65 | 5722.6 | 3951.35 | 92 |
| H55C | 12712.76 | 5275.98 | 3566.7 | 92 |
| H46A | 3289.54 | 5397.36 | 895.31 | 81 |
| H46B | 3869.78 | 5133.08 | 1686.29 | 81 |
| H46C | 3765.75 | 4952.11 | 779.51 | 81 |

**Table 13**: Solvent masking (Olex2) information for **Compound 4**.

| No | x | y | z | V | e | Content |
|---|---|---|---|---|---|---|
| 1 | 0.344 | 0.000 | 0.000 | 759.4 | 135.2 | CH2Cl2 |
| 2 | -0.489 | 0.500 | 0.500 | 759.4 | 135.2 | CH2Cl2 |