Supplementary Information

Triangular Triplatinum(0) Complex with Bridging Germylene Ligands. Insertion of Alkyne into the Pt–Ge Bond Rather Than the Pt–Pt Bond

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General Procedures. All manipulations were carried out using standard Schlenk techniques under an argon or nitrogen atmosphere or in a nitrogen-filled glovebox (Miwa MFG). Hexane, toluene, and THF were purified by using a Grubbs-type solvent purification system (Glass Contour).[1] The ^{1}H, $^{13}C\{^{1}H\}$, and $^{31}P\{^{1}H\}$ NMR spectra were recorded on a Bruker Biospin Avance III 400 MHz NMR spectrometer. Chemical shifts in ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were referenced to the residual peaks of the solvents used.[2] The peak position of the $^{31}P\{^{1}H\}$ NMR spectra was referenced to external 85% H_3PO_4 (δ 0) in deuterated solvents. All deuterated solvents ([D_6]benzene, [D_8]toluene, [D_2]dichloromethane) were carefully deoxygenated by three freeze-thaw-pump cycles before use. The signals of **4** and **5** in the ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were assigned by 2D HMQC NMR experiments. IR spectra were recorded on a JASCO FTIR-4100 spectrometer. Elemental analyses were performed using a LECO CHNS-932 or Yanaco MT-5 CHN autorecorder at the Center for Advanced Materials Analysis, Technical Department, Tokyo Institute of Technology. The compounds, *cis*-[$PtMe_2(PMe_3)_2$][3] and [$Pt(PCy_3)_2$][4], were prepared according to the literature. H_2GePh_2 was synthesized from reduction of Cl_2GePh_2 (Sigma-Aldrich) by $LiAlH_4$. Dimethyl acetylenedicarboxylate (DMAD) and methyl propiolate were purchased from Sigma-Aldrich and used as received.

Preparation of *trans*-[$Pt(GeHPh_2)_2(PMe_3)_2$] (2). To a hexane solution (3 mL) of *cis*-[$PtMe_2(PMe_3)_2$] (752 mg, 1.99 mmol) was added H_2GePh_2 (750 μL, 4.00 mmol) in 1:2 ratio. The reaction mixture was stirred for 1.5 h at room temperature, giving a white precipitate. The white solid was collected by filtration, washed with hexane (1 mL × 3), and then dried *in vacuo* to afford **2** (1.29 g, 81%). Colorless crystals of **2** suitable for X-ray crystallography were obtained from recrystallization from THF/hexane (1:5). Anal. Calcd for $C_{30}H_{40}Ge_2P_2Pt$: C, 44.87; H, 5.02; Found: C, 44.71; H, 4.98; ^{1}H NMR (400 MHz, [D_6]benzene, rt): δ=7.93 (d, J(H,H)=7.2 Hz, 8H; C_6H_5 *ortho*), 7.29 (t, J(H,H)=7.2 Hz, 8H; C_6H_5 *meta*), 7.20 (t, J(H,H)=7.2 Hz, 4H; C_6H_5 *para*), 5.32 (apparent triplet, J(P,H) = 12 Hz, J(Pt,H) = 67 Hz, 2H; Ge*H*), 1.19 ppm (s, J(Pt, H) = 30 Hz, 18H; PCH_3); $^{13}C\{^{1}H\}$ NMR (400 MHz, [D_6]benzene, rt): δ=147.6 (J(Pt,C)=37 Hz; C_6H_5 *ipso*), 136.9 (J(Pt,C)=14 Hz; C_6H_5 *ortho*), 128.1 (C_6H_5 *meta*), 127.8 (C_6H_5 *para*), 17.3 ppm (br; PCH_3); $^{31}P\{^{1}H\}$ NMR (162 MHz, [D_6]benzene, rt): δ=–24.5 ppm (J(Pt,P)=2362 Hz); IR (KBr): $\tilde{\nu}$= 1915 cm^{-1} (s; ν(GeH)).

Preparation of [{$Pt(PMe_3)$}$_3$(μ-$GePh_2$)$_3$] (3). *Trans*-[$Pt(GeHPh_2)_2(PMe_3)_2$] (1.00 g, 1.25

mmol) and [$Pt(PCy_3)_2$] (0.94 g, 1.24 mmol) in 1:1 ratio were dissolved in toluene (3 mL). The reaction mixture was stirred for 12 h at 100 ºC, giving a dark red solution. The solvent was removed under reduced pressure. The resulting material was washed with hexane (1 mL × 3) and dried *in vacuo* to afford **3** (836 mg, 67%). Orange crystals of **3** suitable for X-ray crystallography were obtained from recrystallization from THF/hexane (1:10). Anal. Calcd for $C_{45}H_{57}Ge_3P_3Pt_3$: C, 36.18; H, 3.85; Found: C, 36.54; H, 3.94; ^{1}H NMR (400 MHz, [D_2]dichloromethane, rt): δ=7.96 (m, 12H; C_6H_5 *ortho*), 7.36 (m, 18H; C_6H_5 *meta* and *para*), 1.16 ppm (m, J(Pt,H)=35 Hz, 27H; PCH_3); $^{13}C\{^1H\}$ NMR (101 MHz, [D_2]dichloromethane, rt): δ=158.6 (J(Pt,C)=58 Hz; C_6H_5 *ipso*), 135.5 (C_6H_5 *ortho*), 128.6 (C_6H_5 *meta*), 128.3 (C_6H_5 *para*), 22.4 ppm (m; PCH_3); $^{31}P\{^1H\}$ NMR (162 MHz, [D_2]dichloromethane, rt): δ=27.5 ppm (J(Pt,P) = 2900 Hz, ^2J(Pt,P) = 410 Hz, ^3J(P,P) = 94 Hz); $^{195}Pt\{^1H\}$ NMR (86 MHz, [D_2] dichloromethane, rt): δ –4195 ppm (J(Pt,Pt)=2633 Hz, J(P,Pt)=2900 Hz, ^2J(P,Pt)=410 Hz).

Preparation of [{Pt(PMe$_3$)}$_3$(μ_3-η^2(||)-CZ=CZ-GePh$_2$)(μ-GePh$_2$)$_2$] (4: Z = COOMe). To a THF (2 mL) solution of [{Pt(PMe_3)}$_3$(μ-$GePh_2$)$_3$] (50 mg, 0.033 mmol) was added DMAD (4.1 μL, 0.033 mmol) in an equimolar ratio. The reaction mixture was stirred for 1 h at 50 ºC, giving a dark red solution. The solvent was removed under reduced pressure to give the resulting material, which was washed with hexane (1 mL × 3) and dried *in vacuo* to afford **4** (43 mg, 78%). Red crystals of **4** suitable for X-ray crystallography were obtained from recrystallization from THF/hexane (1:10). Anal. Calcd for $C_{51}H_{63}Ge_3O_4P_3Pt_3$•1/2 C_6H_{14}: C, 38.62; H, 4.20; Found: C, 38.25; H, 4.00; ^{1}H NMR (400 MHz, [D_8]toluene, 27 ºC): δ=8.27 (d, J(H,H) = 6.4 Hz, 4H; C_6H_5 *ortho*), 8.18 (br, 4H; C_6H_5 *ortho*), 7.80 (br, 4H; C_6H_5 *ortho*), 7.29–7.23 (m, 12H; C_6H_5 *meta* and *para*), 7.13 (m, 6H; C_6H_5 *meta* and *para*), 3.55 (s, 3H; OCH_3), 3.19 (s, 3H; OCH_3), 1.30 (m, 18H; PCH_3), 0.34 ppm (d, J(P,H)=10 Hz, 9H; PCH_3); ^{1}H NMR (400 MHz, [D_8]toluene, –50 °C): δ=8.52 (d, J(H,H)=6.8 Hz, 2H; C_6H_5 *ortho*), 8.39 (m, 4H; C_6H_5 *ortho*), 8.13 (m, 2H; C_6H_5 *ortho*), 7.72 (br, 2H; C_6H_5 *ortho*), 7.44 (t, J(H,H)=14.8 Hz, 2H; C_6H_5 *meta*), 7.34–7.07 (m, 16H; C_6H_5 *meta* and *para*), 3.54 (s, 3H; OCH_3), 3.20 (s, 3H; OCH_3), 1.38 (d, J(H,H)=9.2 Hz, 9H; PCH_3), 1.13 (d, J(H,H)=9.6 Hz, 9H; PCH_3), 0.34 ppm (d, J(H,H)=10 Hz, 9H; PCH_3), One of C_6H_5 *ortho* hydrogen signals was buried in the baseline at this temperature; $^{13}C\{^1H\}$ NMR (101 MHz, [D_6]benzene, rt): δ=193.3 (J(Pt,C)=394 Hz; Pt*C*Z=), 174.9 (*C*O), 173.8 (*C*O), 151.1 (C_6H_5 *ipso*), 147.7 (C_6H_5 *ipso*), 143.7 (C_6H_5 *ipso*), 136.3 (C_6H_5 *ortho*), 135.8 (br; C_6H_5 *ortho*), 127.7 (C_6H_5 *meta* or *para*), 127.5

(C_6H_5 *meta* or *para*), 119.0 (Ge*C*Z=), 50.7 (O*C*H$_3$), 50.5 (O*C*H$_3$), 19.2 (m, *J*(P,H) = 32 Hz, *J*(Pt,H) = 50 Hz; P*C*H$_3$), 15.6 ppm (d, *J*(P,H) = 32 Hz; *J*(Pt,H)=58 Hz; P*C*H$_3$); $^{31}P\{^1H\}$ NMR (162 MHz, [D$_6$]benzene, rt): δ=–12.8 (*J*(P,Pt)=4012 Hz, ^2J(P,Pt)=348 Hz, ^3J(P,P)=63 Hz, 1P), –17.7 ppm (*J*(P,Pt)=3667 Hz, ^2J(P,Pt)=304 Hz, ^3J(P,P)=63 Hz, 2P); $^{195}Pt\{^1H\}$ NMR (86 MHz, [D$_6$]benzene, rt): δ=–4102 (dt, *J*(Pt,Pt)=1543 Hz, *J*(PPt)=3997 Hz, ^2J(PPt)=307 Hz, 1Pt), –4466 ppm (br d, *J*(P,Pt)=ca. 3600 Hz, 2Pt); IR (KBr): $\tilde{\nu}$=1692 (s; ν(C=O)), 1675 (s; ν(C=O)), 1213 cm^{-1} (s; ν(C–O)).

Preparation of [{Pt(PMe$_3$)}$_3$(μ_3-η^2(||)-CZ=CH-GePh$_2$)(μ_3-η^2(||)-GePh$_2$-CZ=CH- GePh$_2$)] (5: Z = COOMe). To a toluene (5 mL) solution of [{Pt(PMe$_3$)}$_3$(μ-GePh$_2$)$_3$] (100 mg, 0.066 mmol) was added methyl propiolate (12 μL, 0.13 mmol) in 1:2 ratio. The reaction mixture was stirred for 2 h at room temperature, giving a dark red solution. The solvent was removed under reduced pressure to give the resulting material, which was washed with hexane (1 mL × 3) and dried *in vacuo* to afford **5** (72 mg, 65%). Red crystals of **5** suitable for X-ray crystallography were obtained from recrystallization from THF/hexane (1:10). Anal. Calcd for $C_{53}H_{65}Ge_3O_4P_3Pt_3$: C, 38.30; H, 3.94; Found: C, 37.91; H, 3.86; ^1H NMR (400 MHz, [D$_8$]toluene, rt): δ=8.42 (m, 2H; C_6H_5 *ortho*), 8.37 (d, *J*(H,H)=7.2 Hz, 2H; C_6H_5 *ortho*), 8.23 (m, 4H; C_6H_5 *ortho*), 8.03 (m, 3H; C_6H_5 *ortho* and =C*H*), 7.96 (d, *J*(H,H)=7.2 Hz, 2H; C_6H_5 *ortho*), 7.27–7.03 (m, 18H; C_6H_5 *meta* and *para*), 6.90 (d, *J*(H,H)=7.2 Hz, 1H; =C*H*), 3.45 (s, 3H; OC*H*$_3$), 2.94 (s, 3H; OC*H*$_3$), 1.24 (d, *J*(P,H)=10 Hz, *J*(Pt,H)=38 Hz, 9H; PC*H*$_3$), 1.01 (d, *J*(P,H)=10 Hz, *J*(Pt,H)=33 Hz, 9H; PC*H*$_3$), 0.84 ppm (d, *J*(P,H)=9.6 Hz, *J*(Pt,H)=30 Hz, 9H; PC*H*$_3$); $^{13}C\{^1H\}$ NMR (101 MHz, [D$_6$]benzene, rt): δ=185.8 (*J*(Pt,C)=658 Hz; Pt*C*Z=), 175.1 (*C*O), 173.8 (*C*O), 150.5, 148.4, 145.6, 144.8, 144.4, 142.3 (C_6H_5 *ipso*), 138.7, 136.8, 136.3 (overlapped), 136.0, 135.3 (C_6H_5 *ortho*), 126.2 (C_6H_5 *meta* or *para*), 116.3 (Ge*C*H=), 113.1 (Ge*C*H=), 50.8 (O*C*H$_3$, overlapped), 19.3 (d, *J*(P,H)=34 Hz, *J*(Pt,H)=53 Hz; P*C*H$_3$), 18.2 (d, *J*(P,H)=32 Hz, *J*(Pt,H)=51 Hz; P*C*H$_3$), 16.5 ppm (d, *J*(P,H)=31 Hz, *J*(Pt,H)=47 Hz; P*C*H$_3$), The Ge*C*Z= carbon signal could not be assigned; $^{31}P\{^1H\}$ NMR (162 MHz, [D$_6$]benzene, rt): δ=–17.1 (apparent triplet, *J*(Pt,P)=3733 Hz, ^2J(Pt,P)=270, 443 Hz, ^3J(P,P)=82, 85 Hz), –23.2 (dd, *J*(Pt,P)=3609 Hz, ^2J(Pt,P)=211, 230 Hz, ^3J(P,P)=61, 82 Hz), –26.2 ppm (dd, *J*(Pt,P)=3772 Hz, ^2J(Pt,P)=281, 411 Hz, ^3J(P,P)=61, 85 Hz). IR (KBr): $\tilde{\nu}$= 1708 (s; ν(C=O)), 1687 (s; ν(C=O)), 1197 cm^{-1} (s; ν(C–O)).

X-ray Crystal Structure Analyses. Single crystals of **2-5** suitable for X-ray diffraction study were mounted on MicroMounts™ (MiTeGen). The crystallographic data were collected on a Rigaku Saturn CCD area detector or Bruker SMART APEXII ULTRA/CCD diffractometer equipped with monochromated Mo Kα radiation (λ = 0.71073 Å) at 113 K or 90 K. Calculations were carried out using the program package, respectively. The positional and thermal parameters of non-hydrogen atoms were refined anisotropically on F^2 by the full-matrix least-squares method using SHELXL-97.[5] Hydrogen atoms, except for the Ge–H hydrogens of **2**, were placed at calculated positions and refined with a riding mode on their corresponding carbon atoms. The GeH hydrogens of **2** were found from the Fourier-difference electron-density and refined isotropically. Figures S1 and S2 show the molecular structures of **2** and **3**. Crystallographic data of **2-5** are listed in Table S1.

Molecular Orbital Calculations. Calculation of **3** and [{Pt(PMe$_3$)}$_3$(μ-CO)$_3$] has been performed with *Gaussian 09*, *revision B.01*.[6] Geometry optimization was performed by MPWB95 functional conjunction with 6-31G(d,p) basis set (for H, C, O, P, Ge) and SDD basis set (for Pt). The geometry of the complex **3** was optimized using the actual atom positions obtained by X-ray crystallography. For accretion of the DFT calculations, the density fitting was applied with the W06 auxiliary basis set that implemented in *Gaussian 09*. All optimized structures were verified to be local minima by hessian calculation. NBO analysis was also performed by same level of theory. The HOMO-LUMO energy gaps of **3** and [{Pt(PMe$_3$)}$_3$(μ-CO)$_3$] were calculated as 2.07 and 2.07 eV, respectively.

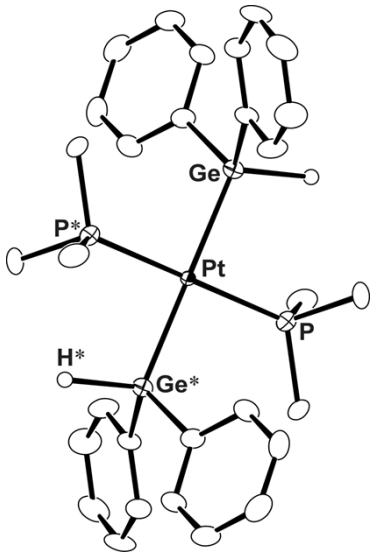

Figure S1. Thermal ellipsoidal plot of **2** (50% probability level). Hydrogen atoms, except GeH hydrogens, are omitted for clarity. Selected bond distances [Å] and angles [º]: Pt–Ge 2.4576(8), Pt–P 2.294(2), Ge–Pt–P 87.63(5).

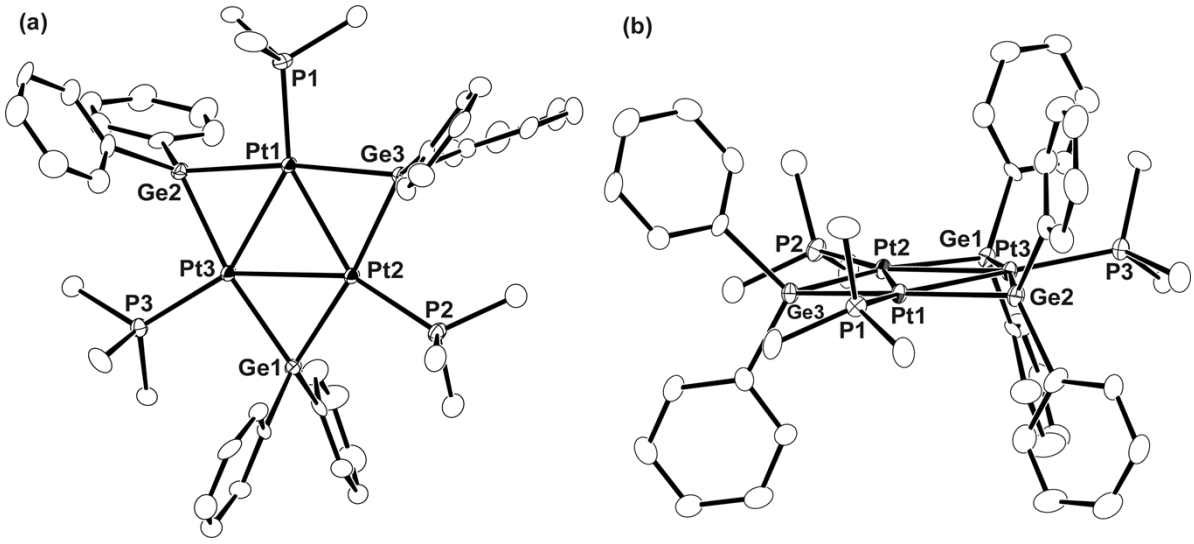

Figure S2. Thermal ellipsoidal plot (50% probability level) of **3** viewed from (a) the above and (b) in the plane of the Pt_3Ge_3 core. All hydrogen atoms have been omitted for clarity. Selected bond distances [Å] and angles [º]: Pt1–Pt2 2.7194(6), Pt1–Pt3 2.7081(6), Pt2–Pt3 2.7150(6), Pt1–Ge2 2.423(1), Pt1–Ge3 2.423(1), Pt2–Ge1 2.412(1), Pt2–Ge3 2.416(1), Pt3–Ge1 2.4209(9), Pt3–Ge2 2.4131(9), Pt1–P1 2.243(2), Pt2–P2 2.247(3), Pt3–P3 2.242(3), Pt2–Ge1–Pt3 68.36(3), Pt1–Ge2–Pt3 68.10(3), Pt1–Ge3–Pt2 68.38(3).

Table S1. Crystallographic Data and Details of Refinement of **2-5**

	2	**3**	**4**	**5**
formula	$C_{30}H_{40}Ge_2P_2Pt$	$C_{45}H_{57}Ge_3P_3Pt_3$	$2(C_{51}H_{63}Ge_3O_4P_3Pt_3)\cdot C_6H_{14}$	$C_{53}H_{65}Ge_3O_4P_3Pt_3$
formula wt	802.86	1493.91	3358.09	1662.00
cryst size/mm	0.28×0.41×0.56	0.18×0.15×0.15	0.20×0.20×0.10	0.13×0.15×0.23
cryst syst	monoclinic	triclinic	monoclinic	monoclinic
cryst color	colorless	red	red	red
space group	C2/c (*No*. 15)	*P*-1 (*No*. 2)	$P2_1$ (*No*. 4)	$P2_1/c$ (*No*. 14)
a/Å	22.985(6)	12.539(2)	12.053(3)	21.046(6)
b/Å	8.962(2)	13.863(2)	23.593(6)	12.804(4)
c/Å	15.656(4)	15.866(3)	20.308(5)	20.027(5)
α/deg		66.820(8)		
β/deg	107.227(3)	79.027(9)	91.905(4)	93.534(3)
γ/deg		66.814(9)		
V/Å^3	3080(2)	2328.9(8)	5772(3)	5387(3)
Z	4	2	2	4
D_{calcd}/g cm^{-3}	1.731	2.130	1.932	2.049
F(000)	1568	1404	3204	3160
μ/mm^{-1}	6.571	10.983	8.910	9.546
no. of reflns measd	11909	19101	23758	25119
no. of unique reflns	3517	10239	15612	9504
R_{int}	0.0295	0.0351	0.0768	0.4150
no. of obsed reflns ($I > 2\sigma(I)$)	3183	7179	11806	7065
no. of variables	167	496	1231	608
R, R_w ($I > 2\sigma(I)$)	0.0475, 0.0507	0.0310, 0.0869	0.0655, 0.1313	0.0921, 0.2482
R, R_w (all data)	0.1223, 0.1242	0.0460, 0.0925	0.0977, 0.1404	0.1060, 0.2617
GOF on F^2	1.081	1.026	1.336	0.981

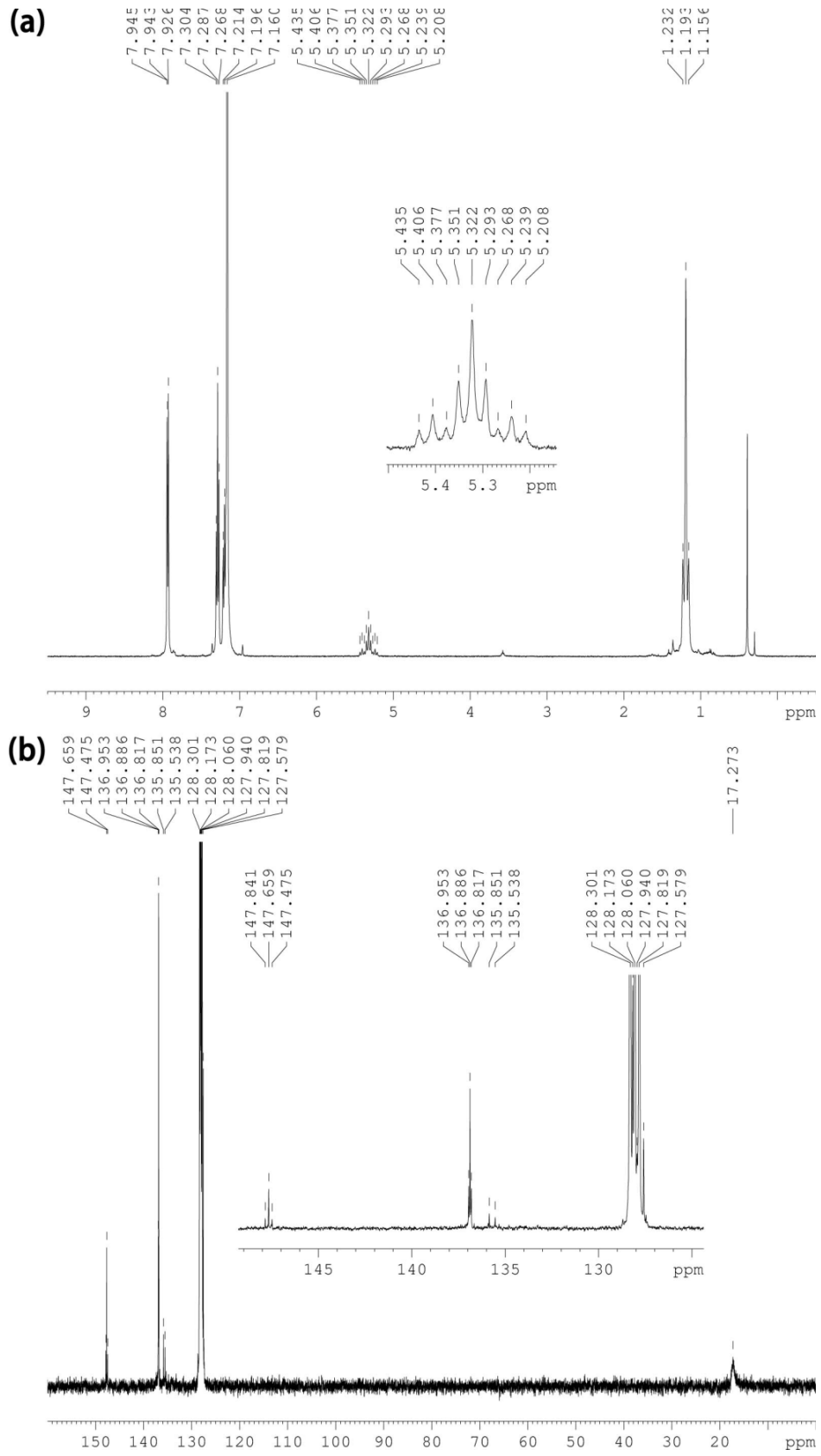

Figure S3 (a) ^{1}H and (b) $^{13}C\{^{1}H\}$ NMR spectra of **2** in C_6D_6.

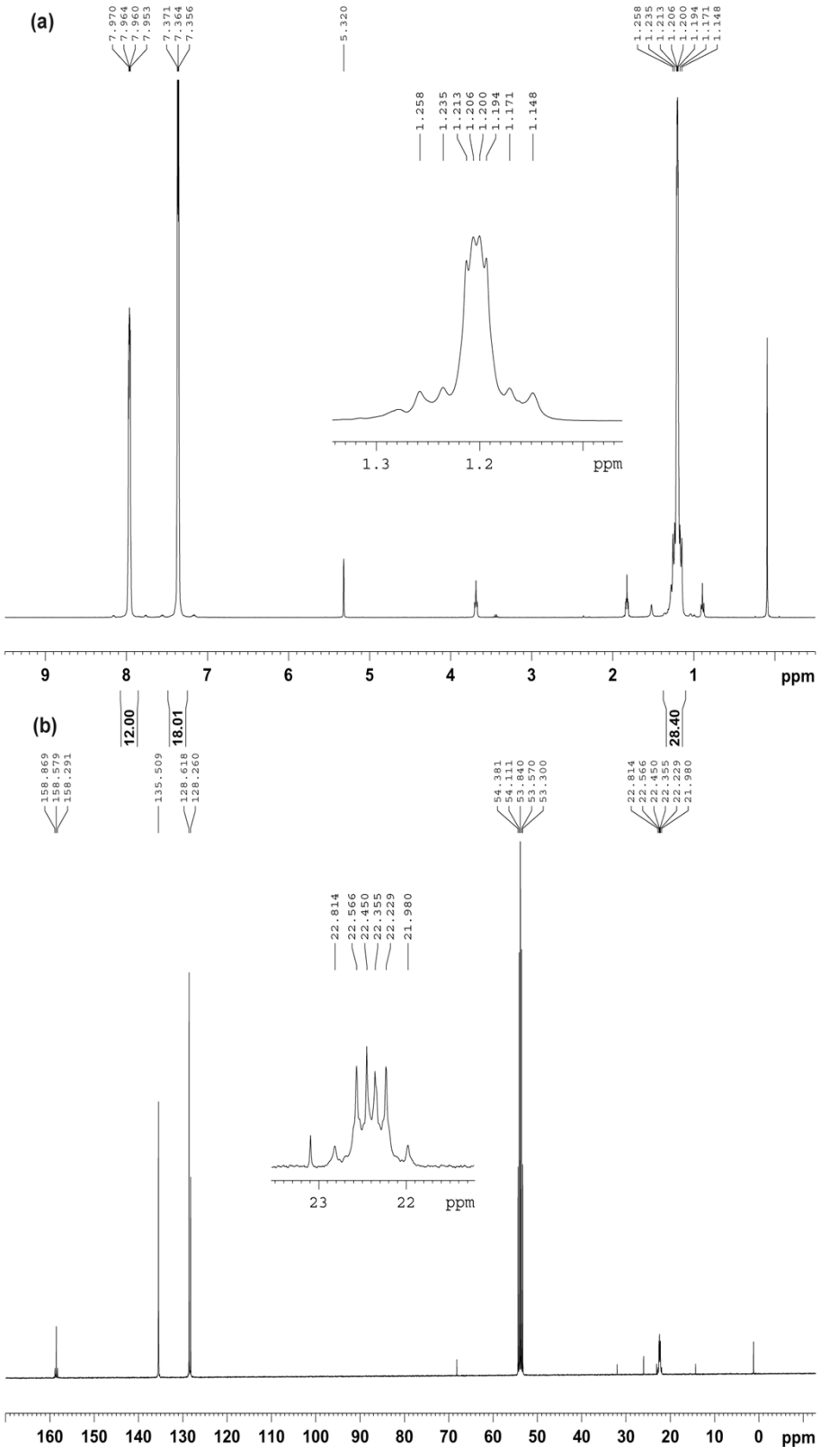

Figure S4 (a) ^{1}H and (b) $^{13}C\{^{1}H\}$ NMR spectra of **3** in CD_2Cl_2.

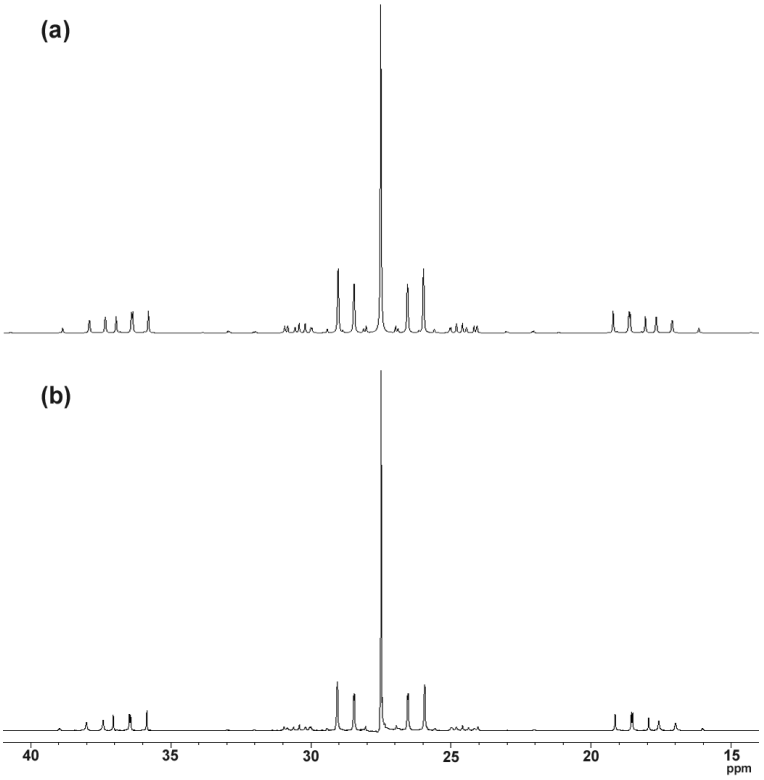

Figure S5 (a) Simulated and (b) experimental $^{31}P\{^{1}H\}$ NMR spectra of **3** in CD_2Cl_2.

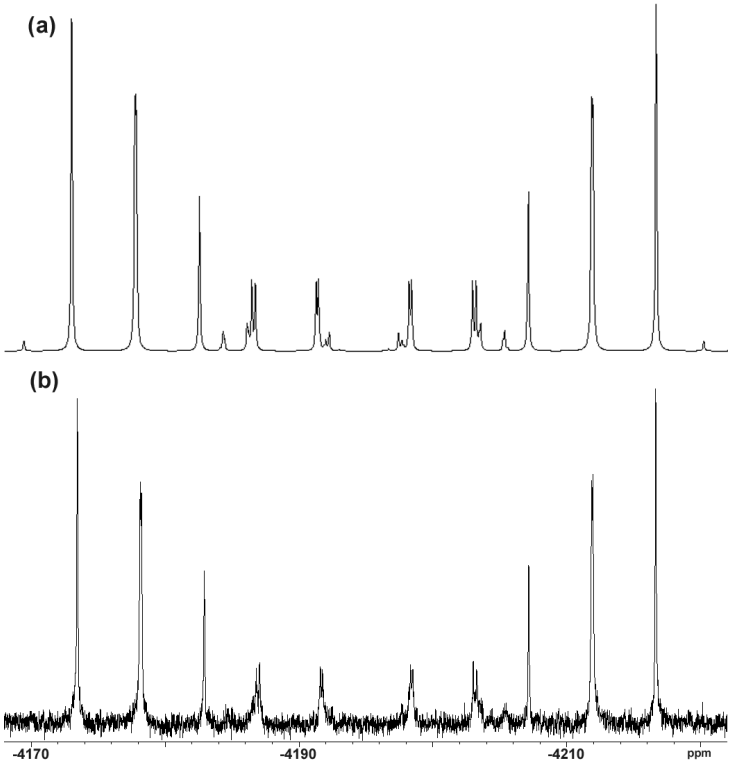

Figure S6 (a) Simulated and (b) experimental $^{195}Pt\{^{1}H\}$ NMR spectra of **3** in CD_2Cl_2.

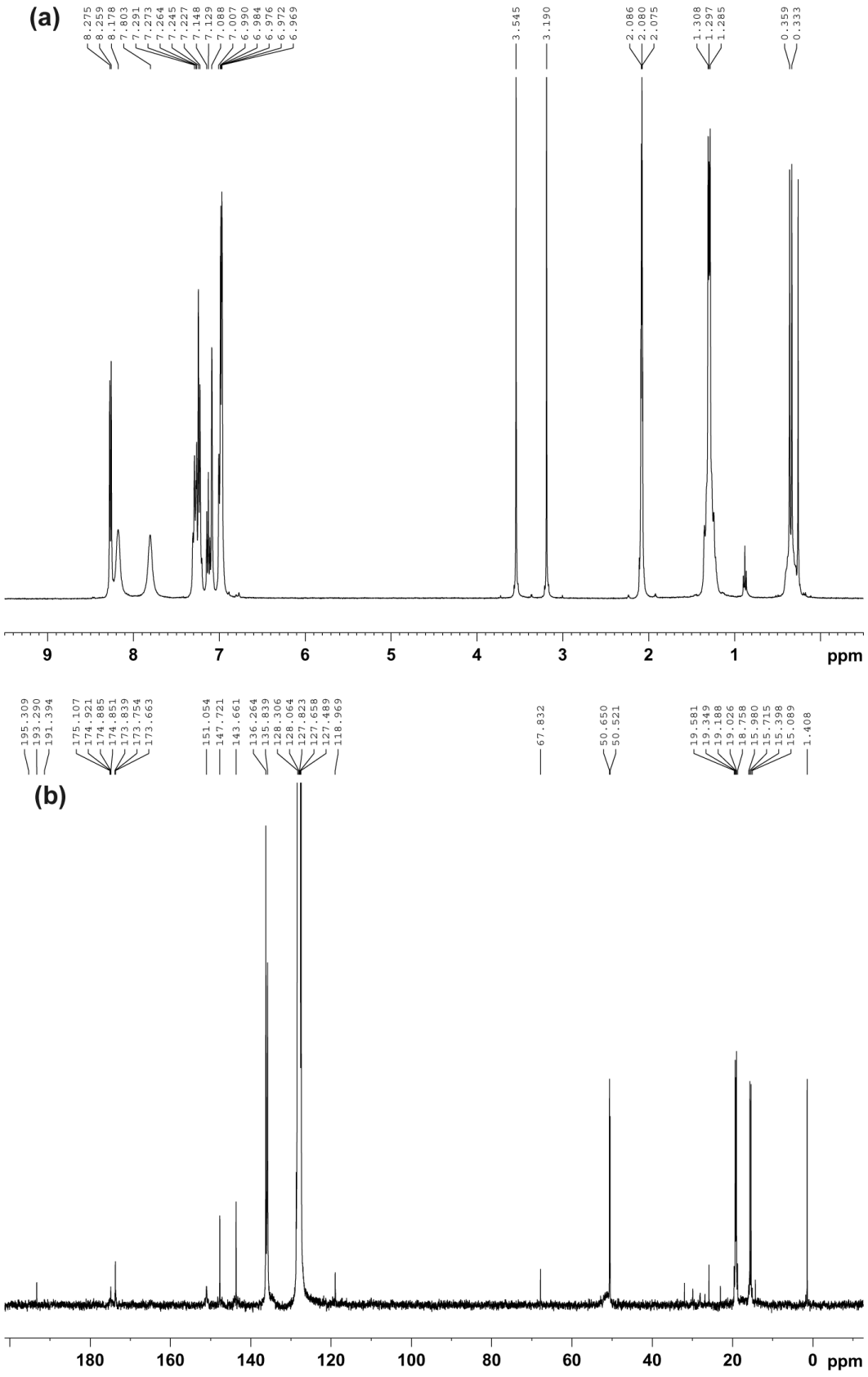

Figure S7 (a) ^{1}H NMR (in C_7D_8) and (b) $^{13}C\{^{1}H\}$ NMR (in C_6D_6) spectra of **4**.

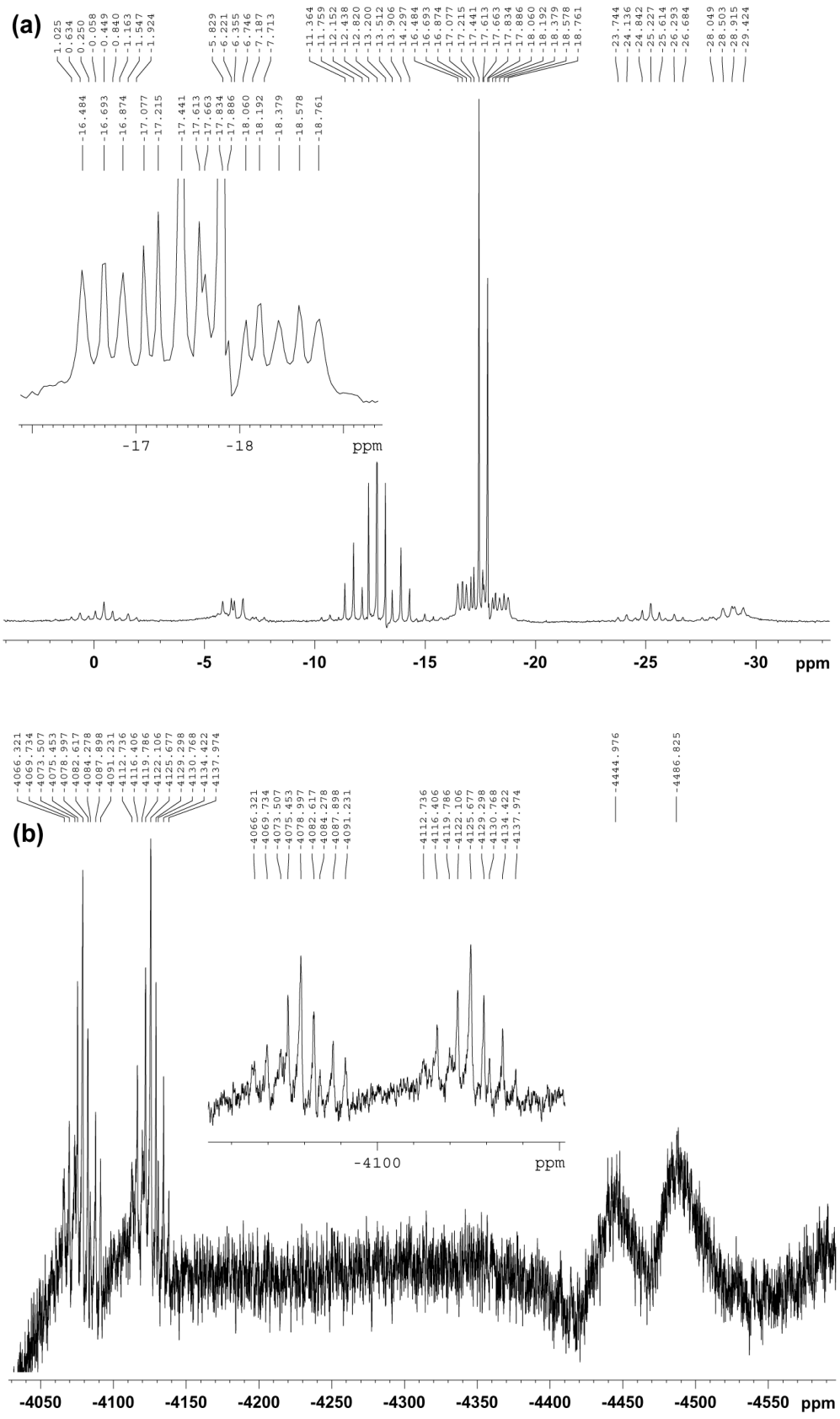

Figure S8 (a) $^{31}P\{^{1}H\}$ and (b) $^{195}Pt\{^{1}H\}$ NMR spectra of **4** in C_6D_6.

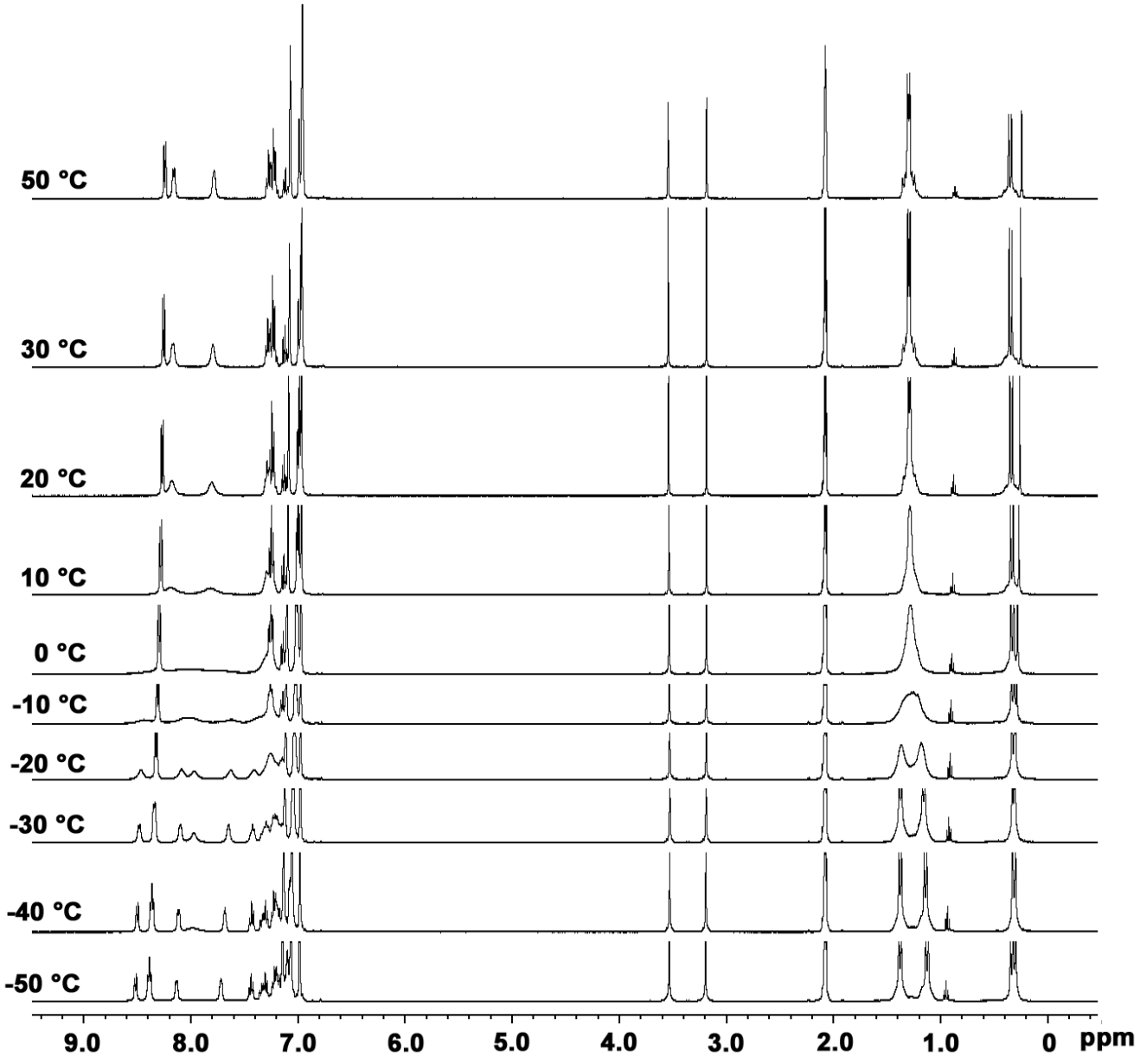

Figure S9 Variable-temperature ^{1}H NMR spectra of **4** in C_7D_8 from –50 to 50 °C.

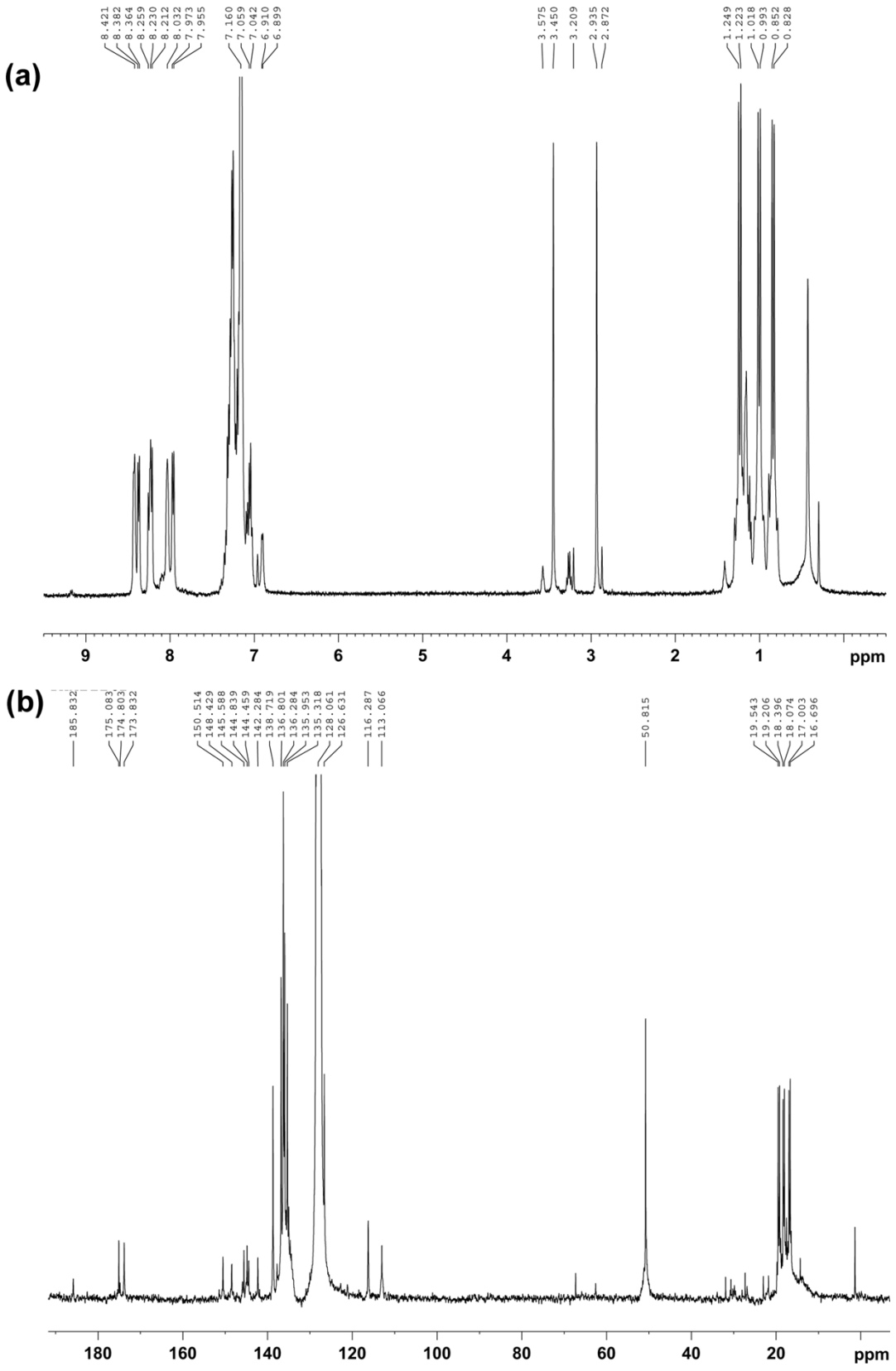

Figure S10 (a) ^{1}H and (b) $^{13}C\{^{1}H\}$ NMR spectra of **5** in C_6D_6.

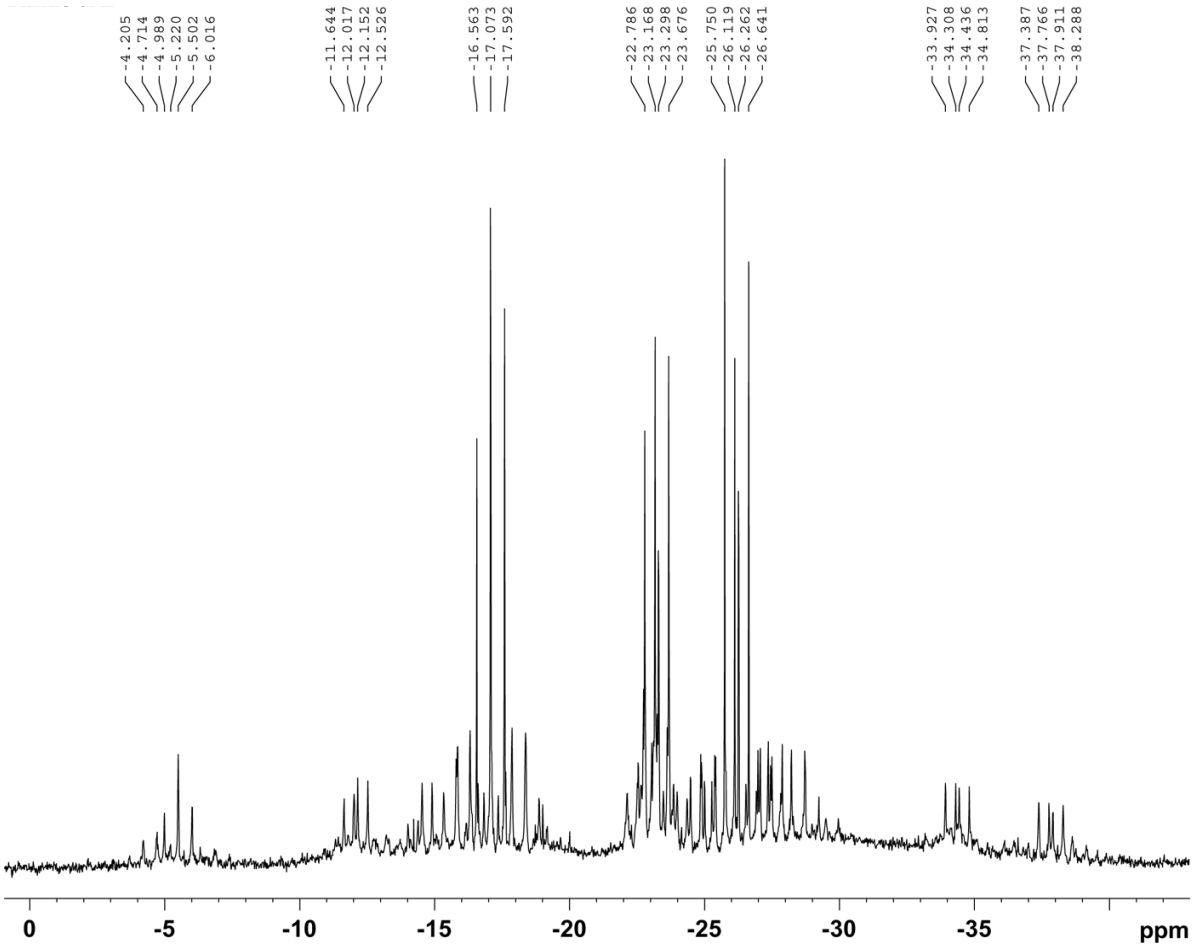

Figure S11 $^{31}P\{^{1}H\}$ NMR spectrum of **5** in C_6D_6.

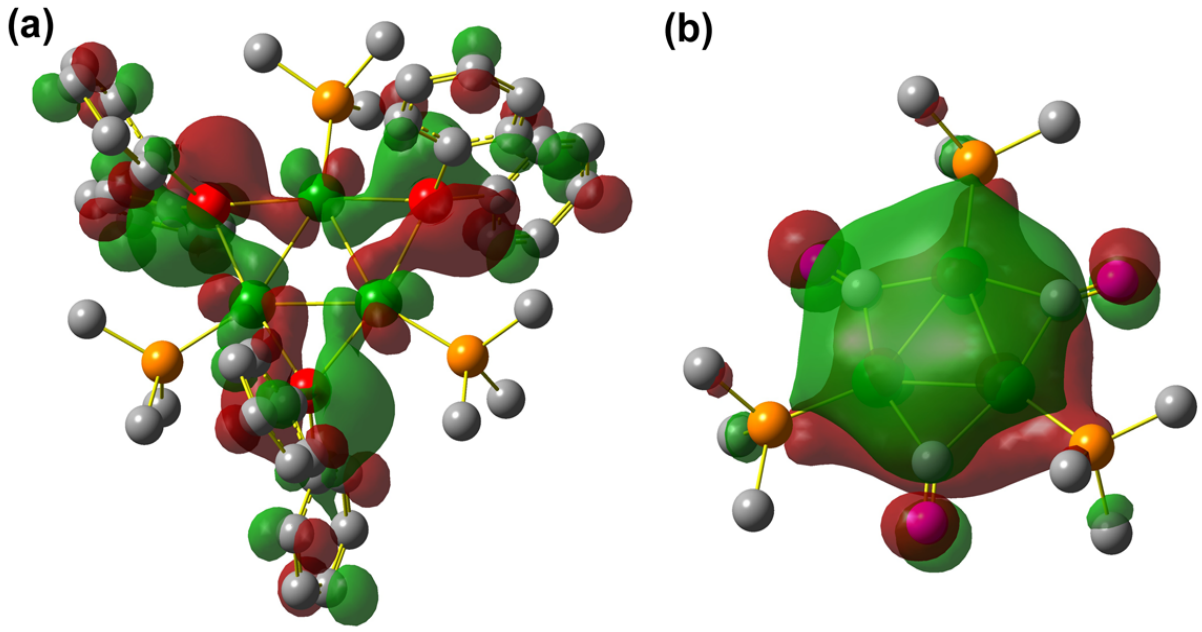

Figure S12. LUMOs of (a) **3** and (b) [{Pt(PMe$_3$)}$_3$(μ-CO)$_3$], optimized by DFT calculations.

Table S2. Experimental and calculated bond distances [Å] and angles [°] of **3** and [{Pt(PMe$_3$)}$_3$(μ-CO)$_3$].[a)]

	3 (E = Ge)		[{Pt(PMe$_3$)}$_3$(μ-CO)$_3$] (E = CO)
	Exp.	Calc.	Calc.
Pt–Pt	2.7142(6)	2.7585	2.7159
Pt–E	2.418(2)	2.450	2.0830
Pt–P	2.244(3)	2.288	2.282
Pt–Pt–Pt	60.00(6)	60.00	60
Pt–E–Pt	68.28(3)	68.52	81.37
Ph–E–Ph	108.8(4)	109.13	—

a) All bond distances and angles are averaged.

Table S3. Optimized geometry of (a) **3** and (b) [{Pt(PMe_3)}$_3$(μ-CO)$_3$]

(a) Complex **3**

atom	x	y	z
Pt	-1.46225357	0.57556076	-0.04653155
Pt	0.23396876	-1.60083087	-0.07181168
Pt	1.25852808	0.96932947	-0.04669669
Ge	2.61439998	-1.06336837	0.13900471
Ge	-0.39262852	2.77756485	0.04341392
Ge	-2.21020268	-1.75236828	0.07159498
P	-3.57339984	1.40693471	-0.34221934
P	0.56005382	-3.85080312	-0.32244036
P	3.08661732	2.3204496	-0.3044485
C	3.88347189	-1.51384821	-1.30831354
C	5.28015373	-1.62508346	-1.15466007
C	6.11250444	-1.87389557	-2.25589079
C	5.56108661	-2.01240845	-3.53627441
C	4.1745205	-1.89084752	-3.71333164
C	3.34975492	-1.64103242	-2.60980431
C	3.48350238	-1.37577714	1.88290285
C	3.04998898	-0.58168616	2.96636008
C	3.57680496	-0.75957994	4.25118389
C	4.54639713	-1.7466967	4.48028282
C	4.97987632	-2.55401873	3.42061471
C	4.45044601	-2.36887739	2.13551041
C	-0.56160572	3.98785776	-1.51188896
C	-0.11696126	3.49120357	-2.75702166
C	-0.23870297	4.25035671	-3.92739998
C	-0.81679667	5.52763219	-3.87585614
C	-1.27614341	6.0333544	-2.65278209
C	-1.14979682	5.26830109	-1.48400108
C	-0.60281124	3.82955509	1.69892064
C	-0.19561879	5.17038111	1.84571304
C	-0.3318209	5.8391364	3.07052791
C	-0.87822574	5.17371791	4.17562144
C	-1.28023759	3.83574068	4.05264651
C	-1.13849328	3.17290491	2.8274856
C	-3.21724272	-2.50630561	-1.45453436
C	-4.51895552	-3.04295658	-1.39093494
C	-5.17297947	-3.49622273	-2.54609051
C	-4.53605449	-3.41632688	-3.79129714
C	-3.24591171	-2.87185601	-3.87883565
C	-2.59909741	-2.42092336	-2.72178708
C	-3.05066348	-2.33596331	1.75935821
C	-2.93771034	-1.47126119	2.86915846
C	-3.47182578	-1.8173469	4.11616329
C	-4.12620017	-3.04676974	4.28089598
C	-4.23714076	-3.92498848	3.19527691
C	-3.70226965	-3.57082561	1.94855923
C	-4.00199551	1.50103905	-2.13555029
C	-3.95753655	3.11882296	0.24301417
C	-5.01295487	0.47819949	0.35497336
C	0.68944469	-4.41180802	-2.07829757
C	-0.74542111	-4.99215673	0.32012651
C	2.08964742	-4.59242002	0.40612935
C	3.72009165	2.34500361	-2.03925359
C	2.91432642	4.12634744	0.05661224
C	4.61795658	1.9180114	0.65184199
H	5.72875452	-1.50806169	-0.16343708
H	7.19346814	-1.95692831	-2.114339
H	6.20895821	-2.20761965	-4.39441725
H	3.73975562	-1.98571604	-4.71213998
H	2.267748	-1.5252508	-2.74413614
H	2.28528331	0.18208061	2.78234162
H	3.22862333	-0.13179462	5.07586887
H	4.95933738	-1.88885315	5.48214596
H	5.72971122	-3.33045894	3.59490736
H	4.79190561	-3.01645308	1.32191588
H	0.32027329	2.4862354	-2.79288086
H	0.11204539	3.84636593	-4.88107584
H	-0.91322651	6.12356726	-4.7868369
H	-1.73558797	7.02452439	-2.60873288
H	-1.52325179	5.67387418	-0.53862278
H	0.24247884	5.7011783	0.99466428
H	-0.01010434	6.88005292	3.16242313
H	-0.98734377	5.69428709	5.13032932
H	-1.70090037	3.30939392	4.9138289
H	-1.44324567	2.12436491	2.72654587
H	-5.03687906	-3.0996451	-0.42873158
H	-6.18258661	-3.90966257	-2.47402716
H	-5.04472818	-3.77033063	-4.69141058
H	-2.74862914	-2.79527236	-4.84967848
H	-1.59685623	-1.98040965	-2.78481324
H	-2.41769444	-0.51511678	2.73561391
H	-3.37480474	-1.13131745	4.96204303
H	-4.54406922	-3.32065332	5.25286137
H	-4.73935916	-4.88821697	3.31937896
H	-3.78840002	-4.27462411	1.11502345
H	-3.27074538	2.14908437	-2.63950128
H	-5.01778025	1.89956291	-2.2849149
H	-3.93051435	0.49244838	-2.56735917
H	-5.01049457	3.37611645	0.04710669
H	-3.3041679	3.83468514	-0.27616357
H	-3.75468468	3.19051019	1.32080315
H	-5.95756579	1.00936746	0.15794676
H	-4.87834445	0.35383831	1.43856077
H	-5.05465163	-0.52147722	-0.10085512
H	-0.22963702	-4.1350366	-2.61303854
H	0.82963645	-5.50310884	-2.1293843
H	1.54279215	-3.91069293	-2.55549591
H	-0.93650257	-4.77658951	1.38055744
H	-0.44920359	-6.04645	0.20112937
H	-1.67477864	-4.8083622	-0.24045095
H	2.10032308	-5.68720606	0.28483054
H	2.15343075	-4.33540897	1.47261829
H	2.96437263	-4.15999251	-0.10324322
H	2.93148973	2.72849049	-2.70168325
H	3.96657671	1.3183192	-2.34438205
H	4.61299583	2.98418241	-2.12422504
H	2.60354485	4.25967563	1.10257395
H	2.13148099	4.54715322	-0.5921121
H	3.86219165	4.66017053	-0.11713504
H	5.4015103	2.67202888	0.47662414
H	4.98643661	0.92872833	0.3436923
H	4.38056384	1.87247502	1.72374729

(b) [{Pt(PMe_3)}$_3$(μ-CO)$_3$].

atom	x	y	z
Pt	-1.07821383	1.13823713	0.00338738
Pt	1.53642546	0.41948784	0.0061117
Pt	-0.39116257	-1.49380325	0.00500865
P	-2.7445334	2.69542139	0.08562992
P	3.76667413	0.89824234	0.0924222
P	-1.09574583	-3.66256448	0.07436591
C	4.27536089	2.66978592	0.16965041
H	3.85413553	3.1240823	1.07745781
C	4.72945129	0.25333555	-1.34484022
H	4.36942689	0.7318692	-2.26598269
C	4.66813912	0.15073584	1.521515
H	4.52384488	-0.9387162	1.4932647
C	-2.19451059	-4.07940514	1.49992894
H	-1.6526259	-3.91175144	2.44082832
C	0.18048986	-4.992674	0.13844633
H	0.77882979	-4.87083474	1.05226523
C	-2.13871996	-4.15386299	-1.36744485
H	-2.98091739	-3.45053963	-1.43734887
C	-2.26763641	4.47656506	0.13300487
H	-1.65797294	4.65997463	1.02890384
C	-3.91869114	2.6166396	-1.3367839
H	-4.31678718	1.59368088	-1.39749098
C	-3.88435319	2.53729528	1.53107475
H	-4.32213771	1.52893757	1.5212067
C	0.64860089	2.29173673	-0.19891407
C	-2.25157988	-0.57049276	-0.16110216
C	1.6700704	-1.65930265	-0.17395747
O	0.95916803	3.41035953	-0.47491566
O	2.50628411	-2.47604424	-0.42320009
O	-3.38845601	-0.86519056	-0.39310363
H	5.74425296	0.38068625	1.48395913
H	4.24370637	0.53089449	2.46088122
H	5.80756007	0.44343611	-1.22755728
H	4.54786163	-0.82803372	-1.42320526
H	5.37083829	2.7765487	0.1771927
H	3.85493496	3.20070866	-0.69547453
H	-0.27703563	-5.99367626	0.12764004
H	0.85642901	-4.88209877	-0.72064314
H	-3.06433835	-3.40753904	1.4777012
H	-2.53598734	-5.12508814	1.4529377
H	-2.5182922	-5.18185544	-1.26091778
H	-1.54476714	-4.07434709	-2.28831635
H	-3.31296039	2.65639337	2.46186728
H	-4.68880545	3.28814643	1.49410021
H	-4.74622283	3.33325425	-1.21906811
H	-3.37544855	2.8315704	-2.26727446
H	-3.15145791	5.1324332	0.14630508
H	-1.64751079	4.70434406	-0.74481531

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