Supporting information

Trinuclear ReFePt clusters with μ_3-phenylvinylidene ligand: synthetic approaches, characterization and their redox-induced transformations

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General information

All operations and manipulations were carried out under an argon atmosphere. Solvents (dichloromethane, petroleum ether, hexane, benzene) were purified by distillation from appropriate drying agents and stored under argon. The course of reactions was monitored by TLC on Silufol plates and IR spectroscopy. Neutral alumina was used for column chromatography. The initial binuclear compounds $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)(LL')$ [L = L' = $P(OPr^i)_3$, $P(OEt)_3$, $P(OPh)_3$; L' = CO, L = $P(OPr^i)_3$, $P(OEt)_3$, $P(OPh)_3$; L' = PPh_3, L = $P(OPr^i)_3$, $P(OEt)_3$, $P(OPh)_3$] were synthesized according to our recent published work [1].

Physical-chemical characteristics were obtained in the Krasnoyarsk Regional Centre of Research Equipment, Siberian Branch of the Russian Academy of Sciences. The IR spectra were recorded on the Shimadzu IR Tracer-100 spectrometer (Japan). The ^1H, $^{13}C\{^1H\}$ and $^{31}P\{^1H\}$ NMR spectra were obtained using NMR spectrometer AVANCE III 600 (Bruker, Germany). The X-ray data for **2a** and **2b** were obtained with the Smart Photon II diffractometer, (Bruker AXS, Germany). The EPR experiments were conducted by using a Bruker ELEXSYS E-580 spectrometer. The experimental EPR spectra were simulated using a Bruker Xsophe program.

Synthetic procedures

1. Reactions of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OR)_3](CO)$ with $Fe_2(CO)_9$

Reaction of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OPr^i)_3](CO)$ (2c) with $Fe_2(CO)_9$.

To a stirred solution of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OPr^i)_3](CO)$ (**2c**) (70 mg, 0.083 mmol) in 5 mL of benzene was added 33 mg of diiron nonacarbonyl (0.091 mmol). The reaction mixture was stirred for 1 hour at 24ºC and then was transferred via cannula into 50 mL flask. The solvent was removed *in vacuo* and the residue was dissolved in a minimum volume of hexane-Et_2O mixture (4:1). This solution was stored at -18°C for 48 hours to give the cluster $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OPr^i)_3]$ (**2a**) as dark-violet crystals. Yield 73 mg (90 %).

Reaction of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OEt)_3](CO)$ (3c) with $Fe_2(CO)_9$.

An identical procedure to the reaction of **2c** with $Fe_2(CO)_9$ was followed using $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OEt)_3](CO)$ (**3c**) (64 mg, 0.080 mmol), diiron nonacarbonyl (30 mg, 0.082 mmol) and benzene (5 mL). The cluster $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OEt)_3]$ (**3a**) was isolated as a dark solid. Yield of **3a**: 68% (51 mg, 0.054 mmol).

Reaction of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OPh)_3](CO)$ (4c) with $Fe_2(CO)_9$.

Treatment of a solution of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OPh)_3](CO)$ (**4c**) with $Fe_2(CO)_9$ did not result in any products as indicated by IR and NMR spectra.

2. Reactions of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OR)_3](PPh_3)$ with $Fe_2(CO)_9$

Reaction of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OPr^i)_3](PPh_3)$ (2d) with $Fe_2(CO)_9$

Diiron nonacarbonyl (34 mg, 0.093 mmol) was added to the solution of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OPr^i)_3](PPh_3)$ (**2d**) (84 mg, 0.078 mmol) in 6 mL of benzene. A reaction mixture was stirred for 2 hours at room temperature and then was filtered through 1 cm of alumina pad. The solvent was removed *in vacuo* and the residue was dissolved in hexane-benzene mixture (2:1) and chromatographed on an alumina column (14 × 2 cm). The column was eluted with petroleum ether and petroleum ether : benzene (7:3) mixture. The first colorless fraction, after evaporation of solvent, gave 24 mg (0.056 mmol, 72%) of pale complex $Fe(CO)_4(PPh_3)$, identified by IR. The second brown-green fraction, after removal of solvent and crystallization from hexane-Et_2O

mixture (4:1), afforded 59 mg (0.060 mmol, 77%) of dark-violet microcrystals of cluster $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OPr^i)_3]$ (**2a**).

Reaction of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OEt)_3](PPh_3)$ (3d) with $Fe_2(CO)_9$

An identical procedure to the reaction of **2d** with $Fe_2(CO)_9$ was followed using $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OEt)_3](PPh_3)$ (**3d**) (79 mg, 0.076 mmol), diiron nonacarbonyl (28 mg, 0.077 mmol) and benzene (6 mL). The cluster $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OEt)_3]$ (**3a**) was isolated as a dark solid. Yield of **3a**: 82% (58 mg, 0.062 mmol). Yield of $Fe(CO)_4(PPh_3)$: 70% (23 mg, 0.053 mmol).

Reaction of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OPh)_3](PPh_3)$ (4d) with $Fe_2(CO)_9$

To a stirred solution of $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)[P(OPh)_3](PPh_3)$ (**4d**) (51 mg, 0.043 mmol) in 5 mL of benzene was added 17 mg of diiron nonacarbonyl (0.047 mmol). The reaction mixture was stirred for 2 hours at room temperature and then was transferred via cannula into 50 mL flask. The solvent was removed *in vacuo* and the orange residue was dissolved in hexane-benzene mixture (2:1) and chromatographed on an alumina column (10 × 2 cm) using petroleum ether and petroleum ether : benzene (7:3) mixture. The first colorless zone contained 14 mg (0.033 mmol, 77 %) of complex $Fe(CO)_4(PPh_3)$. The second yellow-brown major band, after removal of solvent, gave complex $Cp(CO)_2RePt(\mu\text{-}C{=}CHPh)(CO)[P(OPh)_3]$ (**4c**) as a brown oil. Yield of **4c**: 79% (32 mg, 0.034 mmol). The complex **4c** was identified by IR and NMR spectra [1].

3. Reaction of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OPr^i)_3]_2$ (2b) with $Fe_2(CO)_9$

To a solution of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OPr^i)_3]_2$ (**2b**) (74 mg, 0.064 mmol) in 6 mL of benzene was added 47 mg of $Fe_2(CO)_9$ (0.129 mmol). A resulting reaction mixture was stirred for 6 hours at room temperature and then was transferred via cannula into 50 mL flask. The solvent was removed *in vacuo* and the residue was dissolved in hexane-benzene mixture (2:1) and chromatographed on an alumina column (14 × 2 cm). Three main fractions were successively eluted with petroleum ether, petroleum ether-benzene (7:3) and (3:2) mixtures and finally with benzene. The first rose fraction contained 2 mg (0.003 mmol, 5%) of $Cp(CO)_2ReFe_2(\mu\text{-}C{=}CHPh)(CO)_6$ identified by IR spectra [2]. The second brown-green fraction, after removal of solvent and crystallization from hexane-Et_2O mixture (4:1), gave 30 mg (0.031 mmol ,48%) of dark-violet microcrystals of cluster $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OPr^i)_3]$(**2a**). 32 mg (0.028 mmol) of the initial cluster **2b** were obtained from the third orange fraction after it's treatment 33 mg (0.028 mmol). Conversion of the reaction calculated from the amount of unreacted **2b** recovered by column chromatography is 44%.

4. Reactions of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OR)_3]$ with $P(OR)_3$

Reaction of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OPr^i)_3]$ (2a) with $P(OPr^i)_3$.

Triisopropyl phosphite (0.015 mL, 13 mg, 0.063 mmol) was added to the solution of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OPr^i)_3]$ (**2a**) (59 mg, 0.060 mmol) in 5 mL of benzene. A reaction mixture was stirred for 1 hour at room temperature and then was filtered through 1 cm of alumina pad into 50 mL flask. The solvent was removed *in vacuo* and the residue was dissolved in a minimum volume of benzene-hexane mixture (1:1). This solution was stored at -18°C for 48 hours to give the cluster $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OPr^i)_3]_2$ (**2b**) as red crystals. Yield 97% (67 mg, 0.058 mmol).

Reaction of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OEt)_3]$ (3a) with $P(OEt)_3$.

An identical procedure to the reaction of **3a** with $P(OPr^i)_3$ was followed using $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OEt)_3]$ (**3a**) (64 mg, 0.068 mmol), triethyl phosphite (0.072 mL, 12

mg, 0.072 mmol) and benzene (6 mL). The cluster CpReFePt(μ_3-C=CHPh)$(CO)_5[P(OEt)_3]_2$ (**3b**) was isolated as a black crystals. Yield of **3b**: 94% (69 mg, 0.064 mmol).

Reaction of CpReFePt(μ_3-C=CHPh)$(CO)_6[P(OPr^i)_3]$ (2a) with PPh_3.

Triphenylphosphane (7 mg, 0.024 mmol) was added to the solution of CpReFePt(μ_3-C=CHPh)$(CO)_6[P(OPr^i)_3]$ (**2a**) (24 mg, 0.024 mmol) in 4 mL of benzene. A reaction mixture was stirred for 1 hous at room temperature and then was concentrated to ca. 1 mL under reduced pressure. The product was precipitated by adding 10 mL of hexane, the supernatant was decanted, and the bright-red solid was washed with 2 mL of hexane. The residue was dried *in vacuo*, giving CpReFePt(μ_3-C=CHPh)$(CO)_5[P(OPr^i)_3](PPh_3)$ (**2e**) as bright-red solid. Yield 88% (26 mg, 0.021 mmol).

5. Reaction of CpReFePt(μ_3-C=CHPh)$(CO)_6[P(OEt)_3]$ (3a) with dppe

1,2-Bis(diphenylphosphino)ethane (15 mg, 0.038 mmol) was added to the solution of CpReFePt(μ_3-C=CHPh)$(CO)_6[P(OEt)_3]$ (**3a**) (34 mg, 0.036 mmol) in 6 mL of benzene. A reaction mixture was stirred for 2 hours at room temperature and then was concentrated to ca. 1 mL under reduced pressure. The product was precipitated by adding 10 mL of hexane, the supernatant was decanted, and the bright-red solid was washed twice with 2 mL of hexane. The residue was dried *in vacuo*, giving CpReFePt(μ_3-C=CHPh)$(CO)_5$(dppe) (**5**) as bright-red solid. Yield 86% (41 mg, 0.031 mmol). The cluster **5** was identified by IR and NMR spectra [3].

6. Reaction of CpReFePt(μ_3-C=CHPh)$(CO)_5[P(OEt)_3]_2$ (3b) with dppp

The cluster CpReFePt(μ_3-C=CHPh)$(CO)_5$(dppp) (**6**) was obtained as a bright-red solid with 84% yield (24 mg, 0.021 mmol), from reaction of CpReFePt(μ_3-C=CHPh)$(CO)_5[P(OEt)_3]_2$ (3b) (27 mg, 0.025 mmol) and 1,3-bis(diphenylphosphino)propane (11 mg, 0.027 mmol) in 5 mL of benzene following the procedure used for preparation of the cluster 5. The cluster 6 was identified by IR and NMR spectra [3].

Analytical data for CpReFePt(μ_3-C=CHPh)$(CO)_6[P(OPr^i)_3]$ (2a)

Anal. Found: C, 34.43; H, 3.35%. Calc. for $C_{28}H_{32}O_9P_1PtReFe$ (980.65): C, 34.29; H, 3.29%.

IR (ν(CO), cm^{-1}): 2049 s, 2013 s., 1970 sh, 1960 s., 1949 m, 1938 s, 1923 m, 1898 m, 1873 m (C_6H_{12}); 2046 v.s, 2007 s, 1949 v.s, 1927 s, 1901 m, 1855 m (tabl. KBr).

^{1}H NMR (CD_2Cl_2, 25ºC) δ, ppm [*J*, Hz]:

Isomer 2a_π-Pt: 1.10 (d, 9H, J_{HH} = 6.1, -C$\underline{H}_3$); 1.20 (d, 9H, J_{HH} = 6.0, -C$\underline{H}_3$); 4.55 (m, 3H, -C$\underline{H}$); 5.07 (s, 5H, $C_5\underline{H}_5$); 6.19 (d, 1H, $^2J_{PtH}$ = 56.3, =$C^2\underline{H}$Ph); 7.26 (t, 1H, J_{HH} = 7.7, H_{para} =$C^2HC_6\underline{H}_5$); 7.36 (t, 2H, J_{HH} = 7.7, H_{meta} =$C^2HC_6\underline{H}_5$); 7.43 (d, 2H, J_{HH} = 7.7, H_{ortho} =$C^2HC_6\underline{H}_5$).

Isomer 2a_π-Fe: 1.30 (d, 9H, J_{HH} = 6.3, -C$\underline{H}_3$); 1.41 (d, 9H, J_{HH} = 6.3, -C$\underline{H}_3$); 4.77 (m, 3H, -C$\underline{H}$); 5.86 (s, 5H, $C_5\underline{H}_5$); 6.41 (s, 1H, $^3J_{PtH}$ = 68.6, =$C^2\underline{H}$Ph); 7.11 (t, 1H, J_{HH} = 7.0, H_{para} =$C^2HC_6\underline{H}_5$); 7.22 (t, 2H, J_{HH} = 7.4, H_{meta} =$C^2HC_6\underline{H}_5$); 7.56 (d, 2H, J_{HH} = 7.7, H_{ortho} =$C^2HC_6\underline{H}_5$).

Isomer 2a*: 1.29 (d, J_{HH} = 6.5, -C$\underline{H}_3$, *overlap with –CH_3 siganal of isomer π-Fe*); 1.32 (d, J_{HH} = 6.5, -C$\underline{H}_3$, *overlap with –CH_3 siganal of isomer π-Fe*); 4.55 (m, C$\underline{H}$, *overlap with –CH siganal of isomer π-Pt*) 5.43 (s, 5H, $C_5\underline{H}_5$); 7.24 (t, H_{meta} =$C^2HC_6\underline{H}_5$, *overlap with H_{meta} siganal of isomer π-Fe*), 7.27 (t, H_{para} =$C^2HC_6\underline{H}_5$, *overlap with H_{para} siganal of isomer π-Pt*), 7.65 (d, 2H, J_{HH} = 6.7, H_{ortho} =$C^2HC_6\underline{H}_5$), 7.68 (d, 1H, $^2J_{PtH}$ = 62.0, $^3J_{PH}$ = 12.0, =$C^2\underline{H}$Ph, *overlap with H_{ortho} signal of isomer X*).

$^{13}C\{^1H\}$ NMR (CD_2Cl_2, 25ºC) δ, ppm [*J*, Hz]:

Isomer 2a_π-Pt: 23.2 (d, $^3J_{PC}$ = 4.8, -$\underline{C}H_3$); 23.4 (d, $^3J_{PC}$ = 4.0, -$\underline{C}H_3$); 71.0 (d, br, $^2J_{PC}$ = 3.2, $^3J_{PtC}$ = 16.0, -$\underline{C}$H); 88.9 (s, $\underline{C}_5H_5$); 92.9 (d, $^2J_{CP}$ = 4.7, =$\underline{C}^2$HPh); 125.9 (s, C_{para} of =$C^2H\underline{C}_6H_5$); 127.0 (s,

C_{meta} of $=C^2H\underline{C}_6H_5$); 129.7 (d, J_{PtC} = 20.0, C_{ortho} of $=C^2H\underline{C}_6H_5$); 146.3 (s, C_{ipso} of $=C^2H\underline{C}_6H_5$); 188.5 (s, Pt-$\underline{C}$O); 204.5 (s, br, Re-$\underline{C}$O); 214.4 (s, 3(Fe-$\underline{C}$O)).

Isomer 2a_π-Fe: 23.4 (d, $^3J_{PC}$ = 3.8, -$\underline{C}H_3$); 23.6 (d, $^3J_{PC}$ = 4.2, -$\underline{C}H_3$); 71.6 (d, $^2J_{PC}$ = 3.3, $^3J_{PtC}$ = 11.0, -$\underline{C}$H); 88.3 (s, $\underline{C}_5H_5$); 98.3 (d, $^3J_{CP}$ = 1.8, $^2J_{PtC}$ = 23.0, $=\underline{C}^2$HPh); 125.2 (s, C_{para} of $=C^2H\underline{C}_6H_5$); 127.6 (s, C_{meta} of $=C^2H\underline{C}_6H_5$); 128.1 (s, C_{ortho} of $=C^2H\underline{C}_6H_5$); 147.4 (s, C_{ipso} of $=C^2H\underline{C}_6H_5$); 186.8 (d, $^2J_{PC}$ = 12.6, Pt-$\underline{C}$O); 202.2 (s, br 2(Re-$\underline{C}$O)); 213.7 (s, br, 3(Fe-$\underline{C}$O)); 261.2 (s, μ-$\underline{C}^1$).

Isomer 2*: 23.5 (d, $^3J_{PC}$ = 4.3, -$\underline{C}H_3$); 71.1 (s,-$\underline{C}$H); 88.0 (s, $\underline{C}_5H_5$), 126.0 (s, C_{para} of $=C^2H\underline{C}_6H_5$); 127.6 (s, C_{meta} of $=C^2H\underline{C}_6H_5$); 128.1 (s, C_{ortho} of $=C^2H\underline{C}_6H_5$).

$^{31}P\{^1H\}$ NMR (CD_2Cl_2, 25ºC) δ, ppm [J, Hz]:

Isomer 2a_π-Pt: 112.8 (s, 1*P*, J_{PtP}= 5725), 35%.

Isomer 2a_π-Fe: 110.2 (s, 1*P*, J_{PtP}= 5710), 51%.

Isomer 2*: 111.4 (s, 1*P*, J_{PtP}= 5694), 14%.

^1H NMR (CD_2Cl_2, -70ºC) δ, ppm [J, Hz]:

Isomer 2a_π-Pt: 0.99 (d, 9H, J_{HH} = 4.8, -C$\underline{H}_3$); 1.12 (d, 9H, J_{HH} = 4.8, -C$\underline{H}_3$); 4.47 (s, 3H, -C$\underline{H}$); 5.04 (s, 5H, $C_5\underline{H}_5$); 6.09 (s, 1H, $^2J_{PtH}$ = 52.5, $=C^2\underline{H}$Ph); 7.20 - 7.25 (br, 1H, H_{para} of $=C^2HC_6\underline{H}_5$), 7.29 – 7.37 (br, 4H, H_{meta} and H_{ortho} of $=C^2HC_6\underline{H}_5$).

Isomer 2a_π-Fe: 1.24 (d, 9H, J_{HH} = 4.7, -C$\underline{H}_3$); 1.34 (d, 9H, J_{HH} = 4.7, -C$\underline{H}_3$); 4.70 (s, 3H, -C$\underline{H}$); 5.83 (s, 5H, $C_5\underline{H}_5$); 6.32 (s, 1H, $^3J_{PtH}$ = 66.0, $=C^2\underline{H}$Ph); 7.08 (br, 1H, H_{para} of $=C^2HC_6\underline{H}_5$); 7.20 (br, 2H, H_{meta} of $=C^2HC_6\underline{H}_5$); 7.48 (br, 2H, H_{ortho} of $=C^2HC_6\underline{H}_5$).

$^{13}C\{^1H\}$ NMR (CD_2Cl_2, -70ºC) δ, ppm [J, Hz]:

Isomer 2a_π-Pt: 23.2 (d, $^3J_{PC}$ = 4.6, -$\underline{C}H_3$); 23.5 (d, $^3J_{PC}$ = 3.3, -$\underline{C}H_3$); 71.2 (s, -$\underline{C}$H); 89.2 (s, $\underline{C}_5H_5$); 92.9 (d, $^2J_{CP}$ = 4.4, $=\underline{C}^2$HPh); 126.0 (s, C_{para} of = $C^2H\underline{C}_6H_5$); 127.2 (s, C_{meta} of $=C^2H\underline{C}_6H_5$); 129.4 (s, C_{ortho} of $=C^2H\underline{C}_6H_5$); 146.2 (d, J_{CP} = 5.3, C_{ipso} of $=C^2H\underline{C}_6H_5$); 188.5 (d, $^2J_{PC}$ = 10.0, Pt-$\underline{C}$O); 207.2 (s, Re-$\underline{C}$O); 208.9 (s, Re-$\underline{C}$O); 213.7 (s, Fe-$\underline{C}$O); 214.2 (s, Fe-$\underline{C}$O); 216.5 (s, Fe-$\underline{C}$O); 271.1 (d, J_{CP} = 4.0, μ-$\underline{C}^1$).

$^{31}P\{^1H\}$ NMR (CD_2Cl_2, -70ºC) δ, ppm [J, Hz]:

Isomer 2a_π-Pt: 112.2 (s, J_{PtP} = 5660), 96%.

Isomer 2a_π-Fe: 111.3 (s, J_{PtP} = 5566), 4%.

^{195}Pt NMR (CD_2Cl_2, -70ºC) Ξ, ppm [J, Hz]:

Isomer 2a_π-Pt:-4960 (dd, J_{PtP} = 5662, $^3J_{PtH}$ = 57.2).

Analytical data for $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OPr^i)_3]_2$ (2b)

Anal. Found: C, 37.19%; H, 4.37%. Calc. for $C_{36}H_{53}O_{11}P_2PtReFe$ (1160.88): C, 37.25; H, 4.60%.

IR (ν(CO), cm^{-1}): 2014 s, 1994 s, 1944 s, 1888 m (C_6H_{12},); 2006s, 1946 br.s., 1869 m (CH_2Cl_2); 2006 s, 1946 br.s., 1869 m (CH_2Cl_2); 2003 s, 1948 s, 1932 s, 1869 s (tabl. KBr).

^1H NMR (CD_2Cl_2, 25ºC) δ, ppm [J, Hz]:

1.23 (d, 9H, J_{HH} = 6.0, -C$\underline{H}_3$); 1.36 (d, 9H, J_{HH} = 6.0, -CH_3); 1.38 (d, 9H, J_{HH} = 6.0, -C$\underline{H}_3$), 1.39 (d, 9H, J_{HH} = 6.0, -C$\underline{H}$); 4.85 (m, 3H, -C$\underline{H}$); 4.94 (m, 3H, -C$\underline{H}$); 5.84 (s, 5H, $C_5\underline{H}_5$); 5.99 (d, 1H, $^4J_{PH}$ = 16.0, $^3J_{PtH}$ = 60.4, $=C^2\underline{H}$Ph); 7.04 (t, 1H, J_{HH} = 7.5, H_{para} of $=C^2HC_6\underline{H}_5$); 7.14 (t, 2H, J_{HH} = 7.5, H_{meta} of $=C^2HC_6\underline{H}_5$); 7.65 (d, 2H, J_{HH} = 7.8, H_{ortho} of $=C^2HC_6\underline{H}_5$).

$^{13}C\{^1H\}$ NMR (CD_2Cl_2, 25ºC) δ, ppm [J, Hz]:

24.0 (d, $^3J_{PC}$ = 4.0, -$\underline{C}H_3$); 24.1 (d, $^3J_{PC}$ = 4.0, -$\underline{C}H_3$); 69.3 (d, $^2J_{PC}$ = 5.0, -$\underline{C}$H); 71.1 (d, $^2J_{PC}$ = 7.0, -$\underline{C}$H); 88.9 (s, $\underline{C}_5H_5$); 95.9 (dd, $^3J_{PC}$ = 2.8, $^3J_{PC}$ = 7.3, $^2J_{PtC}$ = 22.0, $=\underline{C}^2$HPh); 124.5 (s, C_{para} of $=C^2H\underline{C}_6H_5$); 127.4 (s, C_{meta} of $=C^2H\underline{C}_6H_5$); 128.6 (s, C_{ortho} of $=C^2H\underline{C}_6H_5$); 148.6 (d, $^4J_{PC}$ = 6.0, C_{ipso} of $=C^2H\underline{C}_6H_5$); 204.4 (s, Re-$\underline{C}$O); 207.3 (s, Re-$\underline{C}$O); 216.8 (s, 3(Fe-$\underline{C}$O)); 262.7 (s, μ-$\underline{C}^1$).

$^{31}P\{^1H\}$ NMR (CD_2Cl_2, 25ºC) δ, ppm [J, Hz]:

114.3 (dd, P^1, $^2J_{PP}$ = 47.4, J_{PtP} = 6264); 126.5 (d, P^2, $^2J_{PP}$ = 47.2, J_{PtP} = 4076).

Analytical data for CpReFePt(μ₃-C=CHPh)(CO)₆[P(OEt)₃] (3a)

Anal. Found: C, 32.22; H, 2.88%. Calc. for $C_{25}H_{26}O_9P_1PtReFe$ (938.57): C, 31.99; H, 2.79%.

IR (ν(CO), cm^{-1}): 2066 sh, 2055 s, 2017 v.s., 1975 sh, 1962 v.s., 1952 s, 1941 s, 1925 s, 1900 w, 1975 m (C_6H_{12}); 2047 s, 2009 v.s., 1952 br.v.s., 1880 m, 1861 m (CH_2Cl_2); 2051 s, 2010 s, 1948 v.s, 1902 s, 1870 s, 1846 s (tabl. KBr).

^{1}H NMR (CD_2Cl_2, 25ºC) δ, ppm [*J*, Hz]:

Isomer 3a_π-Pt: 1.37 (t, 9H J_{HH} = 7.1, -CH_3); 4.11 (m, -C$\underline{H}_2$-, *overlap with –CH_2- siganal of isomer X*); 5.10 (s, $C_5\underline{H}_5$); 6.20 (s, 1H, $^2J_{PtH}$ = 57.6, =$C^2\underline{H}$); 7.28 (t, 1H, J_{HH} = 7.4 H_{para} of =$C^2HC_6\underline{H}_5$, *overlap with H_{meta} siganal of isomer π-Fe*); 7.38 (t, 2H, J_{HH} = 7.7, H_{meta} of =$C^2HC_6\underline{H}_5$); 7.45 (d, 2H, J_{HH} = 7.4, H_{ortho} of =$C^2HC_6\underline{H}_5$).

Isomer 3a_π-Fe: 1.18(t, 9H, J_{HH} = 6.9, -C$\underline{H}_3$); 3.90 (dq, 6H, J_{HH} = 7.3, J_{HP} = 7.4, -C$\underline{H}_2$-); 5.84 (s, $C_5\underline{H}_5$); 6.46 (d, $^4J_{PH}$ = 1.5, $^3J_{PtH}$ =67.1, =$C^2\underline{H}$Ph); 7.11 (t, 1H, J_{HH} = 7.51 H_{para} of =$C^2HC_6\underline{H}_5$); 7.21 (t, J_{HH} = 7.5, H_{meta} of =$C^2HC_6\underline{H}_5$, *overlap with H_{para} siganal of isomer π-Pt*); 7.53 (d, 2H, J_{HH} = 7.8, H_{ortho} of =$C^2HC_6\underline{H}_5$).

Isomer 3a*:1.29 (t, $^3J_{HH}$ = 7.2, -C$\underline{H}_3$); 3.96 (m, -C$\underline{H}_2$-, *overlap with –CH_2- siganal of isomer π-Pt*); 5.44 (s, C_5H_5); 7.59 (d, 2H, J_{HH} = 7.8, H_{ortho} =$C^2HC_6\underline{H}_5$), 7.66 (d, $^2J_{PtH}$ = 69.0, J_{PH} = 13.8, =$C^2\underline{H}$Ph, *overlap with H_{ortho} signal of isomer X*).

$^{13}C\{^1H\}$ NMR (CD_2Cl_2, 25ºC) δ, ppm [*J*, Hz]:

Isomer 3a_π-Pt: 15.6 (d,$^3J_{PC}$ = 7.1, -$\underline{C}H_3$); 61.9 (s, br, -$\underline{C}H_2$-); 89.1 (s, C_5H_5); 92.4 (s, =$\underline{C}^2H$); 124.9 – 129.5 (C_{para}, C_{meta}, C_{ortho} of =$C^2H\underline{C}_6H_5$); 145.7 (s, br, C_{ipso} of =$C^2H\underline{C}_6H_5$); 205.8 (s, Re-$\underline{C}$O); 210.6 (s, Re-$\underline{C}$O); 214.6 (s, 3(Fe-$\underline{C}$O)); 269.3 (s, μ-$\underline{C}^1$).

Isomer 3a_π-Fe: 15.8 (d,$^3J_{PC}$ = 6.9, -$\underline{C}H_3$); 62.5 (s, br, -$\underline{C}H_2$-); 88.4 (s, $\underline{C}_5H_5$); 98.3 (s, $^2J_{PtC}$= 25, =$\underline{C}^2H$); 124.9 – 129.5 (C_{para}, C_{meta}, C_{ortho} of =$C^2H\underline{C}_6H_5$); 147.6 (s, C_{ipso} of =$C^2H\underline{C}_6H_5$); 187.3 (d, $^2J_{PtC}$ = 10.9, Pt-$\underline{C}$O); 202.1 (s, Re-$\underline{C}$O); 204.4 (s, Re-$\underline{C}$O); 213.7 (s, 3(Fe-$\underline{C}$O)); 261.7 (s, μ-$\underline{C}^1$).

Isomer 3a*: 15.8 (d, $^3J_{PC}$ = 5.2, -$\underline{C}H_3$); 62.2 (s, br, -$\underline{C}H_2$-); 88.4 (s, $\underline{C}_5H_5$);

$^{31}P\{^1H\}$ NMR (CD_2Cl_2, 25ºC) δ, ppm [*J*, Hz]:

Isomer 3a_π-Pt: 113.5 (d, J_{PtP} = 5759) 51%.

Isomer 3a_π-Fe: 115.9 (d, J_{PtP} = 5679) 42%.

Isomer 3a*: 114.5 (d, J_{PtP} = 5648) 7%.

Analytical data for CpReFePt(μ₃-C=CHPh)(CO)₆[P(OEt)₃] (3b)

Anal. Found: C, 33.89%; H, 4.01%. Calc. for $C_{30}H_{41}FeO_{11}P_2PtRe$ (1076.73): C, 33.47; H, 3.84%.

IR (ν(CO), cm^{-1}): 2007 s, 1938 s, 1911 s, 1844 m (CH_2Cl_2); 2001 v.s, 1930 s, 1913 s, 1899 s, 1849 s (tabl. KBr).

^{1}H NMR (CD_2Cl_2, 25ºC) δ, ppm [*J*, Hz]:

Isomer 3b_π-Pt:1.15 (t, 9H, J_{HH} = 6.8, -C$\underline{H}_3$); 1.37 (t, 9H, J_{HH} = 7.2, -C$\underline{H}_3$); 3.87 (m, 6H, -C$\underline{H}_2$-); 4.03 (m, -C$\underline{H}_2$-, *overlap with -C$\underline{H}_2$- signal of isomer π-Fe*); 5.03 (s, $C_5\underline{H}_5$); 5.99 (dd, 1H, $^3J_{PH}$ = 14.7, $^3J_{PH}$ = 2.92, $^2J_{PtH}$ = 48.1, =$C^2\underline{H}$Ph); 7.15 (t, 1H, J_{HH} = 7.3, H_{para} of =$C^2HC_6\underline{H}_5$); 7.35 (t, 2H, J_{HH} = 7.9, H_{meta} of =$C^2HC_6\underline{H}_5$, *overlap with =$C^2\underline{H}$Ph signal of isomer 3b**); 7.50 (d, 2H, J_{HH} = 7.9, H_{ortho} of =$C^2HC_6\underline{H}_5$).

Isomer 3b_π-Fe: 1.34 (m, 18H, -CH_3); 4.08 (m, -C$\underline{H}_2$-, *overlap with -C$\underline{H}_2$- signal of isomer π-Pt*); 4.15 (m, 6H, -C$\underline{H}_2$-); 5.83 (s, $C_5\underline{H}_5$); 6.17 (d, $^4J_{PH}$ = 16.9, $^3J_{PtH}$ = 62.8, =$C^2\underline{H}$Ph); 7.04 (t, 1H, J_{HH} = 7.1, H_{para} of =$C^2HC_6\underline{H}_5$); 7.24 (t, J_{HH} = 7.4, H_{meta} of =$C^2HC_6\underline{H}_5$, *overlap with H_{meta} signal of isomer 3b**); 7.64 (d, J_{HH} = 7.2, H_{ortho} of =$C^2HC_6\underline{H}_5$, *overlap with H_{ortho} signal of isomer 3b**).

Isomer 3b*: 5.41 (s, $C_5\underline{H}_5$); 7.11 (m, 1H, H_{para} of $=C^2HC_6\underline{H}_5$); 7.25 (m, H_{meta} of $=C^2HC_6\underline{H}_5$, *overlap with H_{meta} signal of isomer π-Fe*); 7.38 (d, $^3J_{PH}$ = 9.8, $^3J_{PtH}$ = 46.0, $=C^2\underline{H}Ph$, *overlap with H_{meta} signal of isomer π-Pt*); 7.65 (m, H_{ortho} of $=C^2HC_6\underline{H}_5$, *overlap with H_{ortho} signal of isomer π-Fe*).

$^{13}C\{^1H\}$ NMR (CD_2Cl_2, 25ºC) δ, ppm [*J*, Hz]:

Isomer 3b_π-Pt: 15.6 (d, $^3J_{PC}$ = 7.9, $-\underline{C}H_3$); 15.8 (d, $^3J_{PC}$ = 8.7, $-\underline{C}H_3$); 61.1 (s, $^3J_{PtC}$ = 15.7, $-\underline{C}H_2-$); 61.6 (s,$^3J_{PtC}$ = 12.2, $-\underline{C}H_2-$); 89.1 (s, $\underline{C}_5H_5$); 91.8 (dd, $^2J_{PC}$ = 2.1, $^2J_{PC}$ = 47.2, J_{PtC} = 113.1, $=\underline{C}^2HPh$); 125.4 (s, C_{para} of $=C^2H\underline{C}_6H_5$); 126.9 (s, C_{meta} of $=C^2H\underline{C}_6H_5$); 129.6 (dd, $^4J_{PC}$ = 1.6, $^4J_{PC}$ = 5.4, $^3J_{PtC}$ = 18.6, C_{ortho} of $=C^2H\underline{C}_6H_5$); 147.7 (dd, $^3J_{PC}$ = 4.5, $^3J_{PC}$ = 6.2 ,$^2J_{PtC}$ = 21.0, C_{ipso} of $=C^2H\underline{C}_6H_5$); 204.4 (s, Re-$\underline{C}O$); 206.6 (s, Re-$\underline{C}O$); 208.5 (s, Fe-$\underline{C}O$); 210.7 (s, Fe-$\underline{C}O$); 215.9 (s, Fe-$\underline{C}O$); 266.4 (s, J_{PtC} = 71.0, μ-$\underline{C}^1$).

Isomer 3b_π-Fe: 15.9 (br, $-\underline{C}H_3$); 60.9 (d, $^2J_{PC}$ = 3.1, $-\underline{C}H_2-$); 61.8 (d, $^2J_{PC}$ = 4.9, $-\underline{C}H_2-$); 88.5 (s, $\underline{C}_5H_5$); 95.4 (s, br, $=\underline{C}^2HPh$); 124.4 (s, C_{para} of $=C^2H\underline{C}_6H_5$); 127.4 (s, C_{meta} of $=C^2H\underline{C}_6H_5$); 128.3 (s, C_{ortho} of $=C^2H\underline{C}_6H_5$); 149.0 (s, br, C_{ipso} of $=C^2H\underline{C}_6H_5$); 206.1 (s, Re-$\underline{C}O$); 207.1 (s, Re-$\underline{C}O$); 215.6 (s, br, Fe-$\underline{C}O$); 262.4 (s, μ-$\underline{C}^1$).

Isomer 3b*: 15.9 (br, $-\underline{C}H_3$, *overlap with $-\underline{C}H_3$ signal of isomer π-Fe*); 61.4 (br, $-\underline{C}H_2-$); 62.2 (br, $-\underline{C}H_2-$); 88.4 (s, $\underline{C}_5H_5$); 95.8 (d, br, $^2J_{PC}$ = 41.0, $=\underline{C}^2HPh$); 125.4 (s, C_{para} of $=C^2H\underline{C}_6H_5$, *overlap with C_{para} signal of isomer π-Pt*); 127.6 (br, s, C_{meta} of $=C^2H\underline{C}_6H_5$); 128.2 (br, s, C_{ortho} of $=C^2H\underline{C}_6H_5$, *overlap with C_{ortho} signal of isomer π-Fe*); 142.6 (s, br, C_{ipso} of $=C^2H\underline{C}_6H_5$); 216.5 (s, br, Fe-$\underline{C}O$); 253.7 (s, br, μ-$\underline{C}^1$).

$^{31}P\{^1H\}$ NMR (CD_2Cl_2, 25ºC) δ, ppm [*J*, Hz]:

Isomer 3b_π-Pt:118.8 (dd, P^1,$^2J_{PP}$ = 72.7, J_{PtP}= 5437); 123.3 (dd, P^2,$^2J_{PP}$ = 72.9, J_{PtP}= 5700), 61%.

Isomer 3b_π-Fe:114.4 (dd, P1, $^2J_{PP}$ = 60.9, J_{PtP}= 6109); 127.4 (dd, P2, $^2J_{PP}$ = 61.0, J_{PtP}= 4000), 23%.

Isomer 3b*:114.6 (d, P^1,$^2J_{PP}$ = 76.3); 118.6 (d, $^2J_{PP}$ = 76.7), 16%.

Analytical data for $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OPr^i)_3](PPh_3)$ (3e)

IR (ν(CO), cm^{-1}): 2001 s, 1957 m, 1938 v.s, 1915 m, 1887 w, 1859 w (C_6H_{12}); 2002 s, 1947 s, 1934 v.s, 1870 m, 1841 w (tabl. KBr).

$^{31}P\{^1H\}$ NMR (CD_2Cl_2, 25ºC) δ, ppm [*J*, Hz]:

120.4 (dd, P^1,$^2J_{PP}$ = 47, J_{PtP}= 5829); 26.1 (dd, P^2,$^2J_{PP}$ = 47, J_{PtP}= 3432), 61%.

X-ray diffraction studies of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OEt)_3]$ (3a) and $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OEt)_3]_6$ (3b).

The crystal data and refinement parameters of experiments for complex **3a, b** are provided in Table 1S. Dark red crystals of (1,1,2,2,2,3-hexacarbonyl)-(1-η^5-cyclopentadienyl)-μ_3-[1,2-η^1,η^1,3-η^2-(phenyl)ethenylidene]-(tri-ethyl phosphite-3κP)–rhenium–iron–platinum(Fe–Re, Fe–Pt) **3a** and (1,1,2,2,2,-pentacarbonyl)-(1-η^5-cyclopentadienyl)-μ_3-[1,2-η^1,η^1,3-η^2-(phenyl)-ethenylidene]-(bis-triethylphosphite-3κP)–rhenium–iron–platinum(Fe–Re, Fe–Pt) **3b** suitable for X-ray diffraction analysis were grown from a hexane and hexane:diethyl ether mixture under argon atmosphere at -18°C.

The experimental data were collected with a Smart Photon II diffractometer (Bruker AXS, CCD area detector). The experimental completeness is 99.8%. Absorption corrections have been applied using multiscan procedure [4]. The structure was solved by direct methods and refined by full-matrix least squares on F^2, using SHELXTL program [5,6]. Hydrogen atoms have been placed in calculated positions and taken into account in the final stages of refinement in the "riding model" approximation. All hexa- and pentagonal cyclic groups were refined in idealized form. The OEt groups in molecules have significant vibrational mobility, and in **3a** one of them is

disordered over two positions. The interatomic distances in the groups were adjusted to idealized values during refinement. The supplementary crystallographic data for the compound **3a** and **3b** have been deposited with the Cambridge Crystallographic Data Centre, CCDC No. 2093592 and 2093594, respectively.

Table 1S. Crystal data and X-ray experimental details for complex $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OEt)_3]L$ [L = CO (**3a**), $P(OEt)_3$ (**3b**)].

Complex	**3a**	**3b**
Empiricalformula	$C_{25}H_{26}O_9P_1PtReFe$	$C_{30}H_{41}FeO_{11}P_2PtRe$
Formulaweight	938.57	1076.73
Temperature/K	296(2)	296(2)
Crystalsystem	triclinic	monoclinic
Spacegroup	*P*-1	$P2_1/c$
a/Å	9.4887(3)	11.7530(3)
b/Å	9.8037(3)	20.1543(5)
c/Å	16.3209(5)	16.4212(4)
α/°	84.4370(10)	
β/°	83.0240(10)	106.6490(10)
γ/°	74.7760(10)	
Volume/Å^3	1450.76(8)	3726.68(16)
Z	2	4
d_{calc}/(g·cm^{-3})	2.149	1.919
μ/mm^{-1}	9.567	7.507
F(000)	884	2072
Crystal size/mm^3	0.38 × 0.26 × 0.06	0.75 × 0.4 × 0.04
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.520 to 56.678	3.284 to 60.000
Indexranges	-12 ≤ h ≤ 12, -13 ≤ k ≤ 13,-21 ≤ l ≤ 21	-16 ≤ h ≤ 16, -28 ≤ k ≤ 28,-23 ≤ l ≤ 23
Reflections collected	18439	52871
Uniq. refl./R(int)/R(sigma)	7237/0.0704/0.0746	10885/0.0646/0.0483
Data/restraints/parameters	7237/3/348	10885/19/418
Goodness-of-fit on F^2	0.954	1.030
Final R_1 [I>=2σ (I)]	0.0441	0.0466
Final R_1, wR_2 [all data]	0.0625, 0.1130	0.0738, 0.1137
$\Delta\rho_{min}/\Delta\rho_{max}$ (e/Å^3)	-1.14/1.34	-1.04/1.28

Cyclic voltammograms of the clusters

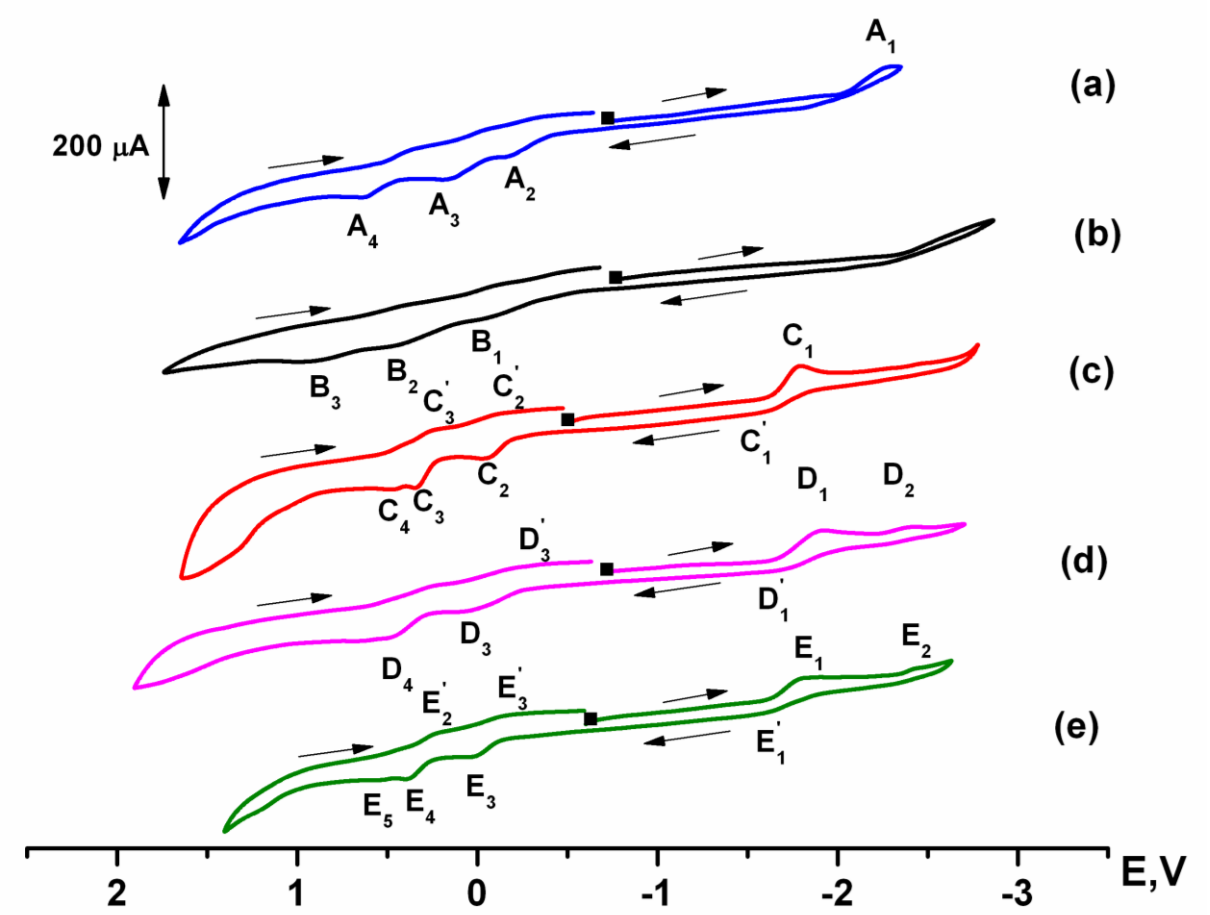

Figure 1S. – Cyclic voltammograms of complexes at GC-electrode: (a) - $CpReFePt(\mu\text{-}C{=}CHPh)(CO)_5[P(OPr^i)_3]_2$ (**2b**), (b) - $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OEt)_3]_2$ (**3b**); (c) - $CpReFePt(\mu\text{-}C{=}CHPh)(CO)_6[P(OPr^i)_3]$ (**2a**), (d) - $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OEt)_3]$ (**3a**); (e) - $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[PPh_3]$ (**1a**) (MeCN, 0.1 M Et_4NBF_4, 2 mM, Ag/0.1 M $AgNO_3$ in MeCN, scan rate 25 mV s^{-1})

Table 2S. IR spectroscopic data for the clusters CpReFePt(μ3-C=CHPh)(CO)5LL'.

		(**2a**)	(**2b**)	(**3a**)	(**3b**)
IR, ν(CO), cm^{-1}	KBr	2046 v.s., 2007 s, 1949 v.s., 1927 s, 1901 m, 1855 m	2003 s, 1948 s, 1932 v.s., 1869 m	2051 s, 2010 s, 1948 v.s., 1902 s, 1870 s, 1846 s	2001 v.s., 1930 s, 1913 s, 1899 s, 1849 s
	C_6H_{12}	2049 s, 2013 s, 1970 sh, 1960 s, 1949 m, 1938 s, 1923 m, 1898 m, 1873 m	2014 s 1994 s 1944 s 1888 m	2066 sh, 2055s, 2017 v.s., 1975 sh, 1962 v.s., 1952 s, 1941 s, 1925 s, 1900 w, 1875 m	2007 s, 1973 m, 1938 s, 1911 s, 1891 m, 1844 w

Computational details

A geometry optimizations of the **2a** cluster isomers were carried out by DF method with the hybrid exchange-correlation (XC) functionals TPSSh [7], B3LYP [8,9] and M06 [10] implemented in the Gaussian 09 program package [11], in spin-restricted fashion. To describe all elements the electron basis sets of the triple-ζ quality with polarization functions (def2-TZVP) [12] and two sets of polarization functions (def2-TZVPP) [12] were used: all-electron for H, C, O, P and Fe and the pseudopotential for Pt and Re [13]. The **UltraFine** integration grid was used for numerical integration and the **Tight** convergence option was used for geometry optimization. The vibrational analysis was performed to ensure that the final structure represent true minimum.

Computational results

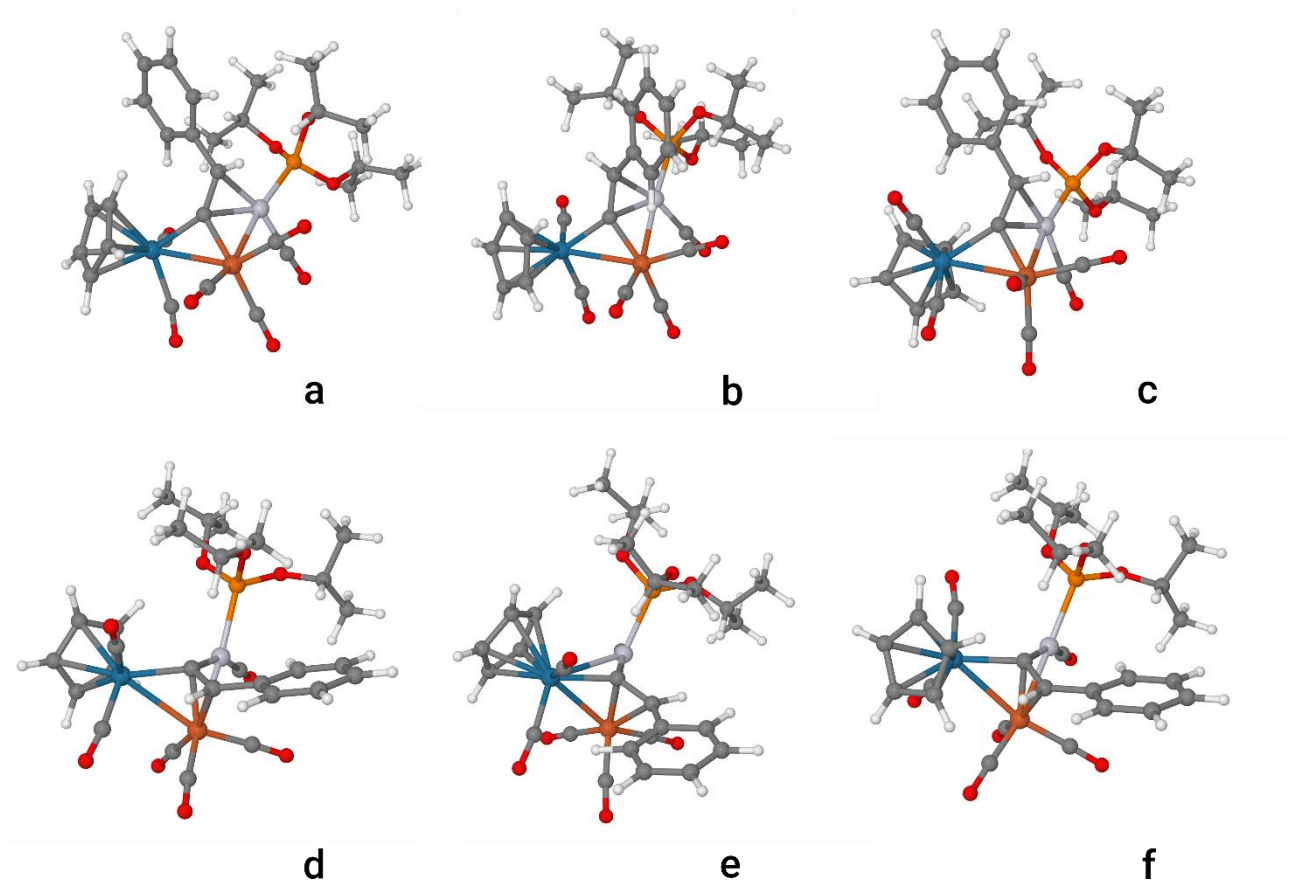

Figure 2S. The sketches of TPSSh/def2-TZVPP calculated structures of the **2a** cluster isomers: **2a_π-Pt** (a), **2a1_π-Pt** (b), **2a2_π-Pt** (c), **2a_π-Fe** (d), **2a1_π-Fe** (e), **2a2_π-Fe** (f)

Atomic coordinates (Å) of the **2a** cluster isomers calculated at TPSSh/def2-TZVPP DFT level

2a_π-Pt

Pt	0.79163	-0.71616	0.05543
Re	-2.75340	0.33750	-0.58607
Fe	-1.52949	-1.69515	0.88363
P	2.98981	-0.10523	-0.29389
O	-0.97876	0.72979	-3.05155
O	-3.59049	-2.34274	-1.85796
O	-3.96602	-1.97544	2.45886
O	-1.67865	-4.42097	-0.28254
O	0.12226	-2.27055	3.21586
O	1.16663	-3.30665	-1.47895
O	3.80488	0.62259	0.89163
O	3.78736	-1.44291	-0.64361
O	3.42918	0.80847	-1.53135
C	-1.14700	0.12600	0.72302
C	-0.10418	0.89281	1.31032
H	0.18140	0.57464	2.31424
C	-1.61359	0.53722	-2.09245
C	-3.16967	-1.41004	-1.30743
C	-3.01691	-1.85930	1.81458
C	-1.62490	-3.35089	0.12663
C	-0.50492	-2.04637	2.27373
C	0.97500	-2.34917	-0.88432
C	-3.49780	2.51361	-0.55263
H	-2.92062	3.31665	-0.98119
C	-3.45516	2.08930	0.80209
H	-2.81526	2.50019	1.56681
C	-4.38753	1.02726	0.97338
H	-4.60115	0.50581	1.89167
C	-4.99989	0.78710	-0.29182
H	-5.75323	0.04121	-0.49343
C	-4.46388	1.70741	-1.23913
H	-4.75488	1.80452	-2.27268
C	0.10325	2.35625	1.13371
C	0.42511	3.12487	2.26049
H	0.53519	2.63138	3.22101
C	0.59088	4.50388	2.17441
H	0.83533	5.07263	3.06437
C	0.43623	5.15040	0.95238
H	0.56084	6.22430	0.88021
C	0.12103	4.39959	-0.17854
H	0.00620	4.89061	-1.13874
C	-0.03977	3.02126	-0.09056
H	-0.27256	2.44923	-0.97885
C	3.48870	0.44146	2.30855
H	2.40081	0.37093	2.38526
C	4.12362	-0.83514	2.83433
H	3.88089	-0.95389	3.89271
H	5.21048	-0.79290	2.73274
H	3.75077	-1.71085	2.30192

C	5.19131	-1.47751	-1.08167
H	5.64149	-0.51408	-0.83308
C	5.86834	-2.59340	-0.30654
H	6.91421	-2.67148	-0.61253
H	5.37747	-3.54729	-0.50954
H	5.83583	-2.40589	0.76665
C	3.12940	2.24160	-1.62385
H	2.43135	2.49329	-0.82278
C	4.42816	3.00730	-1.43939
H	4.23497	4.08072	-1.50381
H	5.14245	2.73856	-2.22109
H	4.87038	2.79127	-0.46687
C	3.98799	1.68797	3.01600
H	3.74778	1.62976	4.07996
H	3.52123	2.58234	2.60303
H	5.07191	1.77556	2.91300
C	5.21547	-1.70224	-2.58380
H	4.72833	-2.64744	-2.83193
H	4.70346	-0.89434	-3.10467
H	6.25019	-1.74480	-2.93311
C	2.47914	2.47298	-2.97527
H	2.23094	3.53079	-3.08908
H	3.16500	2.19296	-3.77802
H	1.56509	1.88775	-3.07674

2a*1_π-Pt

Pt	-0.71528	-0.19490	-0.54732
Re	2.66300	-0.69899	0.72929
Fe	1.60994	0.47156	-1.60419
P	-2.82006	-0.65707	0.25656
O	0.63707	-2.67177	1.90615
O	3.18879	-2.85920	-1.40583
O	3.96220	2.15730	-1.94138
O	2.12944	-1.30583	-3.92358
O	-0.08436	2.28472	-3.13459
O	-1.09089	-1.92070	-3.01246
O	-3.89619	0.54030	0.19955
O	-3.41729	-1.85922	-0.60447
O	-3.09730	-1.22400	1.72913
C	1.15566	0.66678	0.18320
C	0.13059	1.25516	0.96135
H	0.02798	0.85632	1.97079
C	1.35841	-1.90656	1.40337
C	2.92489	-2.00035	-0.67170
C	3.05487	1.45931	-1.80007
C	1.92781	-0.65245	-3.00325
C	0.56485	1.57314	-2.50110
C	-0.89988	-1.26010	-2.09816
C	3.31145	0.23374	2.73035

H	2.61654	0.41477	3.53481
C	3.68454	1.16019	1.71636
H	3.28821	2.15640	1.59667
C	4.66231	0.55115	0.88278
H	5.15724	1.00803	0.04205
C	4.88492	-0.76927	1.37562
H	5.56659	-1.49174	0.95404
C	4.05943	-0.97242	2.51453
H	4.02747	-1.85859	3.12803
C	-0.33747	2.66996	0.89290
C	-1.27317	3.11956	1.83602
H	-1.67459	2.41869	2.56003
C	-1.68558	4.44573	1.87282
H	-2.40703	4.76372	2.61720
C	-1.16873	5.36442	0.96331
H	-1.48644	6.40000	0.98893
C	-0.22401	4.93916	0.03383
H	0.20480	5.64682	-0.66645
C	0.19204	3.61285	0.00397
H	0.95295	3.30456	-0.69912
C	-3.80225	1.63870	-0.77122
H	-2.74731	1.91975	-0.83391
C	-4.30094	1.18781	-2.13373
H	-4.21294	2.01372	-2.84305
H	-5.35055	0.88992	-2.07967
H	-3.71598	0.35033	-2.51576
C	-4.69103	-2.53476	-0.31273
H	-5.25054	-1.90507	0.38225
C	-5.43571	-2.65938	-1.62959
H	-6.38429	-3.17682	-1.46824
H	-4.84574	-3.23494	-2.34561
H	-5.64544	-1.67948	-2.05848
C	-2.78616	-0.50427	2.96235
H	-2.04697	0.26240	2.71723
C	-4.05633	0.14049	3.49283
H	-3.83719	0.68079	4.41716
H	-4.80291	-0.62559	3.71364
H	-4.47405	0.83842	2.76809
C	-4.61905	2.77984	-0.19563
H	-4.55976	3.64397	-0.86046
H	-4.24016	3.07505	0.78224
H	-5.66721	2.48747	-0.09909
C	-4.37990	-3.87864	0.32277
H	-3.79006	-4.49216	-0.36128
H	-3.82161	-3.74928	1.24894
H	-5.31118	-4.40593	0.54451
C	-2.18400	-1.51478	3.92186
H	-1.91408	-1.01922	4.85756
H	-2.91070	-2.29852	4.14742

H	-1.29329	-1.97500	3.49579

2a*2_π-Pt

Pt	0.68849	-0.72330	0.06393
Re	-2.70168	0.45638	-0.60230
Fe	-1.63938	-1.53076	1.01178
P	2.89276	-0.21618	-0.37425
O	-5.21925	-0.96594	0.43493
O	-3.64085	2.82084	1.11653
O	-3.52134	-1.31995	3.22976
O	-2.70952	-3.84648	-0.50544
O	0.23471	-2.77751	2.86788
O	0.72599	-3.38787	-1.38342
O	3.84926	0.00624	0.90455
O	3.50385	-1.43860	-1.20210
O	3.37248	0.99631	-1.30564
C	-1.15671	0.25533	0.84066
C	-0.05160	0.93947	1.39860
H	0.28258	0.54052	2.35755
C	-4.22512	-0.45551	0.12590
C	-3.26836	1.91344	0.49902
C	-2.81666	-1.41610	2.32787
C	-2.27999	-2.96286	0.09160
C	-0.48304	-2.27970	2.11139
C	0.65823	-2.39041	-0.82353
C	-3.31554	-0.28533	-2.70222
H	-4.08603	-1.02968	-2.83080
C	-1.92142	-0.54746	-2.59226
H	-1.45774	-1.51897	-2.63083
C	-1.25378	0.70260	-2.44237
H	-0.18830	0.83607	-2.33688
C	-2.23355	1.73258	-2.46350
H	-2.04574	2.79319	-2.40421
C	-3.51859	1.12522	-2.62960
H	-4.46023	1.64128	-2.72480
C	0.28545	2.38165	1.28439
C	0.99853	2.97848	2.33398
H	1.29030	2.37063	3.18423
C	1.31831	4.33111	2.31526
H	1.86513	4.76594	3.14420
C	0.92350	5.12757	1.24401
H	1.16124	6.18459	1.22940
C	0.20730	4.55146	0.19772
H	-0.11524	5.16371	-0.63715
C	-0.10245	3.19687	0.21590
H	-0.66381	2.75934	-0.59751
C	3.54706	-0.55959	2.22209
H	2.45760	-0.57414	2.32283
C	4.08678	-1.97613	2.31937

H	3.85766	-2.38710	3.30489
H	5.17081	-1.98351	2.18414
H	3.63051	-2.62386	1.56999
C	4.87313	-1.46793	-1.73682
H	5.43820	-0.66868	-1.25266
C	5.45984	-2.82127	-1.37782
H	6.47461	-2.89998	-1.77482
H	4.85695	-3.62255	-1.80982
H	5.50041	-2.95926	-0.29741
C	3.31999	2.41361	-0.92840
H	2.61065	2.52031	-0.10564
C	4.70685	2.85448	-0.49167
H	4.68245	3.91024	-0.21190
H	5.42060	2.73093	-1.30964
H	5.04768	2.27505	0.36534
C	4.15921	0.38167	3.24299
H	3.92852	0.03207	4.25156
H	3.76625	1.39199	3.12641
H	5.24521	0.41365	3.13003
C	4.80237	-1.23148	-3.23563
H	4.20446	-2.01082	-3.71284
H	4.35712	-0.26143	-3.45329
H	5.80818	-1.25897	-3.66210
C	2.82243	3.16408	-2.15013
H	2.76235	4.23119	-1.92882
H	3.50751	3.01923	-2.98854
H	1.83109	2.81872	-2.44461

2a_π-Fe

Pt	-0.61430	0.03389	-0.92882
Re	2.19551	-1.07777	0.54048
Fe	1.72028	1.18206	-1.06143
P	-2.51313	-0.72409	0.09399
O	-2.60053	-2.31686	-0.02380
O	-3.91182	-0.31413	-0.58146
O	-2.85275	-0.34765	1.61864
C	0.74682	0.50050	0.48779
C	0.17811	2.98468	1.10224
O	0.23403	3.10917	-2.68187
C	1.05386	1.80121	0.93982
H	1.94074	1.88736	1.56550
O	4.96505	0.22769	0.62980
C	0.78475	2.33995	-2.02715
O	2.66624	-0.35702	-3.36587
O	2.15670	-0.43180	3.54020
C	2.16705	-0.63952	2.39904
C	0.61141	3.98830	1.98260
H	1.56717	3.87000	2.48250
C	-1.86793	-0.07065	2.66923

H	-0.96282	0.28467	2.17297
C	-1.05692	3.16920	0.46782
H	-1.40148	2.41927	-0.23803
O	4.04416	2.95954	-0.77611
C	-1.82664	4.29989	0.70920
H	-2.77359	4.42343	0.19497
C	3.88127	-0.18565	0.57492
C	2.28160	0.22696	-2.44944
C	2.99829	-2.78528	-0.80224
H	3.85313	-2.64361	-1.44455
C	3.17176	2.22034	-0.86474
C	0.81810	-2.93120	-0.06268
H	-0.25960	-2.91076	-0.03935
C	1.63356	-2.61592	-1.18218
H	1.28320	-2.32863	-2.15897
C	-1.38363	5.28321	1.59128
H	-1.98316	6.16747	1.77252
C	-0.15631	5.12085	2.22638
H	0.20686	5.87837	2.91140
C	-4.45421	1.04451	-0.47827
H	-3.71434	1.66457	0.03398
C	-3.80313	-3.09627	0.32144
H	-4.46531	-2.44397	0.89391
C	-2.45593	1.02499	3.53863
H	-3.38780	0.69119	4.00124
H	-1.74865	1.27977	4.33051
H	-2.64960	1.92405	2.95361
C	-5.72530	0.97543	0.35027
H	-5.51410	0.58942	1.34750
H	-6.16003	1.97304	0.44764
H	-6.45867	0.32645	-0.13371
C	-1.57887	-1.34888	3.43684
H	-1.16064	-2.11369	2.78087
H	-0.85157	-1.14465	4.22504
H	-2.49076	-1.73715	3.89672
C	3.02944	-3.22479	0.55521
H	3.90867	-3.47860	1.12520
C	1.67974	-3.28372	1.01353
H	1.36567	-3.58278	2.00173
C	-4.68245	1.55984	-1.88798
H	-5.37759	0.90921	-2.42269
H	-5.11055	2.56415	-1.84942
H	-3.74789	1.60650	-2.44703
C	-3.34836	-4.26509	1.17609
H	-2.87218	-3.92061	2.09424
H	-4.20993	-4.88049	1.44527
H	-2.64126	-4.88875	0.62486
C	-4.47343	-3.52772	-0.97093
H	-3.79648	-4.14998	-1.56014

H	-5.36921	-4.11159	-0.74491
H	-4.76219	-2.66104	-1.56418
C	-1.28273	-0.26004	-2.69934
O	-1.66025	-0.40103	-3.77258

2a*1_π-Fe

Pt	-0.96969	-0.10139	-0.93614
Re	1.61731	-1.41367	0.61367
Fe	1.47955	0.26736	-1.66140
P	-2.75292	0.33627	0.41892
O	-3.55581	-0.99734	0.78845
O	-3.92039	1.20230	-0.26347
O	-2.59240	1.16935	1.78858
C	0.69711	0.43175	0.11828
C	2.25765	2.53864	0.55653
O	0.16497	2.02944	-3.59089
C	1.15134	1.75838	-0.05453
H	0.39155	2.44907	-0.41531
O	4.56205	-1.30746	-0.21298
C	0.65155	1.32218	-2.82287
O	1.46955	-2.12054	-3.35770
O	2.47903	-0.07391	3.23277
C	2.17104	-0.51723	2.20727
C	2.00572	3.90582	0.75953
H	1.04825	4.31326	0.45024
C	-1.43621	1.09230	2.68362
H	-0.59143	0.73483	2.09132
C	3.51451	2.05412	0.93786
H	3.76879	1.02101	0.76098
O	4.18755	1.20135	-2.32971
C	4.45972	2.88927	1.51989
H	5.42437	2.48267	1.80053
C	3.43336	-1.26060	0.05905
C	1.47010	-1.19023	-2.67723
C	1.59514	-3.64136	-0.02828
H	2.31730	-4.02703	-0.73067
C	3.15664	0.80618	-2.02141
C	-0.35214	-2.77881	0.85267
H	-1.35646	-2.39599	0.93798
C	0.29264	-3.16029	-0.35415
H	-0.13548	-3.12422	-1.34175
C	4.18302	4.23692	1.73171
H	4.92558	4.88484	2.18228
C	2.94761	4.74425	1.34214
H	2.71812	5.79404	1.48536
C	-3.64947	2.54806	-0.78114
H	-2.56262	2.67893	-0.81005
C	-4.89822	-1.00774	1.39740
H	-5.07492	-0.01770	1.82263

C	-1.16679	2.50247	3.17494
H	-2.02094	2.88249	3.74044
H	-0.28953	2.50416	3.82469
H	-0.97054	3.17362	2.33866
C	-4.27797	3.56226	0.15908
H	-3.87017	3.46498	1.16469
H	-4.08135	4.57399	-0.20365
H	-5.35980	3.41721	0.20252
C	-1.73445	0.12065	3.81325
H	-1.91462	-0.88530	3.43149
H	-0.88087	0.08045	4.49350
H	-2.61164	0.44342	4.37872
C	1.75263	-3.57679	1.38757
H	2.60889	-3.90965	1.95171
C	0.55545	-3.01121	1.92222
H	0.35761	-2.83519	2.96831
C	-4.20939	2.61062	-2.19047
H	-5.28559	2.42443	-2.17889
H	-4.03495	3.60229	-2.61364
H	-3.73262	1.87308	-2.83578
C	-4.88207	-2.05817	2.49271
H	-4.15283	-1.81427	3.26529
H	-5.86837	-2.11861	2.95858
H	-4.63914	-3.03795	2.07594
C	-5.91358	-1.30587	0.30795
H	-5.71203	-2.28070	-0.14116
H	-6.91857	-1.32514	0.73702
H	-5.88119	-0.54503	-0.47046
C	-2.03374	-0.74023	-2.40026
O	-2.65687	-1.07772	-3.30202

2a*2_π-Fe

Pt	-0.68846	0.02316	-0.91479
Re	2.25243	-1.06448	0.44899
Fe	1.63512	1.16769	-1.17135
P	-2.56525	-0.73110	0.13918
O	-2.79408	-2.26457	-0.20569
O	-3.96580	-0.11579	-0.35347
O	-2.76692	-0.55548	1.72760
C	0.74361	0.47236	0.42864
C	0.24476	2.93315	1.16410
O	0.52352	3.65092	-2.23123
C	1.10361	1.75713	0.88811
H	2.03636	1.84480	1.43972
O	0.25421	-3.38023	0.28454
C	0.94166	2.66979	-1.80553
O	1.60464	0.04372	-3.87975
O	3.21331	-2.07374	-2.29956
C	2.78801	-1.62690	-1.32002

C	0.74415	3.90153	2.04852
H	1.73616	3.76742	2.46877
C	-1.68995	-0.51704	2.71336
H	-0.77055	-0.26601	2.17766
C	-1.03257	3.14126	0.62938
H	-1.42402	2.41823	-0.07965
O	4.43665	2.04547	-1.06019
C	-1.77918	4.26068	0.97346
H	-2.76071	4.40524	0.53567
C	0.93924	-2.44088	0.28420
C	1.60494	0.43234	-2.79794
C	2.78686	-1.77556	2.57183
H	2.11385	-2.39613	3.14243
C	3.34109	1.69140	-1.08492
C	3.87537	0.07159	1.71879
H	4.19578	1.08594	1.54667
C	2.84479	-0.35780	2.60635
H	2.21191	0.28274	3.19923
C	-1.27152	5.20740	1.86082
H	-1.85534	6.08190	2.12260
C	-0.00069	5.02226	2.39589
H	0.41363	5.75239	3.08169
C	-4.39844	1.24037	-0.01655
H	-3.62264	1.70078	0.59947
C	-4.01236	-3.02157	0.12039
H	-4.58135	-2.44033	0.84938
C	-2.03836	0.58287	3.70079
H	-2.98585	0.36436	4.19895
H	-1.25928	0.65576	4.46323
H	-2.11554	1.54732	3.19853
C	-5.68310	1.12565	0.78604
H	-5.51477	0.55689	1.70091
H	-6.04390	2.12092	1.05636
H	-6.45613	0.62715	0.19697
C	-1.56482	-1.88478	3.36480
H	-1.29625	-2.64658	2.63264
H	-0.78726	-1.85620	4.13242
H	-2.50469	-2.16805	3.84429
C	3.78744	-2.24199	1.66409
H	4.01135	-3.27235	1.43953
C	4.44594	-1.09297	1.12879
H	5.25933	-1.10240	0.41995
C	-4.56564	2.01134	-1.31442
H	-5.30180	1.52116	-1.95486
H	-4.91304	3.02555	-1.10374
H	-3.62138	2.07555	-1.85614
C	-3.56489	-4.33945	0.72589
H	-3.00226	-4.18033	1.64560
H	-4.43889	-4.95381	0.95553

H	-2.93128	-4.88266	0.02270
C	-4.81430	-3.19665	-1.15758
H	-4.22780	-3.74306	-1.89895
H	-5.72333	-3.76604	-0.94775
H	-5.09567	-2.23000	-1.57377
C	-1.49084	-0.24422	-2.63223
O	-1.97058	-0.34802	-3.66718

NMR spectra

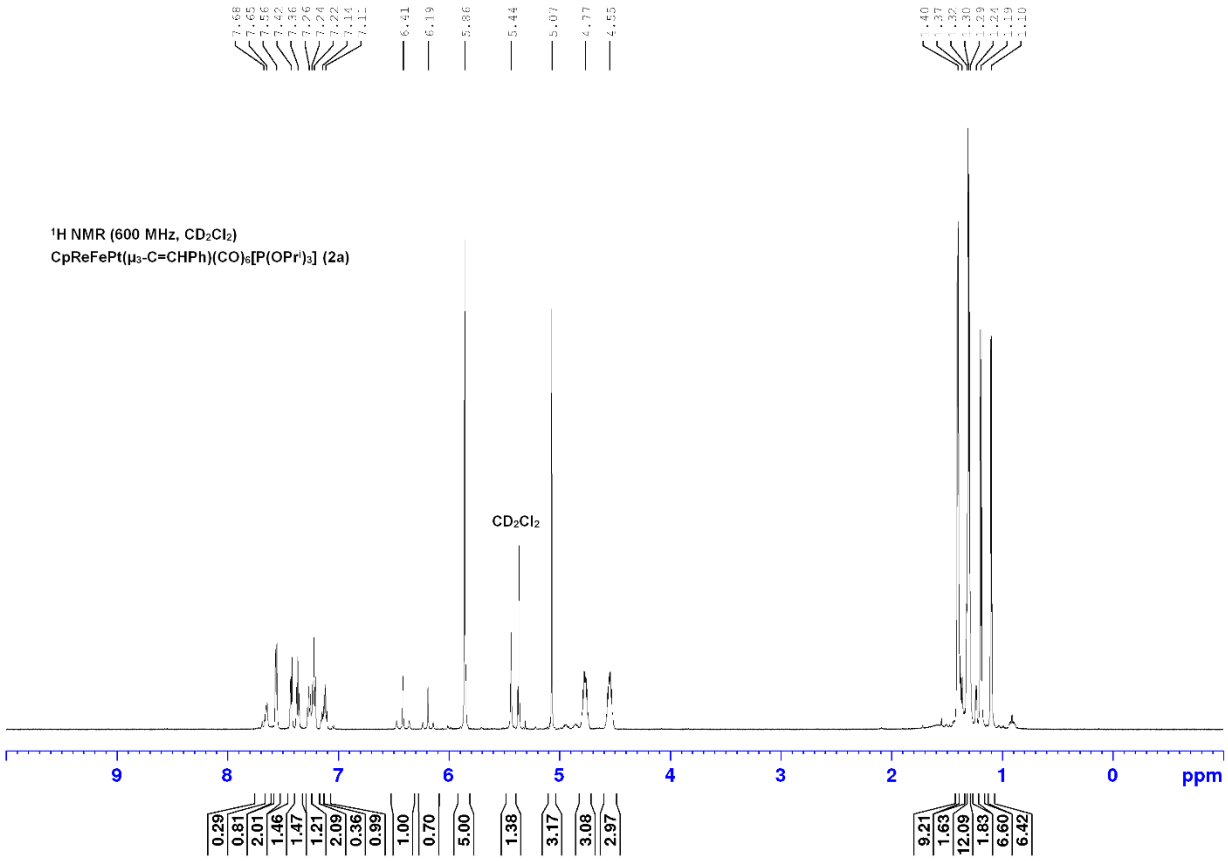

Figure 3S. ^{1}H NMR spectrum of CpReFePt(μ_3-C=CHPh)(CO)$_6$[P(OPr^i)$_3$] (**2a**) (600 MHz, CD_2Cl_2)

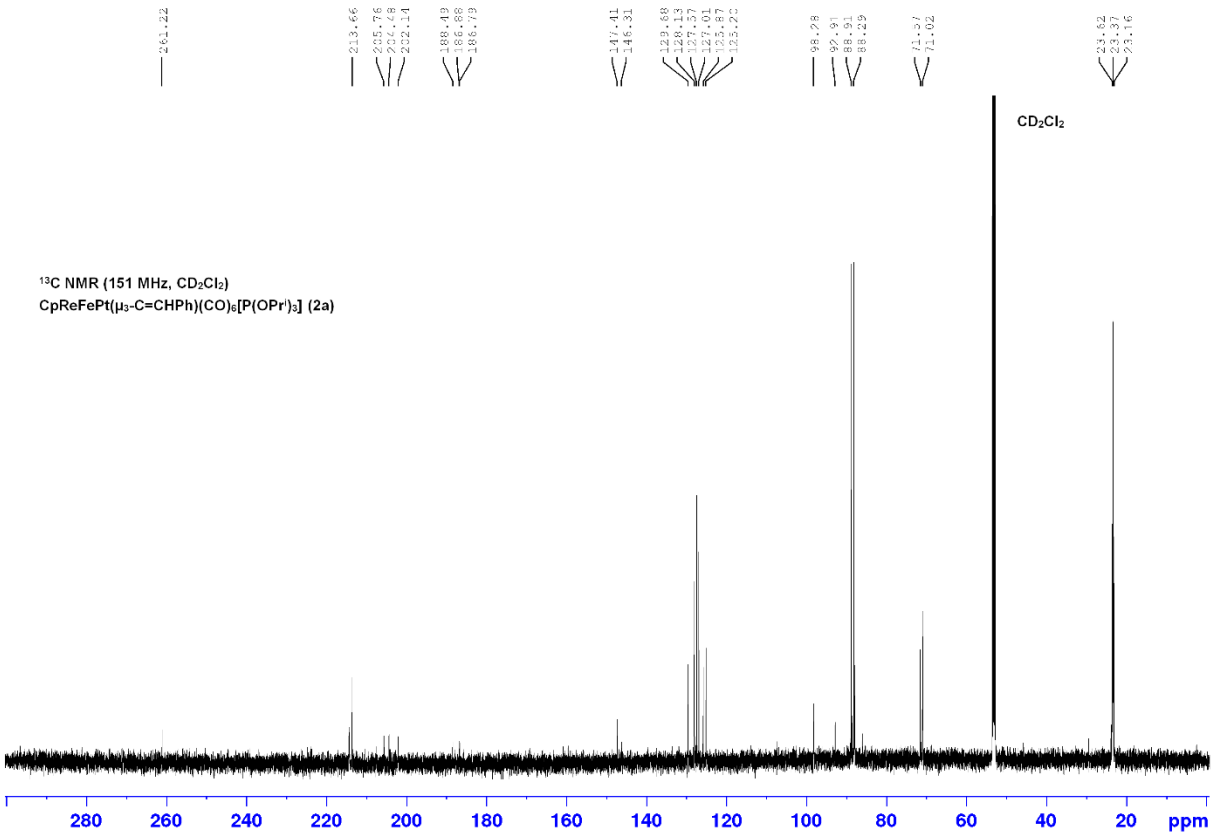

Figure 4S. ^{13}C NMR spectrum of CpReFePt(μ_3-C=CHPh)(CO)$_6$[P(OPr^i)$_3$] (**2a**) (151 MHz, CD_2Cl_2)

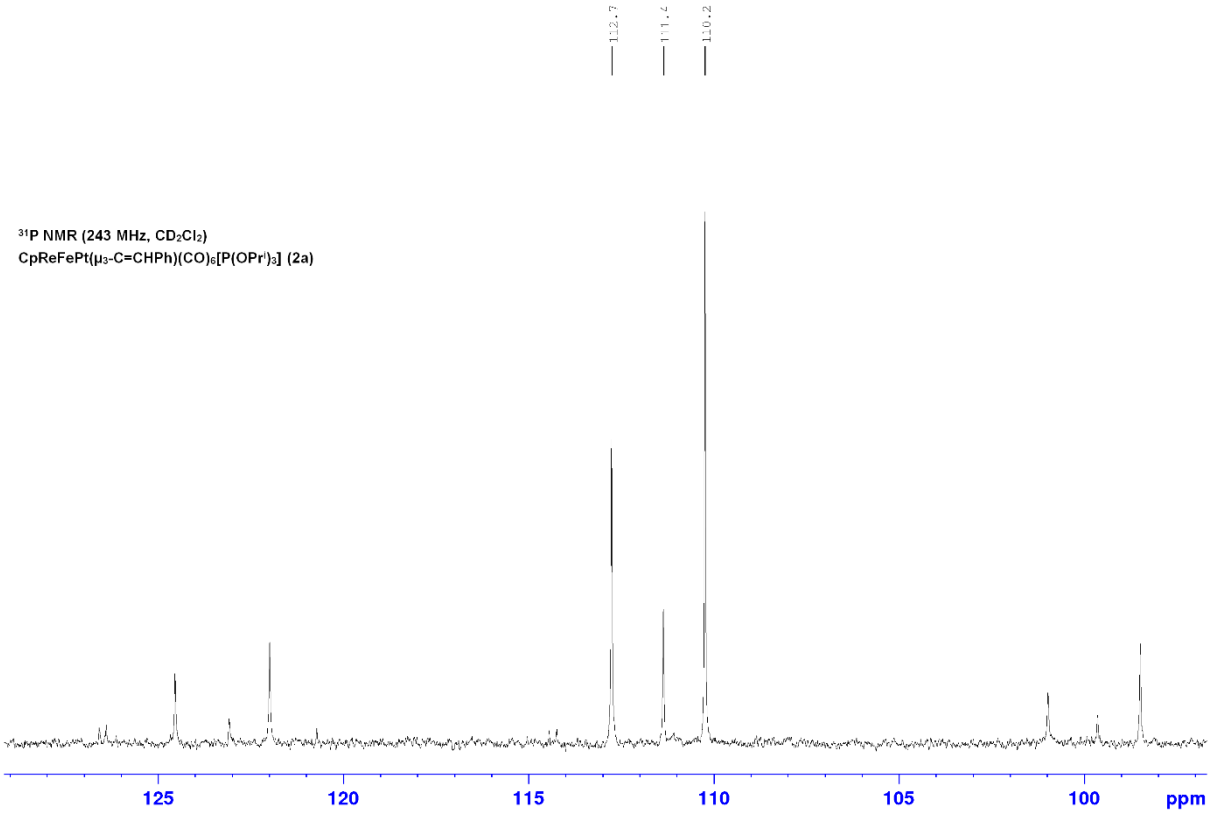

Figure 5S. ^{31}P NMR spectrum of CpReFePt(μ_3-C=CHPh)(CO)$_6$[P(OPr^i)$_3$] (**2a**) (243 MHz, CD_2Cl_2)

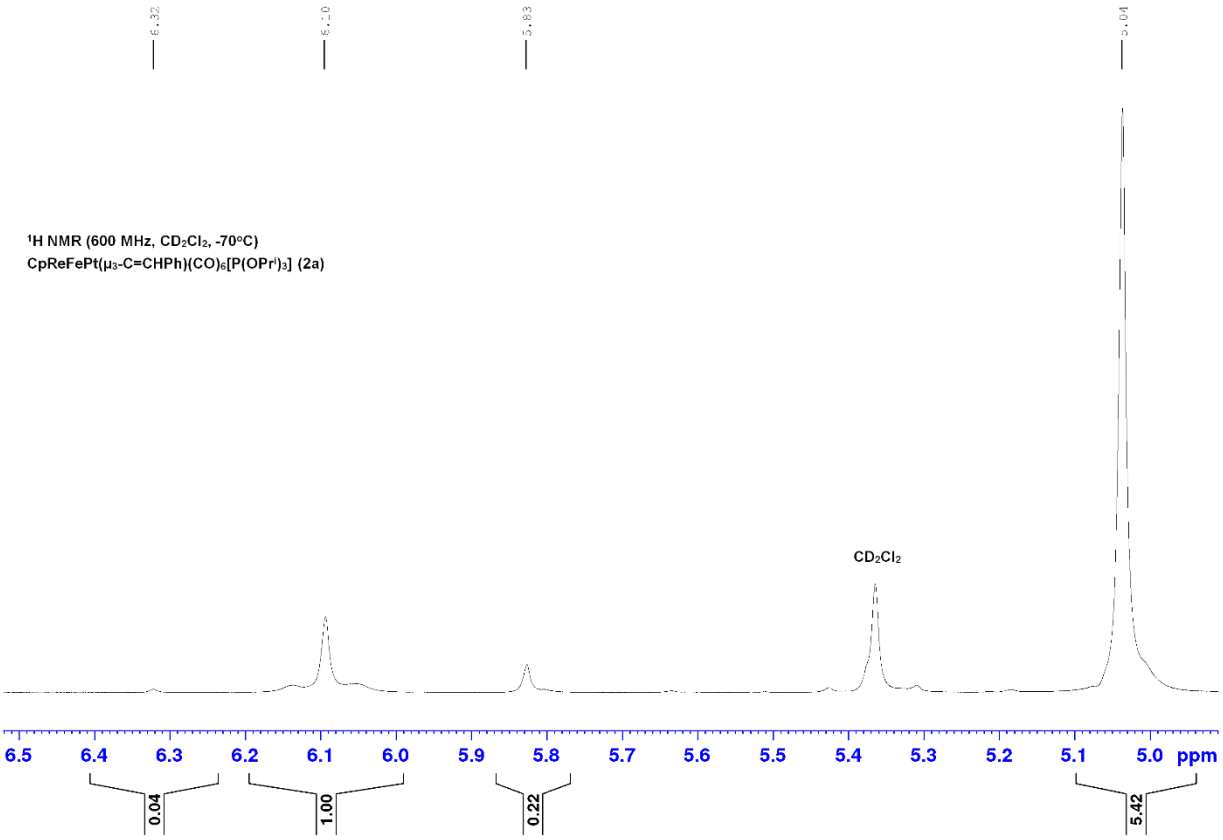

Figure 6S. ^{1}H NMR spectrum of CpReFePt(μ_3-C=CHPh)(CO)$_6$[P(OPr^i)$_3$] (**2a**) (600 MHz, CD_2Cl_2, -70°C)

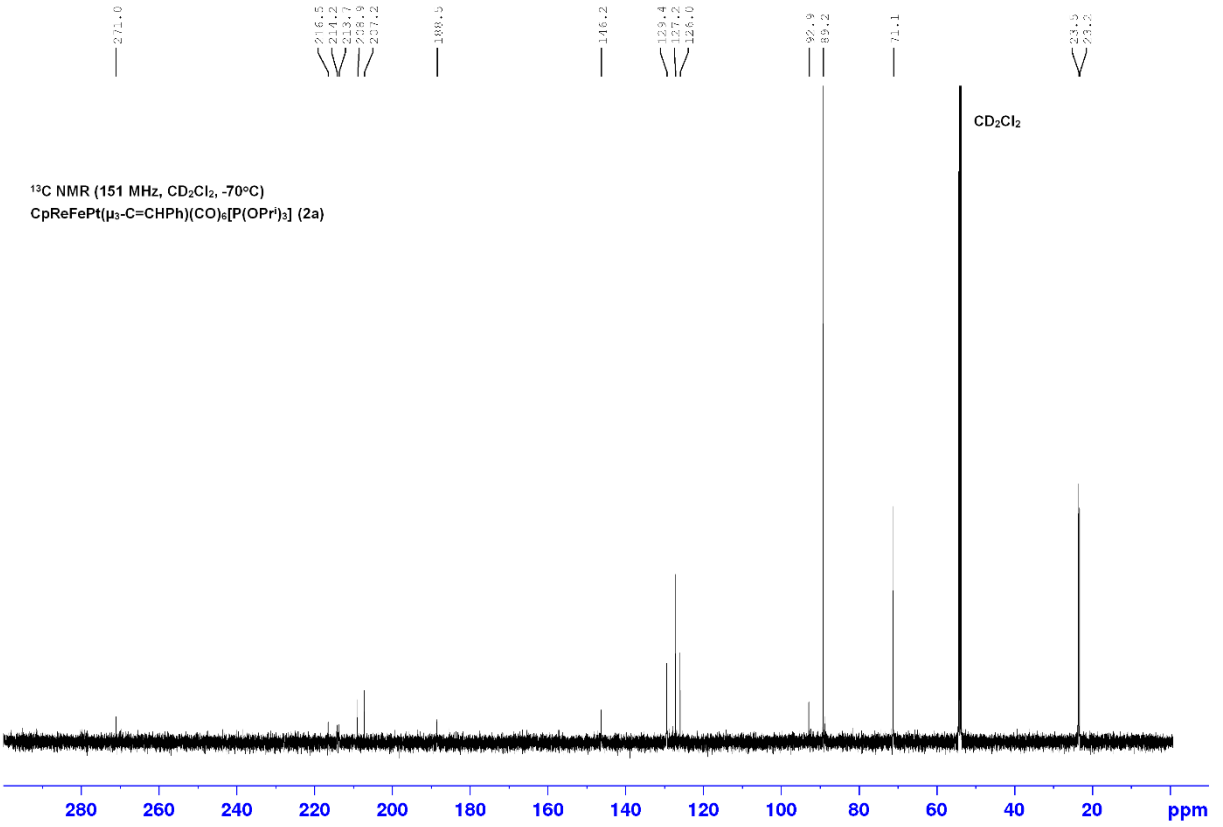

Figure 7S. ^{13}C NMR spectrum of CpReFePt(μ_3-C=CHPh)(CO)$_6$[P(OPr^i)$_3$] (**2a**) (151 MHz, CD_2Cl_2, -70°C)

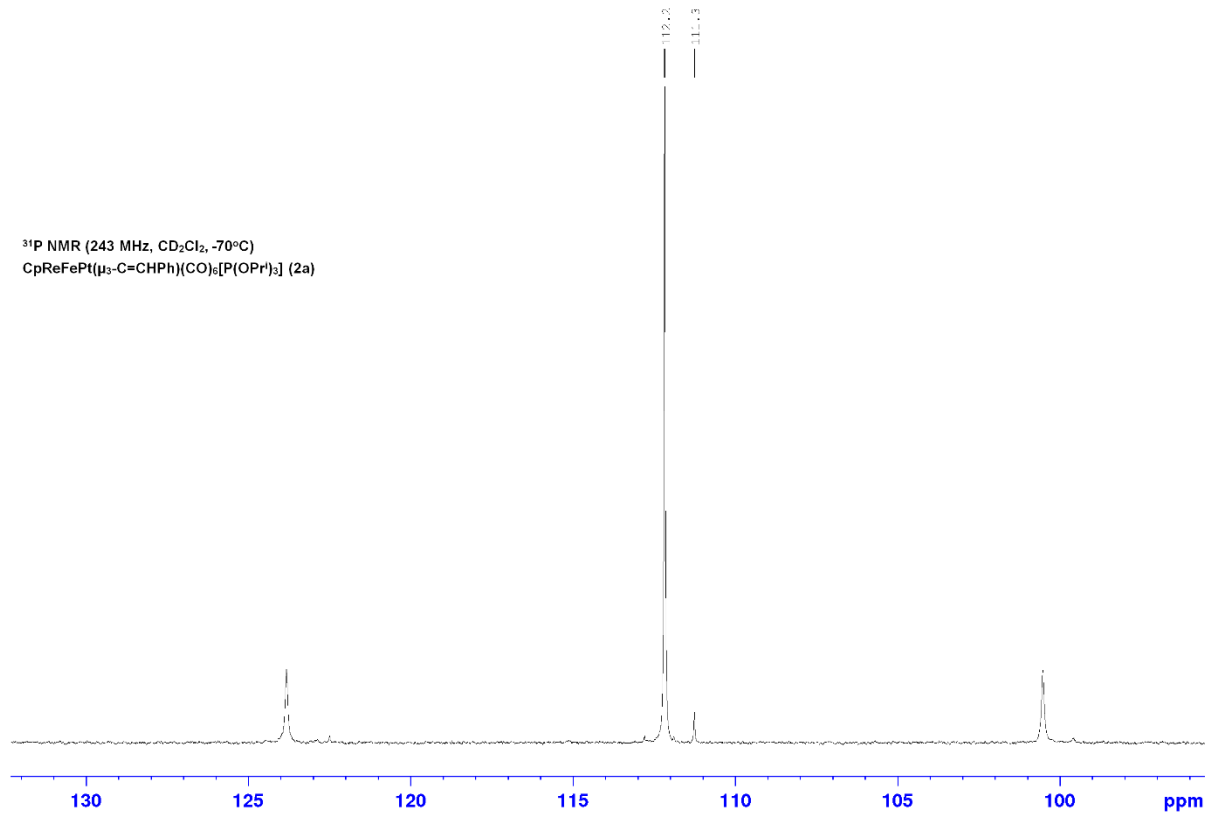

Figure 8S. ^{13}C NMR spectrum of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OPr^i)_3]$ (**2a**) (243 MHz, CD_2Cl_2, -70°C)

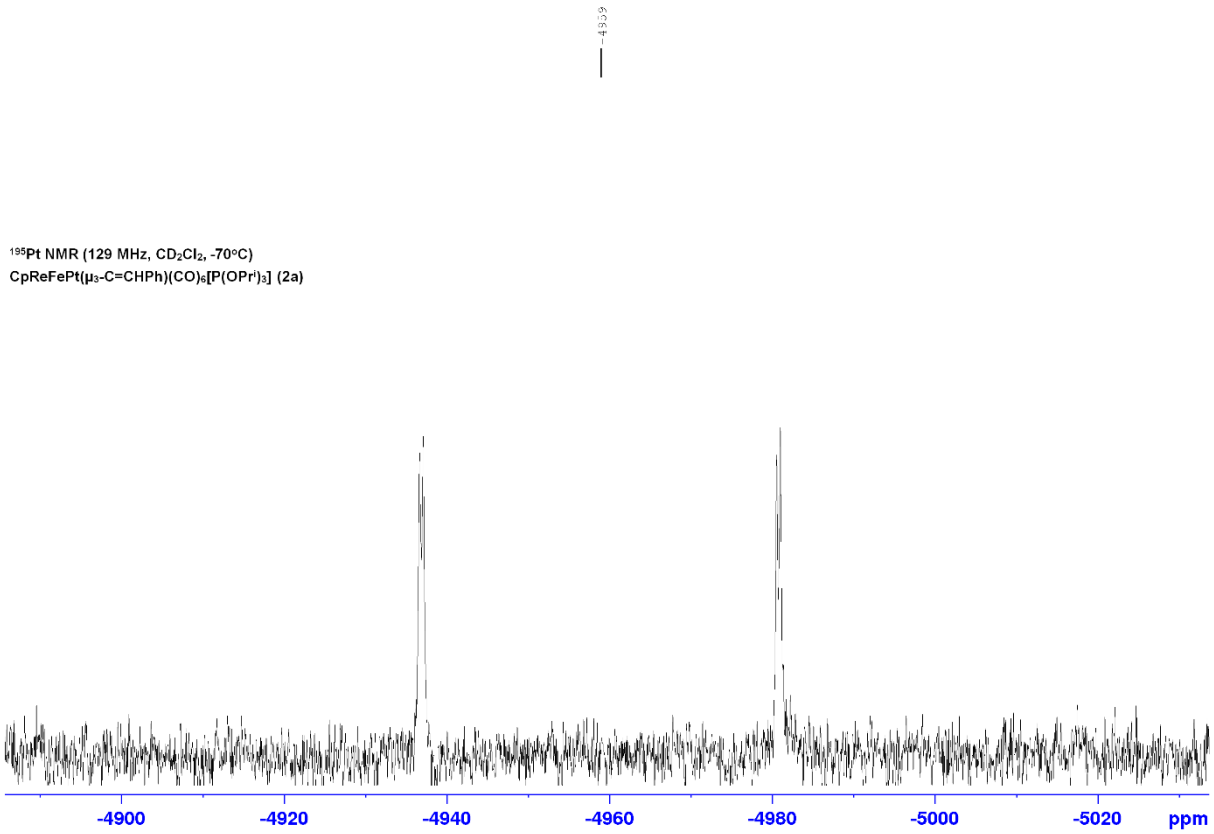

Figure 9S. ^{195}Pt NMR spectrum of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_6[P(OPr^i)_3]$ (**2a**) (129 MHz, Ξ, CD_2Cl_2, -70°C)

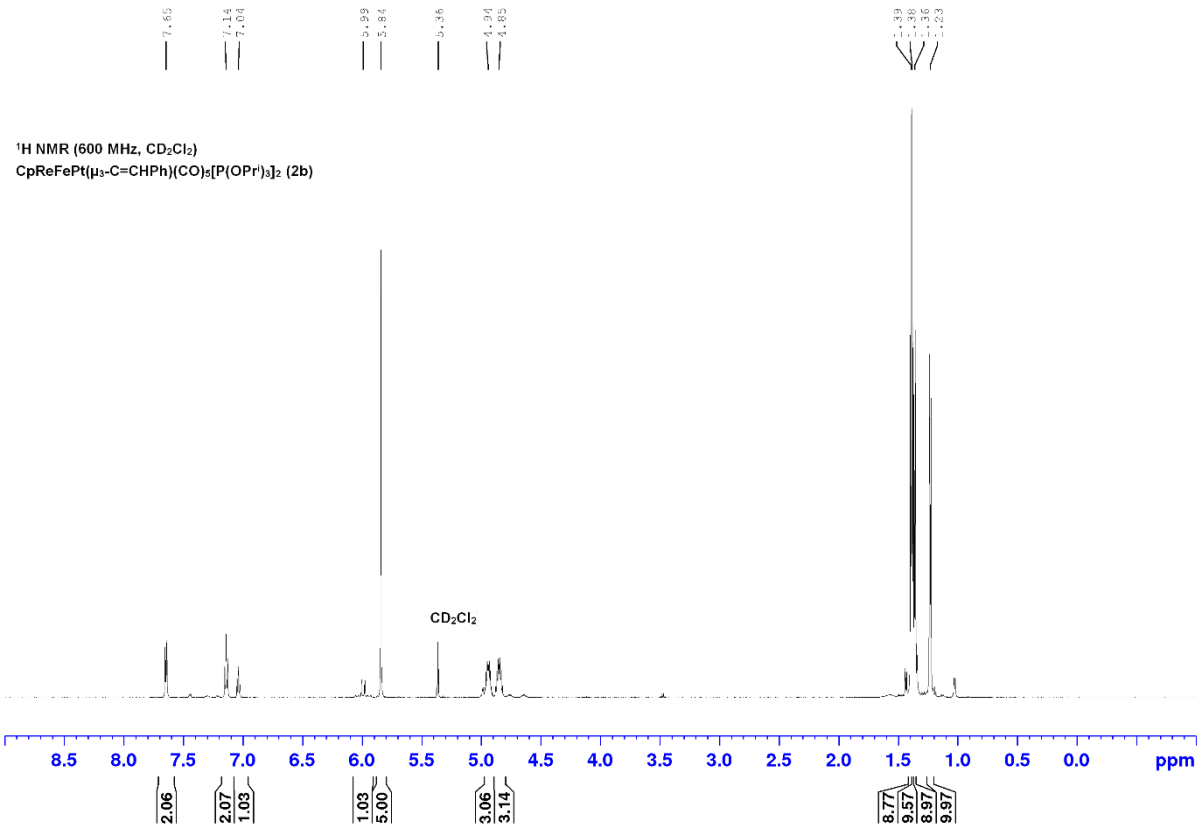

Figure 10S. ^{1}H NMR spectrum of CpReFePt(μ_3-C=CHPh)$(CO)_5[P(OPr^i)_3]_2$ (**2b**) (600 MHz, CD_2Cl_2)

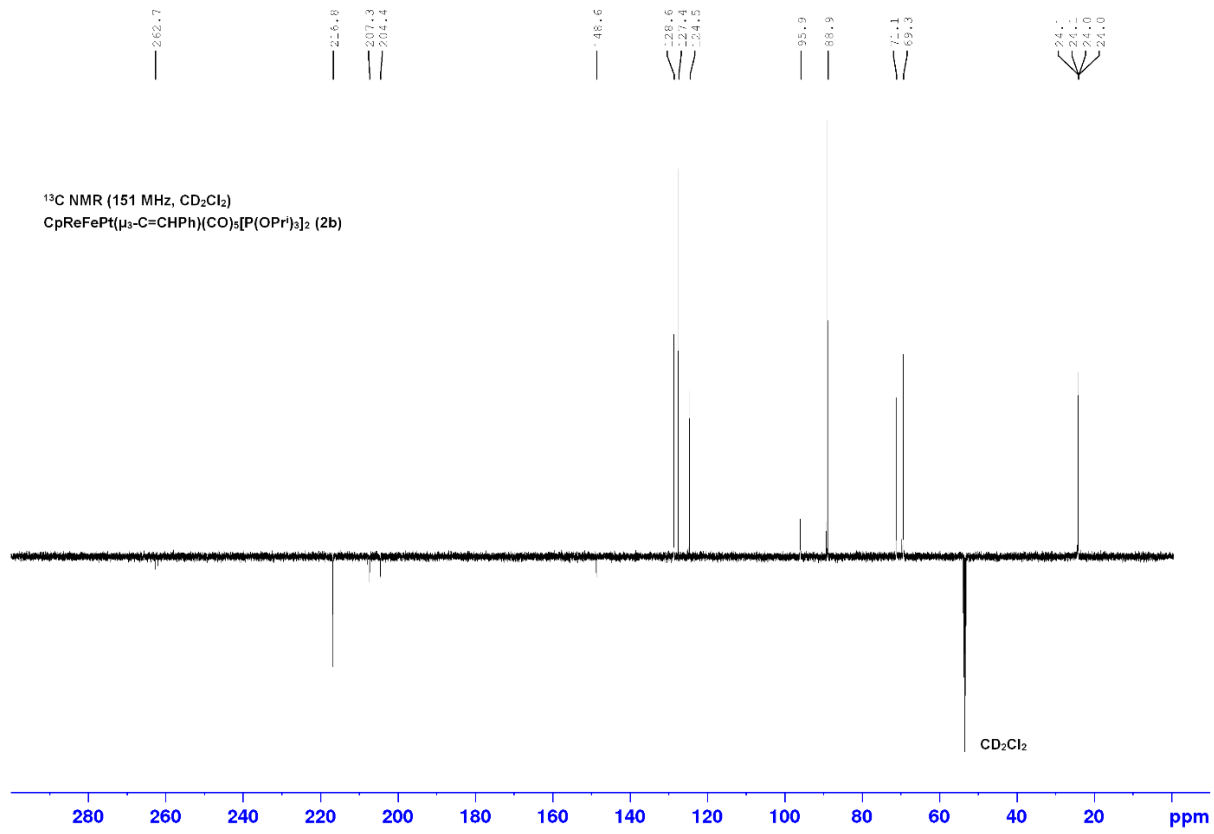

Figure 11S. ^{13}C CQDEPT NMR spectrum of CpReFePt(μ_3-C=CHPh)$(CO)_5[P(OPr^i)_3]_2$ (**2b**) (151 MHz, CD_2Cl_2)

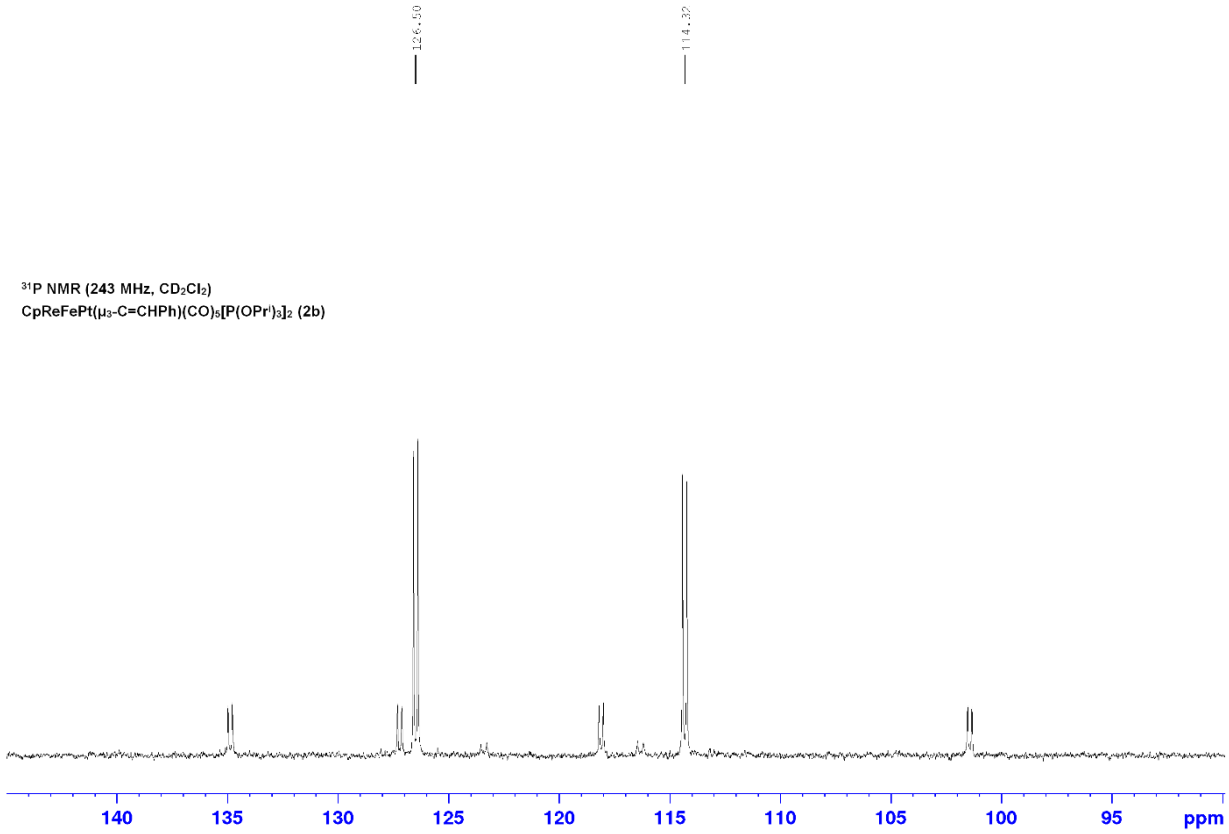

Figure 12S. ^{31}P NMR spectrum of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OPr^i)_3]_2$ (**2b**) (243 MHz, CD_2Cl_2)

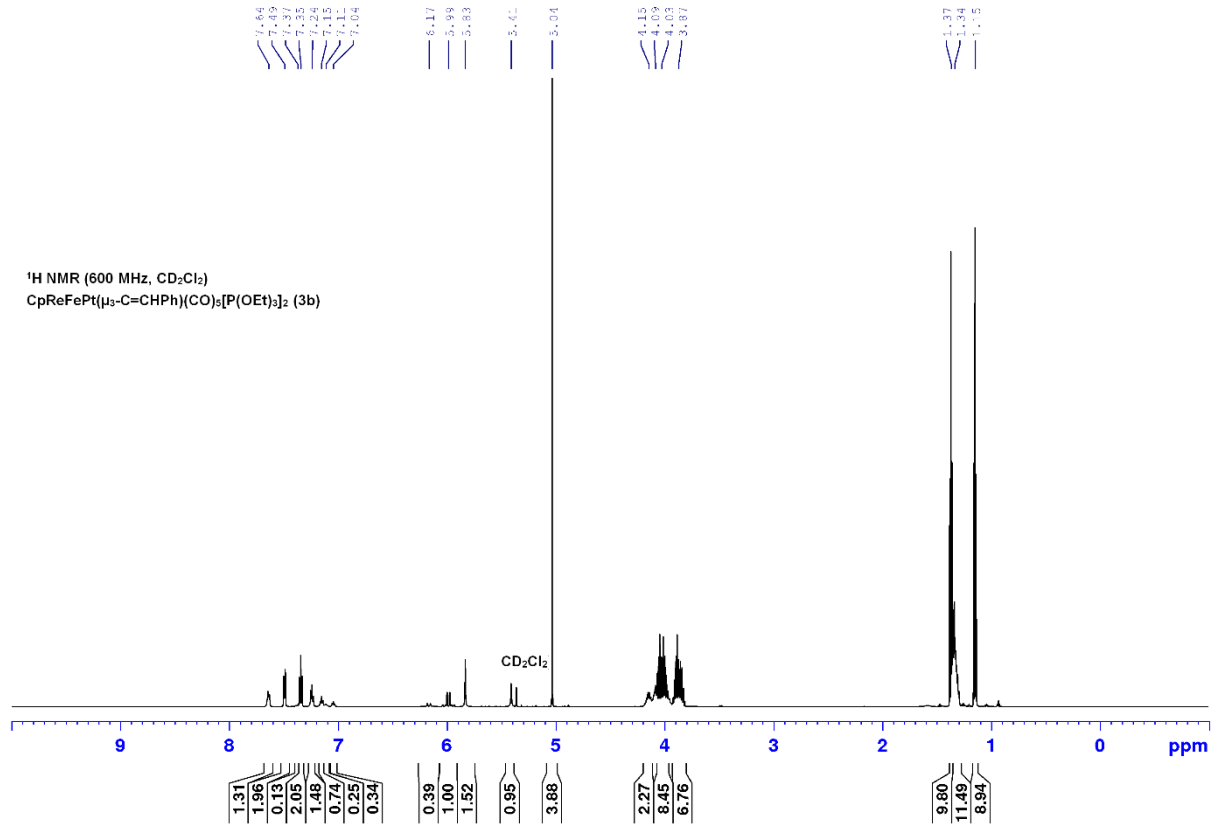

Figure 13S. ^{1}H NMR spectrum of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OEt)_3]_2$ (**3b**) (600 MHz, CD_2Cl_2)

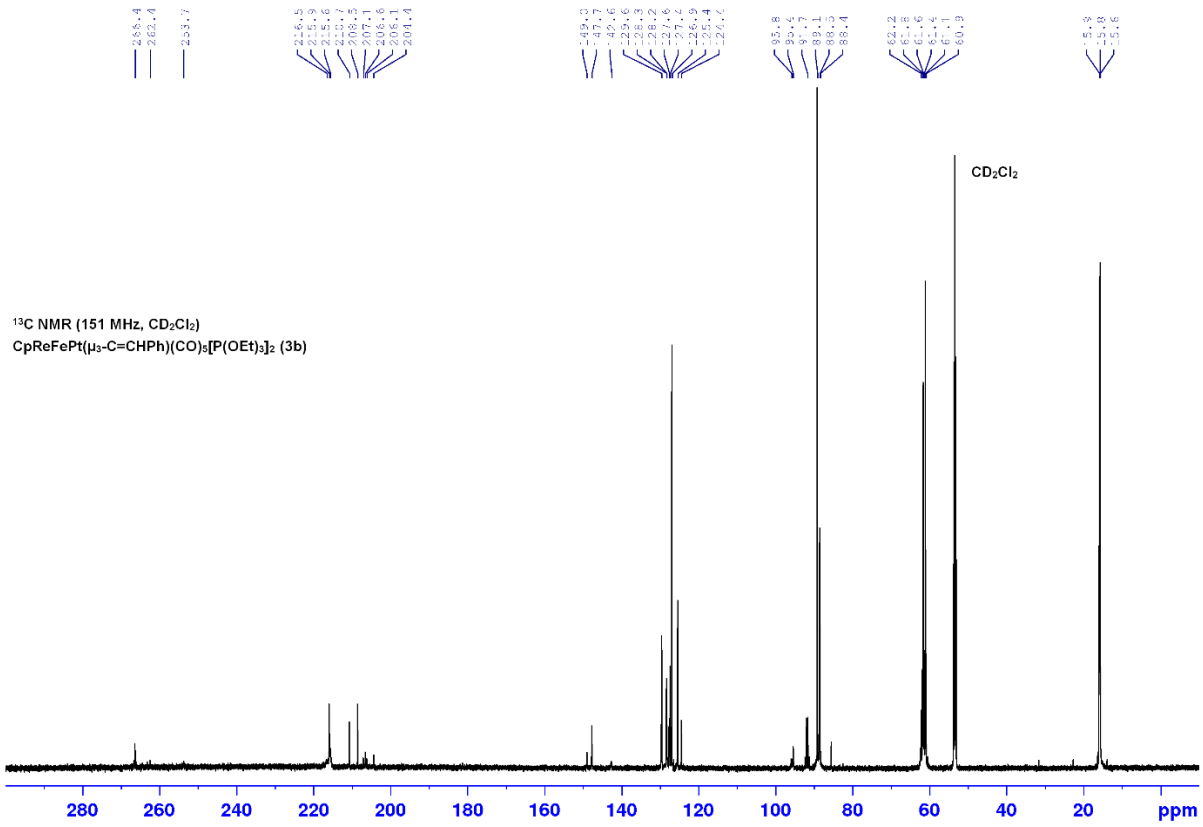

Figure 14S. ^{13}C NMR spectrum of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OEt)_3]_2$ (**3b**) (151 MHz, CD_2Cl_2)

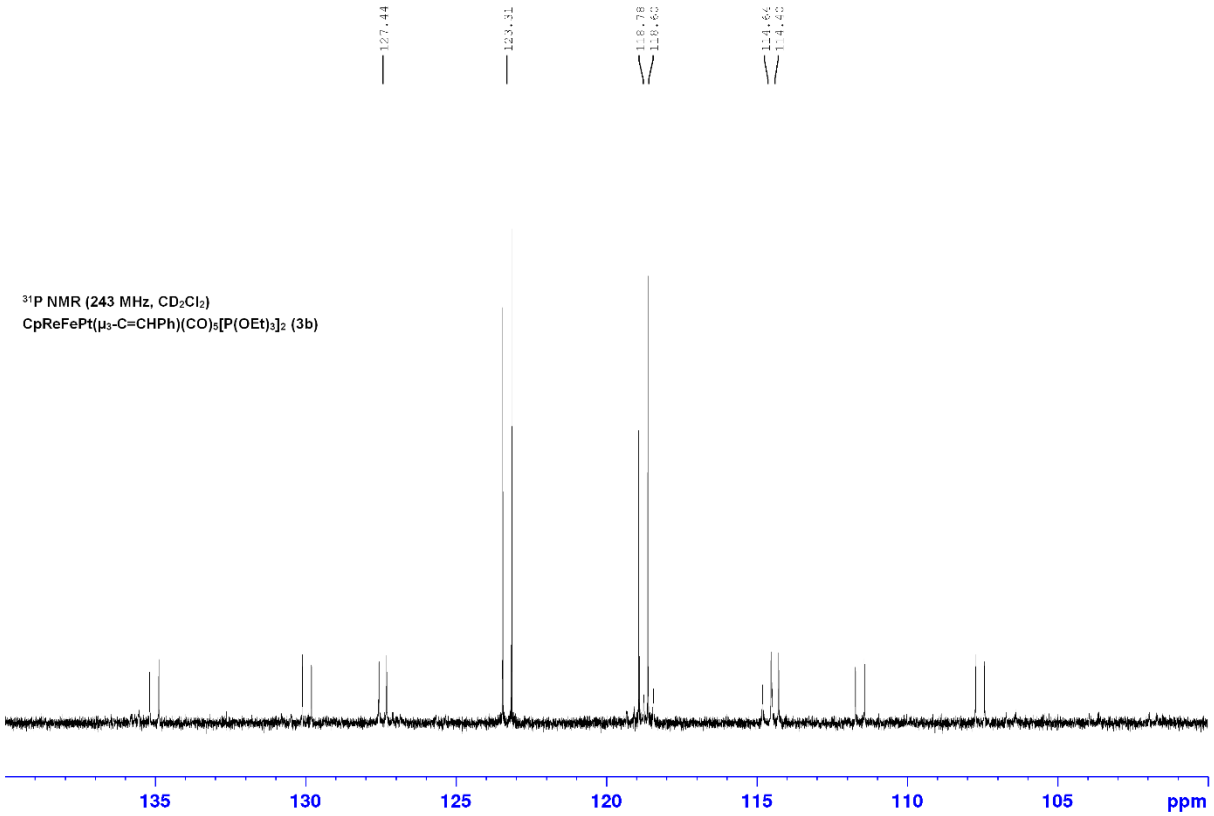

Figure 15S. ^{31}P NMR spectrum of $CpReFePt(\mu_3\text{-}C{=}CHPh)(CO)_5[P(OEt)_3]_2$ (**3b**) (243 MHz, CD_2Cl_2)

References

[1] O.S. Chudin, V. V. Verpekin, A.A. Kondrasenko, G. V. Burmakina, D.A. Piryazev, A.D.

Vasiliev, et al., Chemistry of vinylidene complexes. XXV. Synthesis and reactions of binuclear μ-vinylidene RePt complexes containing phosphite ligands. Spectroscopic, structural and electrochemical study, Inorganica Chim. Acta. 505 (2020) 119463. doi:10.1016/j.ica.2020.119463.

[2] V. V. Verpekin, A.A. Kondrasenko, O.S. Chudin, A.D. Vasiliev, G. V. Burmakina, N.I. Pavlenko, et al., Chemistry of vinylidene complexes. XXIII. Binuclear rhenium–palladium vinylidene bridged complexes, their reactions with diiron nonacarbonyl, J. Organomet. Chem. 770 (2014) 42–50. doi:10.1016/j.jorganchem.2014.07.024.

[3] V. V. Verpekin, A.A. Kondrasenko, R.O. Ergaev, O.S. Chudin, N.I. Pavlenko, A.I. Rubaylo, Phenylvinylidene Clusters Containing ReFePt Metal Cores and Chelate Diphosphine Ligands at the Platinum Atom, J. Sib. Fed. Univ. Chem. 10 (2017) 239–249. doi:10.17516/1998-2836-0021.

[4] G.M. Sheldrick, V. SADABS, 2.01, Bruker AXS Inc, Madison, Wisconsin, USA. (2004).

[5] G.M. Sheldrick, SHELXT – Integrated space-group and crystal-structure determination, Acta Crystallogr. Sect. A Found. Adv. 71 (2015) 3–8. doi:10.1107/S2053273314026370.

[6] G.M. Sheldrick, Crystal structure refinement with SHELXL, Acta Crystallogr. Sect. C Struct. Chem. 71 (2015) 3–8. doi:10.1107/S2053229614024218.

[7] J. Tao, J.P. Perdew, V.N. Staroverov, G.E. Scuseria, Climbing the Density Functional Ladder: Nonempirical Meta–Generalized Gradient Approximation Designed for Molecules and Solids, Phys. Rev. Lett. 91 (2003) 146401. doi:10.1103/PhysRevLett.91.146401.

[8] A.D. Becke, Density-functional thermochemistry. III. The role of exact exchange, J. Chem. Phys. 98 (1993) 5648–5652. doi:10.1063/1.464913.

[9] C. Lee, W. Yang, R.G. Parr, Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density, Phys. Rev. B. 37 (1988) 785–789. doi:10.1103/PhysRevB.37.785.

[10] Y. Zhao, D.G. Truhlar, The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other function, Theor. Chem. Acc. 120 (2008) 215–241. doi:10.1007/s00214-007-0310-x.

[11] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision D.01, (2013) Gaussian, Inc., Wallingford CT, 2013.

[12] F. Weigend, R. Ahlrichs, Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy, Phys. Chem. Chem. Phys. 7 (2005) 3297–3305. doi:10.1039/b508541a.

[13] D. Andrae, U. Häussermann, M. Dolg, H. Stoll, H. Preuß, Energy-adjusted ab initio pseudopotentials for the second and third row transition elements, Theor. Chim. Acta. 77 (1990) 123–141. doi:10.1007/BF01114537.