Supporting Information

γ-Selective Cross-Coupling Reactions of Potassium Allyltrifluoroborates with Haloarenes Catalyzed by a Pd(0)/D-*t*-BPF or Pd(0)/Josiphos ((*R*,*S*)-CyPF-*t*-Bu) Complex: Mechanistic Studies on Transmetalation and Enantioselection

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Instruments

All experiments were carried out under a nitrogen atmosphere. NMR spectra were recorded on a JOEL JNM-A400II (400 MHz) spectrometer. The chemical shifts are reported in ppm (δ) downfield from tetramethylsilane (δ=0 ppm), residual chloroform (δ=7.26 ppm) or residual acetonitrile (δ=1.93 ppm). The signal patterns are indicated as s, singlet; d, doublet; t, triplet; q, quartet; p, pentet; m, multiplet; br s, broad singlet. The coupling constants (*J*) are given in hertz. The ^{13}C NMR spectra were recorded on either a JOEL JNM-A400II (100 MHz) spectrometer. The chemical shifts are reported in δ (ppm) downfield from tetramethylsilane (δ=0 ppm) or residual chloroform (δ=77 ppm). GC analyses were performed on either a Hitachi G-3500 instrument equipped with a glass column (OV-17 on Uniport B, 2 m). Mass spectra were obtained with a Finnigan ITD 800 for the GC-MS analysis and JEOL HX110 and JEOL FABmate for the high-resolution analysis. X–ray analysis was performed using Rigaku R–AXIS RAPID–F. HPLC analysis was directly performed with chiral stationary phase column, Daicel Chiralpak OJ-H purchased from Dicel Co., Ltd.

Regents

Pottasium allyltrifluoroborate: Potassium 2-propenyltrifluoroborate, potassium (*E*)-2-butenyltrifluoroborate, potassium (*Z*)-2-butenyltrifluoroborate, potassium (*E*)-cinnamyltrifluoroborate, were synthesized by reported procedures[1]. Potassium Potassium 3-methyl-2-pentenyltrifluoroborate[2], Potassium 3-methyl-2-heputenyltrifluoroborate[2], and 1-methyl-2-propenyltrifluoroborate.[3-5]were synthesized from the corresponding boronates and KHF_2[6].

Potassium (*E*)-2-butenyltrifluoroborate, **(*E*)-CH_3CH=$CHCH_2BF_3K$** (**2a**): ^{1}H NMR (400 MHz, CD_3CN): 5.55-5.44 (m, 1H), 5.15-5.02 (m, 1H), 1.55 (dq, *J* = 6.5, 1.4 Hz, 3H), 0.98 (br s, 2H); ^{13}C

NMR (100 MHz, CD_3CN): 133.62, 120.13, 12.85; ^{11}B NMR (128 MHz, CD_3CN): 4.94 (q, J = 58.4 Hz); MS m/z (%): 123 (100), 122 (M^+-K^+, 27); HRMS m/z: calcd. for $C_4H_7BF_3$ 123.0593, found 123.0581; Purification by recrystallization from acetonitrile.

Potassium (*Z*)-2-butenyltrifluoroborate, **(*Z*)-$CH_3CH=CHCH_2BF_3K$** (**2b**): ^1H NMR (400 MHz, CD_3CN): 5.64-5.46 (m, 1H), 5.22-5.09 (m, 1H), 1.55 (dd, J = 6.6, 1.0 Hz, 3H), 1.01 (br s, 2H); ^{13}C NMR (100 MHz, CD_3CN): 133.61, 120.12, 12.84; ^{11}B NMR (128 MHz, CD_3CN): 4.99 (q, J = 58.3 Hz); MS m/z (%): 123 (100), 122 (M^+-K^+, 28); HRMS m/z: calcd. for $C_4H_7BF_3$ 123.0593, found 123.0589; Purification by recrystallization from acetonitrile.

Potassium (*E*)-cinnamyltrifluoroborate, **(*E*)-$PhCH=CHCH_2BF_3K$** (**2c**): To a solution of 1-phenyl-1-propene (50 mmol) in THF (50 ml) at -78°C was added potassium *tert*-butoxide (50 mmol). *n*-BuLi (2.6 M in hexanes, 50 mmol) was then added at a rate such that the internal temperature did not exceed -65°C. After the addition was complete, the internal temperature of the reaction mixture was allowed to rise to -50°C. The reaction mixture was stirred for 15 min at this temperature prior to being recooled to -78°C. Triisopropylborate was then added at rate such that the internal temperaturedid not rise above -65°C. The reaction mixture was stirred for an additional 1 h and then rapidly poured into a separatory funnel containing 1N HCl (100 ml) saturated with NaCl. The layers were separated and the aqueous layer extracted with Et_2O (100ml × 3). The combined organic layers were dried ($MgSO_4$), filtered and concentrated in vacuo. The residual was added to a flask containing 80 ml of diethyl ether and $MgSO_4$. Piancol (150 mmol) was added, and the solution was allowed to stir at room temperature for 20h and filtered and concentrated in vacuo. The crude product was redissolved in MeOH (50 ml). KHF_2 (400 mmol, H_2O 5 ml) was then added, the reaction mixture stirred for 2h at room temperature, and subsequently stored at 4°C for 18h. The white precipitate was filtered off and recrystalized from acetonitrile/diethyl ether to afford 2c as white solid (64%).

^1H NMR (400 MHz, CD_3CN): 7.30-7.20 (m, 4H), 7.10-7.05 (m, 1H), 6.45 (dt, J = 15.9, 7.95 Hz, 1H), 6.11 (d, J = 15.9 Hz, 1H), 1.20 (br s, 2H); ^{13}C NMR (100 MHz, CD_3CN): 160.68, 136.62, 129.31, 126.36, 126.24, 126.00; ^{11}B NMR (128 MHz, CD_3CN): 6.11 (q, J = 57.0 Hz); MS m/z (%): 185 (M^+-K^+, 97), 184 (30), 183 (89), 117 (13); HRMS m/z: calcd. for $C_9H_9BF_3$ 185.0749, found 185.0742; Purification by recrystallization from acetonitrile/ether.

Potassium 3-methyl-2-pentenyltrifluoroborate, **(*E*)-$Et(Me)C=CHCH_2BF_3K$** (**2d**): ^1H NMR (400 MHz, CD_3CN): 5.57 (dt, J = 11.6, 2.0 Hz, 1H), 2.26 (q, J = 11.6 Hz , 2H), 1.84 (s, 3H), 1.26 (d, J = 11.2 Hz, 3H), 0.41 (br s, 2H); ^{13}C NMR (100 MHz, CD_3CN): 145.96, 125.45, 118.35, 33.29, 15.68, 13.53; ^{11}B NMR (128 MHz, CD_3CN): 7.97 (q, J = 56.8 Hz); MS m/z (%): 151 (M^+-K^+, 27), 91 (87),

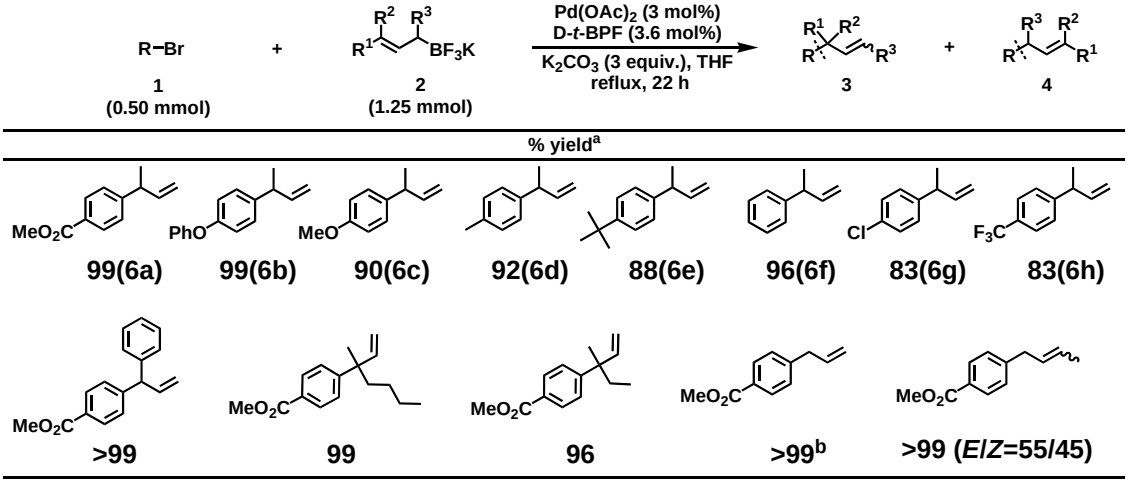
89 (20), 71 (15), 59 (23); HRMS m/z: calcd. for $C_6H_{11}BF_3$ 151.0906, found 151.0909; Purification by recrystallization from acetonitrile/ether.

Potassium 3-methyl-2-heptenyltrifluoroborate, **(*E*)-Bu(Me)C=CHCH$_2$BF$_3$K** (**2e**): ^{1}H NMR (400 MHz, CD_3CN): 5.21 (dt, *J* = 24.9, 7.3 Hz, 1H), 1.95-1.91 (m, 2H), 1.54 (d, *J* = 11.2, 1H), 1.38-1.21 (m, 4H), 0.88 (d, *J* = 7.3 Hz, 3H), 0.87 (br s, 2H); ^{13}C NMR (100 MHz, CD_3CN): 131.07, 127.40, 40.55, 31.39, 23.23, 15.76, 14.34; ^{11}B NMR (128 MHz, CD_3CN): 6.50 (q, *J* = 65.3 Hz); MS m/z (%): 179 (M^+, 100), 178 (30), 137 (12); HRMS m/z: calcd. for $C_8H_{15}BF_3$ 179.1219, found 179.1229.; Purification by recrystallization from acetonitrile.

Potassium 2-propenyltrifluoroborate, **CH$_2$=CHCH$_2$BF$_3$K** (**2f**)
^{1}H NMR (400 MHz, CD_3CN): 6.00-5.88 (m, 1H), 4.75 (d, *J* = 17.2 Hz, 1H), 4.64 (d, *J* = 9.9 Hz, 1H), 1.12 (br s, 2H); ^{13}C NMR (100 MHz, CD_3CN): 142.81, 112.10; ^{11}B NMR (128 MHz, CD_3CN): 4.99 (q, *J* = 58.5 Hz); MS m/z (%): 109 (M^+-K^+, 67); HRMS m/z: calcd. for $C_3H_5BF_3$ 109.0436, found 109.0428; Purification by recrystallization from acetonitrile.

Potassium 3-methyl-2-heptenyltrifluoroborate, **CH$_2$=CHCH(CH$_3$)BF$_3$K** (**2g**): ^{1}H NMR (400 MHz, CD_3CN): 6.09-6.01 (m, 1H), 4.71-4.63 (m, 2H), 2.24 (br s, 1H), 0.87 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, CD_3CN): 149.07, 118.35, 107.37; ^{11}B NMR (128 MHz, CD_3CN): 11.97 (q, *J* = 61.0 Hz); MS m/z (%): 123 (100), 122 (M^+-K^+, 27); HRMS m/z: calcd. for $C_4H_7BF_3$ 123.0593, found 123.0583; Purification by recrystallization from acetonitrile.

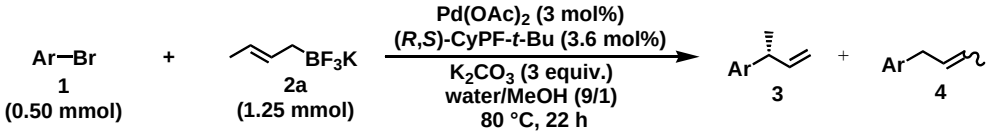
General Procedure for γ-selective cross-coupling (Table 1). A 20 ml flask charged with palladium acetate (0.015 mmol, 3 mol%), 1,1'-bis(di-*tert*-butylphosphino)ferrocene (D-*t*-BPF) (0.018 mmol), potassium allyltrifluoroborates (1.25 mmol), K_2CO_3 (1.5 mmol) was flush with nitrogen. THF (5 ml) and bromoarene (0.5 mmol) were added successively. After being reflux for 22 h, the reaction mixture was treated with 1N HCl (10 ml) at room temperature. Flash chromatography on silica gel gave the coupling product.

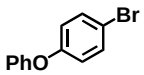
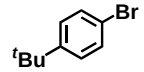
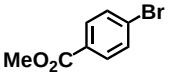
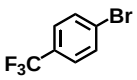


[a] Isolated yield. [b] Walphos was used as ligand.

Table S1. γ-selective cross-coupling of **2**

General procedure for asymmetric cross-coupling (Table 2). A flask charged with potassium (*E*)-2-butenyltrifluoroborate (2.5 mmol), $Pd(OAc)_2$ (3 mol%), 1-dicyclohexylphosphino-2-di-*tert*-butylphosphinoethylferrocene (CyPF-t-Bu) (3.6 mol %) and K_2CO_3 (3.0 mmol) was flushed with nitrogen. H_2O/MeOH (9/1, 5 mL) and bromoarene (1.0 mmol) were then added. The resulting mixture was stirred at 80 °C for 22 h. Isolated yields determined by chromatography on silica gel are shown in Table 2. Enantiomer excess was determined by a chiral stationary column. The absolute configuration was established to be *R* by the specific rotation reported and retention times of two enantiomers in HPLC analysis.[7]



halide	% yield[a]	3/4	%ee of 3
	99 (6b)	84/16	79
	86 (6e)	84/16	86
	93 (6a)	93/7	82 (*R*)
	73 (6h)	90/10	90

[a] Isolated yields.

Table S2. Asymmetric cross-coupling giving **3**

(*R*)-methyl 4-(1-methyl-2-propenyl)benzoate, (4-$MeO_2CC_6H_4$)$CH(CH_3)CH=CH_2$ (**6a**): ^{1}H NMR (400 MHz, $CDCl_3$): 7.97 (dt, *J* = 10.3, 1.9 Hz, 2H), 7.27 (dt, *J* = 10.3, 1.9 Hz, 2H), 6.01 (ddd, *J* = 17.5, 9.8, 6.3 Hz, 1H), 5.06 (dt, *J* = 17.5, 1.4 Hz, 1H), 5.05 (dt, *J* = 9.9, 1.4 Hz, 1H), 3.89 (s, 3H), 3.51 (quin, *J* = 6.8 Hz, 1H), 1.37 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 167.01, 150.87, 142.22, 129.73, 128.04, 127.23, 113.81, 51.91, 43.13, 20.47; MS m/z (%): 190 (M^+, 29), 175 (11), 159 (45), 145 (17), 131 (100), 128 (15), 116 (25), 114 (17), 91 (24); HRMS m/z: calcd. for $C_{12}H_{14}O_2$ 190.0994, found 190.0986; $[\alpha]_D^{23}$: −12.68 (c 0.59, benzene); Purification by silica gel column chromatography (hexane/AcOEt = 15/1); The ee was determined by HPLC on a chiral stationary phase (Daicel Chiralpak OJ-H, hexane/isopropanol = 99.5/0.5, 0.50 mL/min, tR = 31.9, 39.2).

1-(1-methyl-2-propenyl)-4-phenoxybenzene, (4-$PhOC_6H_4$)$CH(CH_3)CH=CH_2$ (**6b**): ^{1}H NMR (400 MHz, $CDCl_3$): 7.28 (t, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.6 Hz, 2H), 7.04 (d, *J* = 7.5 Hz, 1H), 6.98 (d, *J* = 7.9 Hz, 2H), 6.94 (d, *J* = 8.7 Hz, 2H), 5.98 (ddd, *J* = 17.0, 10.4, 6.6 Hz, 1H), 5.04 (dt, *J* = 17.0, 1.5 Hz, 1H), 5.02 (dt, *J* = 10.4, 1.5 Hz, 1H), 3.44 (quin, *J* = 6.8 Hz, 1H), 1.34 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 157.53, 155.30, 143.24, 140.42, 129.62, 128.40, 122.92, 118.93, 118.56, 113.07, 42.46, 20.79; MS m/z (%): 224 (M^+, 100), 209 (58), 131 (55), 116 (63), 91 (18), 77 (18); HRMS m/z: calcd. for $C_{16}H_{16}O$ 224.1201, found 224.1188; $[\alpha]_D^{23}$: −9.46 (c 0.56, benzene); Purification by silica gel column chromatography (hexane/AcOEt = 15/1); The ee was determined by HPLC on a chiral stationary phase (Daicel Chiralpak OJ-H, hexane/isopropanol = 99.5/0.5, 0.50 mL/min, tR = 16.5, 18.0).

1-(1-methyl-2-propenyl)-4-methoxybenzene, (4-$MeOC_6H_4$)$CH(CH_3)CH=CH_2$ (**6c**): ^{1}H NMR (400 MHz, $CDCl_3$): 7.12 (d, *J* = 8.8 Hz, 2H), 6.84 (d, J = 8.8 Hz, 2H), 5.97 (ddd, J = 16.8, 10.5, 6.3 Hz, 1H), 5.03 (dt, *J* = 17.2, 1.6 Hz, 1H), 5.02 (ddd, *J* = 10.9, 1.6 Hz, 1H), 3.76 (s, 3H), 3.41 (quin, *J* = 6.8 Hz, 1H), 1.33 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 157.88, 143.55, 137.59, 128.07, 113.72, 112.73, 55.16, 42.27, 20.79; MS m/z (%): 162 (M^+, 100), 147 (97), 145 (16), 131 (21), 121 (24), 119 (12), 117 (12), 91 (16); HRMS m/z: calcd. for $C_{11}H_{14}O$ 162.1045, found 162.1044; Purification by silica gel column chromatography (hexane/AcOEt = 15/1); The ee was determined by HPLC on a chiral stationary phase (Daicel Chiralpak OJ-H, hexane/isopropanol = 99.5/0.5, 0.50 mL/min, tR = 13.8, 15.2).

1-(1-methyl-2-propenyl)-4-methylbenzene, (4-MeC_6H_4)$CH(CH_3)CH=CH_2$ (**6d**): ^{1}H NMR (400 MHz, $CDCl_3$): 7.11 (s, 4H), 5.99 (ddd, *J* = 17.1, 10.1, 6.3 Hz, 1H), 5.04 (dt, *J* = 17.1, 1.4 Hz, 1H), 5.01 (dt, *J* = 9.9, 1.5 Hz, 1H), 3.43 (quin, *J* = 6.6 Hz, 1H), 2.31 (s, 3H), 1.34 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 143.44, 142.55, 135.57, 129.08, 127.07, 112.86, 42.74, 20.97, 20.76; MS m/z (%): 146 (M^+, 29), 132 (13), 131 (100), 129 (10), 116 (17), 115 (16), 91 (24); HRMS m/z: calcd.

for $C_{11}H_{14}$ 146.1096, found 146.1096.; Purification by silica gel column chromatography (hexane/AcOEt = 15/1).

1-(1-methyl-2-propenyl)-4-*tert*-butylbenzene, (4-*t*-BuC_6H_4)CH(CH_3)CH=CH_2 (**6e**): ^{1}H NMR (400 MHz, $CDCl_3$): 7.32 (d, *J* = 8.3 Hz, 2H), 7.14 (d, *J* = 8.3 Hz, 2H), 6.00 (ddd, *J* = 16.9, 10.3, 6.5 Hz, 1H), 5.05 (dt, *J* = 17.0, 1.5 Hz, 1H), 5.01 (dt, *J* = 10.3, 1.5 Hz, 1H), 3.44 (quin, *J* = 6.7 Hz, 1H), 1.35 (d, *J* = 7.0 Hz, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): 148.81, 143.46, 142.44, 126.80, 125.26, 112.86, 42.69, 34.34, 31.41, 20.68; MS m/z (%): 188 (M+, 27), 173 (100), 131 (36), 55 (16); HRMS m/z: calcd. for $C_{14}H_{20}$ 188.1565, found 188.1570; $[\alpha]_D^{23}$: −9.59 (c 0.57, benzene); Purification by silica gel column chromatography (hexane only); The ee was determined by HPLC on a chiral stationary phase (Daicel Chiralpak OJ-H, hexane only, 0.50 mL/min, tR = 12.3, 13.6).

1-(1-methyl-2-propenyl)benzene, C_6H_5CH(CH_3)CH=CH_2 (**6f**): ^{1}H NMR (400 MHz, $CDCl_3$): 7.32-7.24 (m, 2H), 7.21-7.17 (m, 3H), 6.01 (ddd, *J* = 17.1, 10.5, 6.8 Hz, 1H), 5.05 (dt, *J* = 17.1, 1.5 Hz, 1H), 5.04 (dt, *J* = 10.4, 1.5 Hz, 1H), 3.47 (quin, *J* = 6.8 Hz, 1H), 1.36 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 159.69, 143.22, 128.39, 127.21, 126.09, 113.08, 43.15, 20.71; MS m/z (%): 132 (M^+, 48), 131 (23), 118 (14), 117 (100), 116 (15), 115 (53), 105 (12), 91 (29), 77 (15); HRMS m/z: calcd. for $C_{10}H_{12}$ 132.0939, found 132.0935; Purification by silica gel column chromatography (hexane only).

1-(1-methyl-2-propenyl)-4-chlorobenzene, (4-ClC_6H_4)CH(CH_3)CH=CH_2 (**6g**): ^{1}H NMR (400 MHz, $CDCl_3$): 7.26 (dt, *J* = 8.6, 1.8 Hz, 2H), 7.14 (dt, *J* = 8.8, 2.0 Hz, 2H), 5.95 (ddd, *J* = 17.3, 11.1, 6.3 Hz, 1H), 5.04 (dt, *J* = 17.4, 1.5 Hz, 1H), 5.03 (dt, *J* = 11.2, 1.5 Hz, 1H), 3.44 (quin, *J* = 6.8 Hz, 1H), 1.34 (d, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 143.94, 142.67, 131.74, 128.60, 128.45, 113.53, 42.51, 20.64; MS m/z (%): 166 (M^+, 25), 153 (15), 151 (52), 131 (100), 116 (54), 115 (62), 103 (19), 91 (18); HRMS m/z: calcd. for $C_{10}H_{11}Cl$ 166.0549, found 166.0545.; Purification by silica gel column chromatography (hexane/AcOEt = 15/1).

1-(1-methyl-2-propenyl)-4-(trifluoromethyl)benzene, (4-$CF_3C_6H_4$CH(CH_3)- CH=CH_2 (**6h**): ^{1}H NMR (400 MHz, $CDCl_3$): 7.55 (d, *J* = 8.1 Hz, 2H), 7.32 (d, *J* = 8.1 Hz, 2H), 5.97 (ddd, *J* = 17.8, 9.5, 6.3 Hz, 1H), 5.05 (dt, *J* = 17.8, 1.5 Hz, 1H), 5.04 (dt, *J* = 9.7, 1.5 Hz, 1H), 3.52 (quin, *J* = 6.8 Hz, 1H), 1.37 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 149.60, 142.18, 127.60, 125.70, 125.34, 122.96, 114.01, 43.02, 20.56; MS m/z (%): 200 (M^+, 40), 185 (30), 181 (59), 173 (19), 165 (45), 164 (19), 133 (16), 131 (100), 116 (14), 115 (19); HRMS m/z: calcd. for $C_{11}H_{11}F_3$ 200.0813, found 200.0817; $[\alpha]_D^{23}$: −6.65 (c 0.81, benzene); Purification by silica gel column chromatography (hexane only); The ee was determined by HPLC on a chiral stationary phase (Daicel Chiralpak OJ-H,

hexane only, 0.50 mL/min, tR = 28.9, 31.5).

methyl 4-(1-phenyl-2-propenyl)benzoate, 4-$MeO_2CC_6H_4CH(Ph)CH=CH_2$: ^{1}H NMR (400 MHz, $CDCl_3$): 7.97 (dt, *J* = 8.5, 1.8 Hz, 2H), 7.32-7.20 (m, 5H), 7.17 (dt, *J* = 8.6, 1.8 Hz, 2H), 6.29 (ddd, *J* = 17.1, 10.1, 7.3 Hz, 1H), 5.26 (dt, *J* = 10.1, 1.3 Hz, 1H), 5.00 (dt, *J* = 17.1, 1.5 Hz, 1H), 4.78 (d, *J* = 6.8 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, CDCl3): 167.01, 148.58, 142.41, 139.75, 129.70, 128.61, 128.50, 128.23, 126.60, 116.98, 54.85, 52.01; MS m/z (%): 252 (M^+, 48), 221 (17), 194 (17), 193 (100), 192 (12), 191 (12), 178 (28), 165 (28), 117 (11), 116 (13), 115 (60), 91 (14); HRMS m/z: calcd. for $C_{17}H_{16}O_2$ 252.1150, found 252.1158; Purification by silica gel column chromatography (hexane/AcOEt = 10/1).

methyl 4-(3-methyl-1-hepten-3-yl)benzoate, 4-$MeO_2CC_6H_4C(Me)(Bu)CH=CH_2$: ^{1}H NMR (400 MHz, $CDCl_3$): 7.96 (dt, *J* = 8.3, 2.0 Hz, 2H), 7.38 (dt, *J* = 8.6, 1.8 Hz, 2H), 6.01 (dd, *J* = 17.3, 10.7 Hz, 1H), 5.12 (dd, *J* = 10.7, 1.0 Hz, 1H), 5.04 (dd, *J* = 17.1, 1.0 Hz, 1H), 3.90 (s, 3H), 1.38 (s, 3H), 1.27 (t, *J* = 7.3 Hz, 2H), 1.15-0.88 (m, 4H), 0.84 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 167.12, 153.21, 146.36, 129.35, 128.66, 126.70, 112.21, 51.96, 44.59, 40.81, 26.60, 24.84, 23.32, 14.00; MS m/z (%): 246 (M^+, 22), 190 (22), 189 (100), 187 (12), 176 (18), 157 (29), 145 (52), 143 (10), 131 (27), 130 (44), 129 (52), 128 (26), 117 (15), 115 (36), 105 (21), 91 (16); HRMS m/z: calcd. for $C_{18}H_{22}O_2$ 246.1620, found 246.1628; Purification by silica gel column chromatography (hexane/AcOEt = 10/1).

methyl 4-(3-methyl-1-penten-3-yl)benzoate, 4-$MeO_2CC_6H_4C(Me)(Et)CH=CH_2$: ^{1}H NMR (400 MHz, $CDCl_3$): 7.96 (dt, *J* = 8.5, 2.1 Hz, 2H), 7.38 (dt, *J* = 8.8, 2.0 Hz, 2H), 6.01 (dd, *J* = 17.5, 10.7 Hz, 1H), 5.14 (dd, *J* = 10.7, 1.5 Hz, 1H), 5.05 (dd, *J* = 17.4, 1.3 Hz, 1H), 1.84 (q, *J* = 7.5 Hz, 2H), 1.36 (s, 3H), 0.75 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 167.12, 152.93, 146.06, 129.34, 128.30, 126.79, 112.45, 51.95, 44.86, 33.37, 24.23, 8.80; MS m/z (%): 218 (M^+, 32), 190 (17), 189 (100), 187 (15), 159 (28), 158 (10), 157 (40), 145 (57), 143 (15), 131 (22), 130 (65), 129 (69), 128 (38), 127 (13), 117 (28), 116 (12), 115 (54), 195 (36), 103 (11), 91 (26), 77 (19); HRMS m/z: calcd. for $C_{14}H_{18}O_2$ 218.1307, found 218.1305; Purification by silica gel column chromatography (hexane/AcOEt = 15/1).

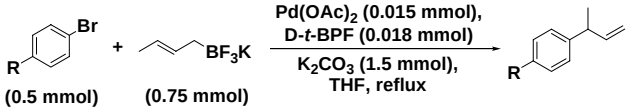
4-allylbenzoic acid methyl ester, 4-$MeO_2CC_6H_4CH_2CH=CH_2$: ^{1}H NMR (400 MHz, $CDCl_3$): 7.97 (d, *J* = 8.3 Hz, 2H), 7.26 (d, *J* = 7.8 Hz, 2H), 5.96 (ddt, *J* = 17.1, 10.1, 6.3

Hz, 1H), 5.11 (d, *J* = 9.9 Hz, 1H), 5.09 (d, *J* = 17.2 Hz, 1H), 3.90 (s, 3H), 3.44 (d, *J* = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 167.06, 145.46, 136.37, 129.73, 128.58, 128.04, 116.56, 51.98, 40.11; MS m/z (%): 176 (M^+, 55), 146 (11), 145 (100), 118 (11), 117 (92), 116 (18), 115 (60), 91 (27), 89 (12), 63 (11); HRMS m/z: calcd. for $C_{11}H_{12}O_2$ 176.0837, found 176.0839; Silica gel column chromatography (hexane/AcOEt = 15/1).

methyl 4-(2-butenyl)benzoate, 4-$MeO_2CC_6H_4CH_2CH$=$CHCH_3$ (E/Z = 55/45): ^{1}H NMR (400 MHz, $CDCl_3$): 7.96 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 5.64-5.51 (m, 2H), 3.90 (s, 3H), 3.45 (d, *J* = 6.6 Hz, 0.9H), 3.36 (d, *J* = 4.3 Hz, 1.1H), 1.74-1.69 (m, 3H).; MS m/z (%): 190 (M^+, 47), 175 (7), 159 (34), 132 (11), 131 (100), 129 (15), 116 (24), 115 (26), 91 (37), 77 (11); HRMS m/z: calcd. for $C_{12}H_{14}O_2$ 190.0994, found 190.0999.; Purification by silica gel column chromatography (hexane/AcOEt = 15/1).

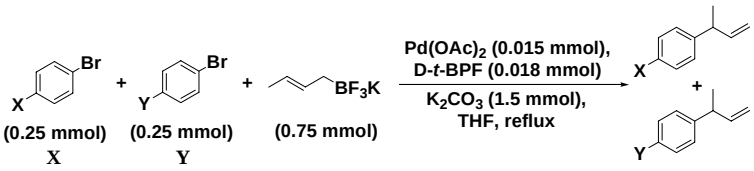
Kinetic measurement of coupling between potassium allyltrifluoroborates and *p*-substituted bromoarenes (Scheme 3): To a solution of $Pd(OAc)_2$ (0.015 mmol), D-*t*-BPF (0.018 mmol), potassium (E)-2-butenyltrifluoroborate (0.75 mmol), and K_2CO_3 (1.5 mmol) in THF (7 ml) was added *p*-substituted bromoarene (0.5 mmol) (*p*-$PhOC_6H_4Br$, *p*-MeC_6H_4Br, PhBr, *p*-ClC_6H_4Br or *p*-$CF_3C_6H_4Br$). The mixture was stirred at 75 ˚C. The reaction progress was followed by GC analysis of the coupling product.

Competitive reactions using Pd(D-t-BPF)(Ar)(Br) or Pd(CyPF-t-Bu)(Ar)(Br) (Schemes 4 and 5): A 20 ml flask was charged with Pd(D-*t*-BPF)(Ph)(Br) (0.25 mmol), Pd(D-*t*-BPF)(Ar)(Br) (0.25 mmol Ar = *p*-$PhOC_6H_4$, *p*-ClC_6H_4, *p*-$CF_3C_6H_4$), potassium (*E*)-2-butenyltrifluoroborate (0.75 mmol), and K_2CO_3 (1.5 mmol) under nitrogen. THF (7 ml) was added and the resulting solution was heated to 75°C. The relative rate was estimated by GC analysis of coupling products (a sum of **6** and **7**).



R	σ_p	initial rate (mmol/min)	log (rate(X)/rate(H))
-OPh	-0.32	2.314	0.364
-Me	-0.17	1.536	0.186
-H	0.00	1.000	0.000
-Cl	0.23	0.547	-0.261
$-CF_3$	0.54	0.256	-0.592

Table S3. Kinetic Measurement of Cross-coupling Reaction

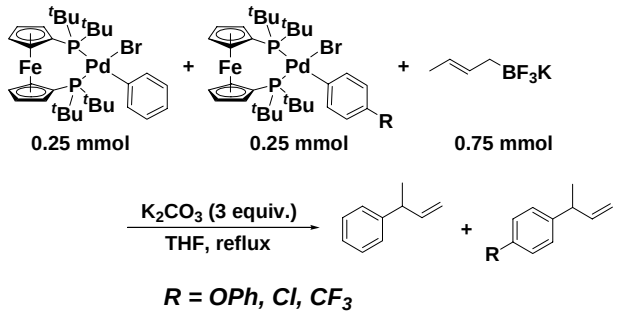


X	Y	time (min)	%conv.[a] X	%conv.[a] Y
-OPh	-Me	10	31	9
-OMe	-Me	80	19	9
-Me	-H	20	19	29
-Me	-*t*-Bu	20	33	27
-H	-Cl	180	13	26
-Cl	$-CF_3$	210	10	16

[a] GC conversions.

R	σ_p	Conv.(X)/Conv.(Y)	log (Conv.(X)/Conv.(Y))
-OPh	-0.32	2.2567	0.353
-OMe	-0.27	1.383	0.141
-^{t}Bu	-0.20	0.536	-0.184
-Me	-0.17	0.655	-0.271
-H	0.00	1.000	0.000
-Cl	0.23	2.000	0.301
$-CF_3$	0.54	3.200	0.505

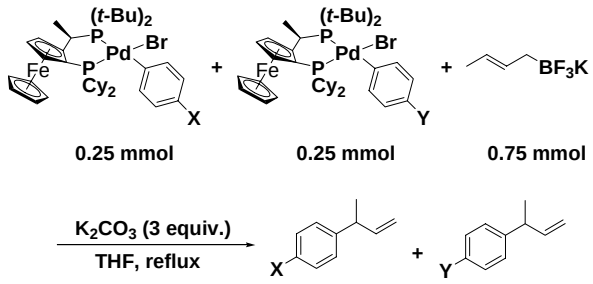
Table S4. Competitive Reactions of 4-Substituted Arylbromide



R = OPh, Cl, CF_3

R	σ_p	log (rate(X)/rate(H))
-OPh	-0.32	0.112
-H	0.00	0.000
-Cl	0.23	-0.120
$-CF_3$	0.54	-0.316

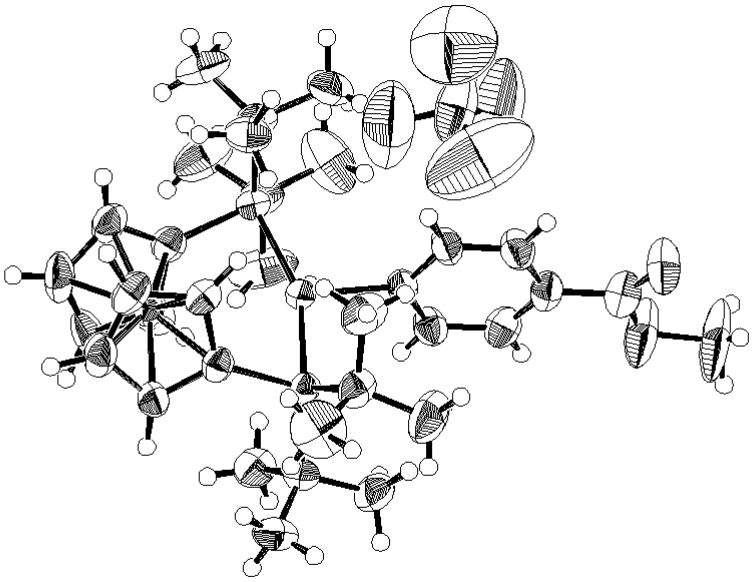
Table S5. Competitive Reactions of Pd(D-t-BPF)(Ar)(Br)



R	σ_p	log (rate(X)/rate(H))
-OPh	-0.32	0.2140
-H	0.00	0.000
-Cl	0.23	-0.120
$-CF_3$	0.54	-0.389

Table S6. Competitive Reactions of Pd(CyPF-t-Bu)(Ar)(Br)

X-ray Structure Report



(D-*t*-BPF)Pd(4-$MeO_2CC_6H_4$)(BF_4)

Experimental

Data Collection

A brown block crystal of $C_{34}H_{51}BF_4FeO_2P_2Pd$ having approximate dimensions of 0.50 x 0.40 x 0.30 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations that were exposed for 90 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 29.477(4) Å
b = 13.529(2) Å β = 39.089(5)°
c = 28.991(4) Å
V = 7289.9(18) Å^3

For Z = 8 and F.W. = 802.77, the calculated density is 1.463 g/cm^3. The systematic absences of:

h0l: l ± 2n
0k0: k ± 2n

uniquely determine the space group to be:

$P2_1/c$ (#14)

The data were collected at a temperature of 23 $\pm$ 1^{o}C to a maximum 2θ value of 55.0^{o}. A total of 44 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0^{o} in 5.0^{o} step, at χ=45.0^{o} and ϕ = 0.0^{o}. The exposure rate was 60.0 [sec./^{o}]. A second sweep was performed using ω scans from 0.0 to 160.0^{o} in 5.0^{o} step, at χ=45.0^{o} and ϕ = 180.0^{o}. The exposure rate was 60.0 [sec./^{o}]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 63791 reflections that were collected, 16670 were unique (R_{int} = 0.032); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 10.282 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.490 to 0.735. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction[1] was applied (coefficient = 0.000060).

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques[3]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[4] on F^2 was based on 16670 observed reflections and 813 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \; | \; |Fo| - |Fc| \; | \; / \Sigma \; |Fo| = 0.0578$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.2488$$

The standard deviation of an observation of unit weight[5] was 0.83. A Sheldrick

weighting scheme was used. The maximum and minimum peaks on the final difference Fourier map corresponded to 3.21 and -1.31 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10] crystallographic software package except for refinement, which was performed using SHELXL-97[11].

References

(1) Larson, A.C. (1970), Crystallographic Computing, 291-294. F.R. Ahmed, ed. Munksgaard, Copenhagen (equation 22, with V replaced by the cell volume).

(2) SIR97: Altomare, A., Burla, M., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A., Polidori, G., and Spagna, R. (1999). J. Appl. Cryst., 32, 115-119.

(3) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(4) Least Squares function minimized: (SHELXL97)

$$\Sigma w(F_o^2-F_c^2)^2 \qquad \text{where w = Least Squares weights.}$$

(5) Standard deviation of an observation of unit weight:

$$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations

N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(10) CrystalStructure 3.8: Crystal Structure Analysis Package, Rigaku and Rigaku Americas (2000-2007). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(11) SHELX97: Sheldrick, G.M. (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{34}H_{51}BF_4FeO_2P_2Pd$
Formula Weight	802.77
Crystal Color, Habit	brown, block
Crystal Dimensions	0.50 X 0.40 X 0.30 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 90.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 29.477(4) Å b = 13.529(2) Å c = 28.991(4) Å β = 39.089(5) ° V = 7289.9(18) $Å^3$
Space Group	$P2_1/c$ (#14)

Z value	8
D_{calc}	1.463 g/cm^3
F_{000}	3312.00
μ(MoKα)	10.282 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Detector Aperture	270 mm x 256 mm
Data Images	44 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0^{o}
Exposure Rate	60.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 160.0^{o}
Exposure Rate	60.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 63791 Unique: 16670 (R_{int} = 0.032)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.490 - 0.735) Secondary Extinction

(coefficient: 6.00000e-005)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR97)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	w = 1/ [$\sigma^2(Fo^2)$ + $(0.2500 \cdot P)^2$ + 6.0000 · P] where P = $(Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	16670
No. Variables	813
Reflection/Parameter Ratio	20.50
Residuals: R1 (I>2.00σ(I))	0.0578
Residuals: R (All reflections)	0.0727
Residuals: wR2 (All reflections)	0.2488
Goodness of Fit Indicator	0.830
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	3.21 $e^-/Å^3$

Minimum peak in Final Diff. Map	-1.31 $e^{-}/Å^{3}$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Pd(1)	1.119141(17)	0.15567(2)	0.310584(17)	3.000(10)
Pd(2)	0.648609(17)	0.18313(3)	0.549613(17)	3.046(10)
Fe(1)	1.26178(4)	0.09681(5)	0.15779(4)	4.236(16)
Fe(2)	0.50450(3)	0.22631(5)	0.70743(4)	3.377(14)
P(1)	1.19641(6)	0.21994(8)	0.30374(6)	3.153(19)
P(2)	1.07944(7)	0.07615(9)	0.27740(7)	3.39(2)
P(3)	0.57115(6)	0.12042(8)	0.55633(6)	3.043(18)
P(4)	0.68522(6)	0.25705(9)	0.58776(7)	3.36(2)
F(1)	0.8145(5)	-0.1740(7)	0.4537(4)	20.1(5)
F(2)	0.7305(8)	-0.2810(11)	0.4993(8)	24.9(6)
F(3)	0.7053(5)	-0.1650(8)	0.5701(4)	18.0(4)
F(4)	0.7706(6)	-0.2907(9)	0.5406(6)	19.2(4)
F(5)	0.4647(6)	-0.3331(8)	0.6362(7)	23.3(6)
F(6)	0.3825(9)	-0.3876(13)	0.6588(10)	27.4(7)
F(7)	0.4213(6)	-0.4839(8)	0.6756(5)	17.8(3)
F(8)	0.4902(9)	-0.4506(8)	0.5685(4)	33.6(11)
O(1)	0.8129(2)	0.3781(3)	0.6467(2)	5.92(9)
O(2)	0.8154(2)	0.2364(3)	0.6825(2)	6.14(10)
O(3)	0.9495(2)	-0.0208(4)	0.2017(2)	7.00(11)
O(4)	0.9459(3)	0.1304(4)	0.1748(2)	8.97(17)
C(1)	1.0251(2)	0.1965(3)	0.4138(2)	3.30(7)
C(2)	0.9938(2)	0.1368(3)	0.4715(2)	3.69(7)
C(3)	0.9331(2)	0.1679(3)	0.5429(2)	3.96(8)
C(4)	0.9040(2)	0.2612(3)	0.5566(2)	3.68(7)
C(5)	0.9340(2)	0.3191(3)	0.4993(2)	3.91(8)
C(6)	0.9948(2)	0.2871(3)	0.4277(2)	3.78(7)
C(7)	0.8400(2)	0.2996(4)	0.6321(3)	4.20(9)
C(8)	0.7515(4)	0.2675(8)	0.7567(3)	8.7(2)
C(9)	1.0174(2)	-0.0341(3)	0.3286(3)	4.14(8)
C(10)	0.9391(3)	-0.0003(6)	0.3935(4)	7.25(18)
C(11)	1.0353(3)	-0.0924(4)	0.3587(3)	5.40(12)

C(12)	1.0291(5)	-0.1017(5)	0.2777(5)	7.7(2)
C(13)	1.0606(3)	0.1604(4)	0.2431(3)	5.10(11)
C(14)	1.1141(4)	0.2467(4)	0.2046(3)	5.98(14)
C(15)	1.0659(5)	0.1122(6)	0.1918(5)	7.7(2)
C(16)	0.9827(4)	0.2035(6)	0.3112(4)	6.59(16)
C(17)	1.1975(2)	0.3546(3)	0.3179(2)	3.84(8)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(18)	1.1781(4)	0.4126(4)	0.2907(4)	6.03(14)
C(19)	1.1413(4)	0.3774(5)	0.3979(3)	7.36(19)
C(20)	1.2704(3)	0.3903(5)	0.2762(5)	7.4(2)
C(21)	1.2121(3)	0.1364(4)	0.3419(3)	4.48(9)
C(22)	1.1501(4)	0.1513(6)	0.4254(4)	6.76(17)
C(23)	1.2836(3)	0.1550(5)	0.3105(4)	6.16(15)
C(24)	1.2079(4)	0.0314(4)	0.3274(4)	6.16(15)
C(25)	1.1711(2)	0.0281(3)	0.1998(2)	3.96(8)
C(26)	1.2258(3)	0.0469(4)	0.1234(2)	4.81(10)
C(27)	1.2887(3)	-0.0031(4)	0.0870(3)	5.37(12)
C(28)	1.2753(2)	-0.0523(4)	0.1395(3)	5.07(11)
C(29)	1.2038(2)	-0.0316(3)	0.2086(2)	4.09(8)
C(30)	1.2687(2)	0.2006(3)	0.2058(2)	4.35(10)
C(31)	1.3289(2)	0.1361(5)	0.1595(3)	6.27(17)
C(32)	1.3644(4)	0.1441(7)	0.0883(3)	9.5(3)
C(33)	1.3292(6)	0.2113(6)	0.0900(4)	9.0(3)
C(34)	1.2672(4)	0.2462(4)	0.1625(3)	6.15(16)
C(35)	0.7428(2)	0.1498(3)	0.4445(2)	3.45(7)
C(36)	0.7712(2)	0.2149(3)	0.3899(2)	4.14(8)
C(37)	0.8317(3)	0.1861(4)	0.3163(3)	4.50(9)
C(38)	0.8621(2)	0.0944(4)	0.2975(2)	4.20(8)
C(39)	0.8344(2)	0.0321(4)	0.3530(3)	4.59(9)
C(40)	0.7761(2)	0.0587(4)	0.4253(2)	4.22(9)
C(41)	0.9231(3)	0.0599(4)	0.2210(3)	5.26(11)
C(42)	1.0058(6)	0.1068(9)	0.0977(4)	12.5(4)
C(43)	0.5486(2)	0.2077(3)	0.5263(2)	3.85(8)
C(44)	0.5469(3)	0.3123(4)	0.5477(3)	5.04(11)
C(45)	0.6099(3)	0.2064(5)	0.4425(3)	5.26(11)
C(46)	0.4776(3)	0.1860(5)	0.5576(4)	5.88(14)
C(47)	0.5712(3)	-0.0119(3)	0.5376(3)	4.46(9)
C(48)	0.6199(5)	-0.0268(5)	0.4581(4)	7.43(19)

C(49)	0.4937(4)	-0.0482(6)	0.5889(5)	8.3(2)
C(50)	0.5998(4)	-0.0737(4)	0.5546(4)	6.32(15)
C(51)	0.7436(3)	0.3717(4)	0.5435(3)	4.62(10)
C(52)	0.7247(5)	0.4344(6)	0.5174(5)	8.1(2)
C(53)	0.7323(5)	0.4326(5)	0.5947(5)	7.5(2)
C(54)	0.8220(4)	0.3448(6)	0.4781(5)	9.3(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(55)	0.7064(3)	0.1671(4)	0.6179(3)	4.51(9)
C(56)	0.6546(3)	0.0814(4)	0.6533(3)	5.17(11)
C(57)	0.7012(4)	0.2119(6)	0.6701(4)	6.40(16)
C(58)	0.7829(3)	0.1268(6)	0.5501(4)	6.64(16)
C(59)	0.5927(2)	0.2991(3)	0.6676(2)	3.86(8)
C(60)	0.5386(2)	0.2793(4)	0.7431(3)	4.68(10)
C(61)	0.4738(3)	0.3255(5)	0.7809(3)	5.67(14)
C(62)	0.4875(3)	0.3752(4)	0.7278(3)	5.53(13)
C(63)	0.5584(3)	0.3584(3)	0.6592(3)	4.32(9)
C(64)	0.5011(2)	0.1283(3)	0.6549(2)	3.40(7)
C(65)	0.5082(2)	0.0769(3)	0.6924(2)	3.73(7)
C(66)	0.4477(3)	0.0994(4)	0.7672(2)	4.75(10)
C(67)	0.4047(2)	0.1667(4)	0.7770(2)	4.72(10)
C(68)	0.4374(2)	0.1840(4)	0.7079(2)	3.86(8)
B(1)	0.7578(4)	-0.2289(5)	0.5143(3)	9.0(3)
B(2)	0.4453(7)	-0.4118(9)	0.6321(6)	11.1(4)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq}

atom	x	y	z	B_{eq}
H(1)	1.0137	0.0752	0.4623	4.42
H(2)	0.9117	0.1269	0.5816	4.75
H(3)	0.9136	0.3800	0.5083	4.69
H(4)	1.0151	0.3268	0.3889	4.53
H(5)	0.7646	0.3036	0.7736	10.47
H(6)	0.7237	0.2105	0.7871	10.47
H(7)	0.7235	0.3091	0.7589	10.47
H(8)	0.9340	0.0627	0.3826	8.70
H(9)	0.9255	0.0055	0.4361	8.70
H(10)	0.9087	-0.0479	0.4025	8.70
H(11)	0.9932	-0.1269	0.4023	6.49
H(12)	1.0510	-0.0475	0.3699	6.49
H(13)	1.0729	-0.1391	0.3227	6.49
H(14)	0.9965	-0.0832	0.2792	9.21
H(15)	1.0203	-0.1690	0.2934	9.21
H(16)	1.0777	-0.0951	0.2286	9.21
H(17)	1.1574	0.2242	0.1850	7.17
H(18)	1.0931	0.2988	0.2392	7.17
H(19)	1.1251	0.2709	0.1656	7.17
H(20)	1.1141	0.1189	0.1423	9.30
H(21)	1.0331	0.1439	0.1969	9.30
H(22)	1.0540	0.0434	0.2038	9.30
H(23)	0.9802	0.2682	0.2997	7.91
H(24)	0.9720	0.2077	0.3520	7.91
H(25)	0.9485	0.1608	0.3235	7.91
H(26)	1.1467	0.3739	0.2964	7.23
H(27)	1.2211	0.4282	0.2399	7.23
H(28)	1.1542	0.4726	0.3184	7.23
H(29)	1.1355	0.3215	0.4226	8.83
H(30)	1.0964	0.3915	0.4184	8.83
H(31)	1.1560	0.4338	0.4040	8.83

H(32)	1.3072	0.3520	0.2323	8.83
H(33)	1.2742	0.3828	0.3060	8.83
H(34)	1.2760	0.4587	0.2637	8.83
H(35)	1.1072	0.1699	0.4429	8.11
H(36)	1.1627	0.2026	0.4369	8.11
H(37)	1.1417	0.0909	0.4485	8.11

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(38)	1.3202	0.1131	0.2688	7.40
H(39)	1.2780	0.1406	0.3472	7.40
H(40)	1.2973	0.2230	0.2959	7.40
H(41)	1.2236	0.0297	0.2834	7.39
H(42)	1.1591	0.0085	0.3677	7.39
H(43)	1.2382	-0.0104	0.3217	7.39
H(44)	1.2201	0.0873	0.1000	5.77
H(45)	1.3340	-0.0045	0.0339	6.44
H(46)	1.3092	-0.0940	0.1297	6.08
H(47)	1.1799	-0.0556	0.2554	4.90
H(48)	1.3431	0.0936	0.1741	7.53
H(49)	1.4083	0.1088	0.0448	11.35
H(50)	1.3436	0.2315	0.0475	10.74
H(51)	1.2327	0.2956	0.1788	7.38
H(52)	0.7504	0.2767	0.4018	4.97
H(53)	0.8516	0.2303	0.2796	5.40
H(54)	0.8559	-0.0290	0.3409	5.51
H(55)	0.7587	0.0159	0.4615	5.07
H(56)	1.0500	0.1233	0.0780	15.03
H(57)	1.0018	0.1441	0.0727	15.03
H(58)	1.0052	0.0375	0.0911	15.03
H(59)	0.5810	0.3170	0.5456	6.05
H(60)	0.4995	0.3263	0.5966	6.05
H(61)	0.5591	0.3592	0.5145	6.05
H(62)	0.6446	0.2561	0.4229	6.31
H(63)	0.5909	0.2196	0.4273	6.31
H(64)	0.6325	0.1426	0.4248	6.31
H(65)	0.4570	0.2468	0.5632	7.06
H(66)	0.4450	0.1546	0.6045	7.06
H(67)	0.4864	0.1430	0.5250	7.06
H(68)	0.6384	-0.0930	0.4437	8.92

H(69)	0.6591	0.0193	0.4286	8.92
H(70)	0.5931	-0.0162	0.4513	8.92
H(71)	0.4950	-0.0991	0.5648	9.97
H(72)	0.4651	0.0061	0.6005	9.97
H(73)	0.4730	-0.0740	0.6331	9.97
H(74)	0.5884	-0.0422	0.5924	7.58

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(75)	0.6511	-0.0800	0.5113	7.58
H(76)	0.5782	-0.1381	0.5708	7.58
H(77)	0.7321	0.5028	0.5190	9.71
H(78)	0.6752	0.4240	0.5484	9.71
H(79)	0.7548	0.4166	0.4680	9.71
H(80)	0.6949	0.4801	0.6187	9.05
H(81)	0.7761	0.4664	0.5678	9.05
H(82)	0.7186	0.3904	0.6307	9.05
H(83)	0.8481	0.3988	0.4440	11.15
H(84)	0.8272	0.2872	0.4550	11.15
H(85)	0.8406	0.3314	0.4936	11.15
H(86)	0.6763	0.0223	0.6480	6.21
H(87)	0.6435	0.0726	0.6300	6.21
H(88)	0.6112	0.0951	0.7043	6.21
H(89)	0.6875	0.1616	0.7025	7.68
H(90)	0.6657	0.2635	0.6981	7.68
H(91)	0.7470	0.2389	0.6425	7.68
H(92)	0.8035	0.1095	0.5631	7.97
H(93)	0.8120	0.1765	0.5126	7.97
H(94)	0.7810	0.0692	0.5323	7.97
H(95)	0.5450	0.2394	0.7659	5.61
H(96)	0.4284	0.3253	0.8339	6.81
H(97)	0.4525	0.4143	0.7379	6.64
H(98)	0.5797	0.3700	0.6202	5.50
H(99)	0.5475	0.0323	0.6700	4.48
H(100)	0.4379	0.0737	0.8059	5.70
H(101)	0.3592	0.1950	0.8236	5.67
H(102)	0.4185	0.2274	0.6985	4.63

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pd(1)	0.0438(2)	0.0335(2)	0.0341(2)	-0.00147(12)	-0.02956(17)	-0.00030(11)
Pd(2)	0.0399(2)	0.0405(2)	0.0371(2)	0.00485(12)	-0.03033(18)	-0.00349(12)
Fe(1)	0.0548(4)	0.0413(3)	0.0344(3)	-0.0103(2)	-0.0268(3)	-0.0035(2)
Fe(2)	0.0423(3)	0.0428(3)	0.0394(3)	0.0045(2)	-0.0307(2)	-0.0086(2)
P(1)	0.0412(5)	0.0369(5)	0.0365(5)	-0.0025(4)	-0.0288(4)	-0.0008(4)
P(2)	0.0560(6)	0.0362(5)	0.0449(5)	-0.0002(4)	-0.0413(5)	-0.0020(4)
P(3)	0.0439(5)	0.0370(5)	0.0395(5)	0.0044(4)	-0.0336(4)	-0.0050(4)
P(4)	0.0466(5)	0.0451(6)	0.0461(5)	-0.0010(4)	-0.0386(5)	0.0018(4)
F(1)	0.242(10)	0.216(10)	0.105(5)	-0.082(8)	-0.083(6)	0.018(5)
F(2)	0.48(2)	0.286(16)	0.40(2)	-0.129(16)	-0.40(2)	0.069(14)
F(3)	0.171(7)	0.278(13)	0.121(6)	0.026(7)	-0.085(6)	-0.054(7)
F(4)	0.259(12)	0.224(11)	0.242(12)	-0.058(9)	-0.193(11)	0.082(9)
F(5)	0.204(10)	0.190(9)	0.285(14)	-0.042(7)	-0.137(10)	-0.080(9)
F(6)	0.41(2)	0.34(2)	0.49(2)	0.114(18)	-0.40(2)	-0.047(19)
F(7)	0.238(10)	0.223(11)	0.180(9)	-0.001(8)	-0.152(8)	0.028(8)
F(8)	0.45(2)	0.156(8)	0.075(4)	-0.046(11)	-0.054(8)	-0.009(5)
O(1)	0.071(2)	0.060(2)	0.062(2)	0.019(2)	-0.043(2)	-0.021(2)
O(2)	0.076(2)	0.089(3)	0.0412(19)	0.025(2)	-0.039(2)	-0.013(2)
O(3)	0.078(2)	0.085(3)	0.056(2)	0.017(2)	-0.040(2)	-0.023(2)
O(4)	0.127(4)	0.089(3)	0.039(2)	0.007(3)	-0.042(2)	-0.006(2)
C(1)	0.045(2)	0.038(2)	0.038(2)	0.0003(16)	-0.0306(18)	-0.0019(16)
C(2)	0.050(2)	0.038(2)	0.043(2)	0.0062(18)	-0.034(2)	-0.0039(18)
C(3)	0.055(2)	0.048(2)	0.044(2)	-0.002(2)	-0.038(2)	0.0028(19)
C(4)	0.042(2)	0.048(2)	0.044(2)	0.0000(18)	-0.0321(19)	-0.0082(19)
C(5)	0.057(2)	0.040(2)	0.054(2)	0.0052(19)	-0.044(2)	-0.0027(19)
C(6)	0.050(2)	0.044(2)	0.045(2)	0.0069(19)	-0.036(2)	-0.0019(19)
C(7)	0.052(2)	0.052(2)	0.052(2)	0.001(2)	-0.039(2)	-0.008(2)
C(8)	0.100(5)	0.132(7)	0.040(3)	0.035(5)	-0.039(3)	-0.011(4)
C(9)	0.051(2)	0.047(2)	0.062(2)	-0.009(2)	-0.045(2)	0.003(2)
C(10)	0.056(3)	0.092(5)	0.092(5)	-0.013(3)	-0.049(3)	0.026(4)
C(11)	0.085(3)	0.049(2)	0.067(3)	-0.020(2)	-0.058(3)	0.020(2)
C(12)	0.167(8)	0.065(4)	0.117(6)	-0.036(4)	-0.125(6)	0.016(4)
C(13)	0.095(4)	0.057(3)	0.068(3)	0.013(2)	-0.070(3)	-0.004(2)

C(14)	0.115(5)	0.048(3)	0.075(3)	0.007(3)	-0.077(4)	0.003(2)
C(15)	0.176(8)	0.078(4)	0.127(6)	0.007(5)	-0.140(7)	-0.005(4)
C(16)	0.093(4)	0.084(4)	0.095(5)	0.025(3)	-0.078(4)	-0.008(3)
C(17)	0.052(2)	0.040(2)	0.050(2)	0.0004(18)	-0.039(2)	-0.0092(19)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(18)	0.117(5)	0.045(2)	0.105(5)	0.002(3)	-0.096(5)	-0.005(3)
C(19)	0.124(6)	0.070(4)	0.063(3)	0.018(4)	-0.067(4)	-0.026(3)
C(20)	0.067(3)	0.050(3)	0.140(6)	-0.001(2)	-0.075(4)	-0.018(3)
C(21)	0.061(2)	0.051(2)	0.070(3)	-0.005(2)	-0.054(2)	0.012(2)
C(22)	0.089(4)	0.111(6)	0.074(4)	-0.019(4)	-0.068(4)	0.029(4)
C(23)	0.069(3)	0.080(4)	0.105(5)	-0.005(3)	-0.073(4)	0.008(3)
C(24)	0.103(4)	0.048(3)	0.121(5)	-0.022(3)	-0.097(5)	0.026(3)
C(25)	0.062(2)	0.040(2)	0.048(2)	-0.002(2)	-0.042(2)	-0.0037(19)
C(26)	0.067(3)	0.052(2)	0.044(2)	-0.002(2)	-0.039(2)	-0.009(2)
C(27)	0.072(3)	0.054(3)	0.050(2)	-0.003(2)	-0.040(2)	-0.017(2)
C(28)	0.053(2)	0.043(2)	0.061(3)	0.008(2)	-0.035(2)	-0.021(2)
C(29)	0.056(2)	0.037(2)	0.053(2)	-0.0072(19)	-0.040(2)	0.0001(19)
C(30)	0.054(2)	0.046(2)	0.038(2)	-0.022(2)	-0.029(2)	0.0053(19)
C(31)	0.041(2)	0.077(4)	0.059(3)	-0.012(2)	-0.023(2)	-0.023(3)
C(32)	0.066(4)	0.113(6)	0.045(3)	-0.046(4)	-0.009(3)	-0.023(4)
C(33)	0.161(8)	0.075(4)	0.047(3)	-0.068(5)	-0.066(5)	0.025(3)
C(34)	0.118(5)	0.041(2)	0.052(3)	-0.029(3)	-0.060(3)	0.008(2)
C(35)	0.040(2)	0.047(2)	0.037(2)	0.0060(17)	-0.0281(18)	-0.0021(17)
C(36)	0.051(2)	0.044(2)	0.047(2)	0.0071(19)	-0.034(2)	0.001(2)
C(37)	0.059(2)	0.057(3)	0.046(2)	-0.007(2)	-0.038(2)	0.007(2)
C(38)	0.046(2)	0.060(2)	0.039(2)	-0.002(2)	-0.029(2)	-0.003(2)
C(39)	0.055(2)	0.051(2)	0.055(2)	0.012(2)	-0.039(2)	-0.008(2)
C(40)	0.048(2)	0.056(2)	0.040(2)	0.015(2)	-0.030(2)	-0.004(2)
C(41)	0.068(3)	0.064(3)	0.053(3)	-0.002(2)	-0.043(2)	-0.004(2)
C(42)	0.173(9)	0.129(8)	0.034(3)	0.031(7)	-0.045(4)	-0.021(4)
C(43)	0.052(2)	0.050(2)	0.053(2)	0.004(2)	-0.043(2)	0.001(2)
C(44)	0.085(3)	0.047(2)	0.072(3)	0.004(2)	-0.064(3)	0.002(2)
C(45)	0.079(3)	0.073(3)	0.056(3)	0.004(3)	-0.054(3)	0.005(2)
C(46)	0.069(3)	0.100(5)	0.081(4)	0.007(3)	-0.065(3)	-0.000(3)
C(47)	0.081(3)	0.039(2)	0.065(3)	0.004(2)	-0.060(3)	-0.008(2)
C(48)	0.144(7)	0.066(4)	0.082(4)	0.027(4)	-0.091(5)	-0.026(3)
C(49)	0.106(5)	0.072(4)	0.139(7)	-0.027(4)	-0.095(6)	-0.003(4)
C(50)	0.136(6)	0.045(3)	0.104(5)	0.023(3)	-0.105(5)	-0.020(3)

C(51)	0.058(2)	0.063(3)	0.068(3)	-0.015(2)	-0.052(2)	0.012(2)
C(52)	0.147(7)	0.091(5)	0.145(7)	-0.062(5)	-0.133(7)	0.069(5)
C(53)	0.160(8)	0.066(4)	0.126(6)	-0.028(4)	-0.128(7)	0.015(4)
C(54)	0.061(4)	0.090(5)	0.123(7)	-0.020(3)	-0.051(4)	0.017(5)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(55)	0.063(3)	0.063(3)	0.062(3)	0.005(2)	-0.053(2)	0.005(2)
C(56)	0.079(3)	0.056(3)	0.081(3)	0.001(2)	-0.067(3)	0.013(2)
C(57)	0.105(5)	0.097(5)	0.094(4)	-0.020(4)	-0.091(4)	0.025(4)
C(58)	0.072(3)	0.109(5)	0.079(4)	0.022(3)	-0.060(3)	0.003(4)
C(59)	0.055(2)	0.046(2)	0.054(2)	0.0006(19)	-0.045(2)	-0.007(2)
C(60)	0.058(2)	0.074(3)	0.051(2)	-0.003(2)	-0.044(2)	-0.010(2)
C(61)	0.056(3)	0.078(4)	0.054(3)	0.007(2)	-0.036(2)	-0.032(3)
C(62)	0.055(2)	0.047(2)	0.081(4)	0.018(2)	-0.046(3)	-0.029(2)
C(63)	0.062(2)	0.037(2)	0.073(3)	0.001(2)	-0.054(2)	-0.003(2)
C(64)	0.044(2)	0.043(2)	0.039(2)	-0.0040(17)	-0.0315(18)	-0.0003(17)
C(65)	0.059(2)	0.039(2)	0.049(2)	-0.0065(19)	-0.044(2)	0.0055(18)
C(66)	0.070(3)	0.062(3)	0.045(2)	-0.018(2)	-0.044(2)	0.012(2)
C(67)	0.042(2)	0.075(3)	0.040(2)	-0.008(2)	-0.026(2)	-0.004(2)
C(68)	0.039(2)	0.057(2)	0.043(2)	0.0043(19)	-0.0299(19)	-0.007(2)
B(1)	0.130(8)	0.089(6)	0.062(5)	-0.022(6)	-0.058(5)	0.006(4)
B(2)	0.138(11)	0.112(10)	0.076(6)	-0.010(8)	-0.058(7)	0.013(6)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Pd(1)	P(1)	2.298(2)	Pd(1)	P(2)	2.280(2)
Pd(1)	C(1)	2.017(3)	Pd(2)	P(3)	2.298(2)
Pd(2)	P(4)	2.289(2)	Pd(2)	C(35)	2.015(3)
Fe(1)	C(25)	2.106(7)	Fe(1)	C(26)	2.053(11)
Fe(1)	C(27)	2.036(8)	Fe(1)	C(28)	2.045(5)
Fe(1)	C(29)	2.050(4)	Fe(1)	C(30)	2.096(8)
Fe(1)	C(31)	2.084(11)	Fe(1)	C(32)	2.040(9)
Fe(1)	C(33)	2.036(8)	Fe(1)	C(34)	2.041(6)
Fe(2)	C(59)	2.099(7)	Fe(2)	C(60)	2.051(11)
Fe(2)	C(61)	2.040(9)	Fe(2)	C(62)	2.048(5)
Fe(2)	C(63)	2.055(4)	Fe(2)	C(64)	2.079(7)
Fe(2)	C(65)	2.052(4)	Fe(2)	C(66)	2.061(5)
Fe(2)	C(67)	2.040(6)	Fe(2)	C(68)	2.051(9)
P(1)	C(17)	1.874(5)	P(1)	C(21)	1.873(10)
P(1)	C(30)	1.811(5)	P(2)	C(9)	1.886(5)
P(2)	C(13)	1.860(12)	P(2)	C(25)	1.831(4)
P(3)	C(43)	1.870(9)	P(3)	C(47)	1.870(6)
P(3)	C(64)	1.812(5)	P(4)	C(51)	1.893(6)
P(4)	C(55)	1.864(10)	P(4)	C(59)	1.822(4)
F(1)	B(1)	1.369(10)	F(2)	B(1)	1.37(3)
F(3)	B(1)	1.370(10)	F(4)	B(1)	1.37(2)
F(5)	B(2)	1.26(2)	F(6)	B(2)	1.38(3)
F(7)	B(2)	1.29(2)	F(8)	B(2)	1.281(16)
O(1)	C(7)	1.191(7)	O(2)	C(7)	1.322(9)
O(2)	C(8)	1.435(7)	O(3)	C(41)	1.198(8)
O(4)	C(41)	1.325(10)	O(4)	C(42)	1.446(8)
C(1)	C(2)	1.381(8)	C(1)	C(6)	1.379(7)
C(2)	C(3)	1.383(6)	C(3)	C(4)	1.400(8)
C(4)	C(5)	1.371(9)	C(4)	C(7)	1.485(6)
C(5)	C(6)	1.391(6)	C(9)	C(10)	1.528(8)
C(9)	C(11)	1.541(15)	C(9)	C(12)	1.532(17)
C(13)	C(14)	1.537(10)	C(13)	C(15)	1.51(2)
C(13)	C(16)	1.572(9)	C(17)	C(18)	1.504(17)

C(17)	C(19)	1.502(9)	C(17)	C(20)	1.509(12)
C(21)	C(22)	1.541(9)	C(21)	C(23)	1.536(15)
C(21)	C(24)	1.513(10)	C(25)	C(26)	1.423(7)
C(25)	C(29)	1.421(12)	C(26)	C(27)	1.404(11)

Table 4. Bond lengths (Å) (continued)

atom	atom	distance	atom	atom	distance
C(27)	C(28)	1.409(14)	C(28)	C(29)	1.406(5)
C(30)	C(31)	1.418(8)	C(30)	C(34)	1.430(15)
C(31)	C(32)	1.416(14)	C(32)	C(33)	1.35(2)
C(33)	C(34)	1.421(8)	C(35)	C(36)	1.387(9)
C(35)	C(40)	1.394(7)	C(36)	C(37)	1.407(6)
C(37)	C(38)	1.372(8)	C(38)	C(39)	1.388(10)
C(38)	C(41)	1.476(7)	C(39)	C(40)	1.372(6)
C(43)	C(44)	1.532(9)	C(43)	C(45)	1.533(8)
C(43)	C(46)	1.527(14)	C(47)	C(48)	1.511(13)
C(47)	C(49)	1.547(13)	C(47)	C(50)	1.517(18)
C(51)	C(52)	1.50(2)	C(51)	C(53)	1.494(18)
C(51)	C(54)	1.505(8)	C(55)	C(56)	1.515(9)
C(55)	C(57)	1.525(18)	C(55)	C(58)	1.539(8)
C(59)	C(60)	1.410(8)	C(59)	C(63)	1.453(13)
C(60)	C(61)	1.410(11)	C(61)	C(62)	1.421(15)
C(62)	C(63)	1.385(6)	C(64)	C(65)	1.435(12)
C(64)	C(68)	1.407(6)	C(65)	C(66)	1.404(6)
C(66)	C(67)	1.399(12)	C(67)	C(68)	1.414(11)

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(2)	H(1)	0.930	C(3)	H(2)	0.930
C(5)	H(3)	0.930	C(6)	H(4)	0.930
C(8)	H(5)	0.960	C(8)	H(6)	0.960
C(8)	H(7)	0.960	C(10)	H(8)	0.960
C(10)	H(9)	0.960	C(10)	H(10)	0.960
C(11)	H(11)	0.960	C(11)	H(12)	0.960
C(11)	H(13)	0.960	C(12)	H(14)	0.960
C(12)	H(15)	0.960	C(12)	H(16)	0.960
C(14)	H(17)	0.960	C(14)	H(18)	0.960
C(14)	H(19)	0.960	C(15)	H(20)	0.960
C(15)	H(21)	0.960	C(15)	H(22)	0.960
C(16)	H(23)	0.960	C(16)	H(24)	0.960
C(16)	H(25)	0.960	C(18)	H(26)	0.960
C(18)	H(27)	0.960	C(18)	H(28)	0.960
C(19)	H(29)	0.960	C(19)	H(30)	0.960
C(19)	H(31)	0.960	C(20)	H(32)	0.960
C(20)	H(33)	0.960	C(20)	H(34)	0.960
C(22)	H(35)	0.960	C(22)	H(36)	0.960
C(22)	H(37)	0.960	C(23)	H(38)	0.960
C(23)	H(39)	0.960	C(23)	H(40)	0.960
C(24)	H(41)	0.960	C(24)	H(42)	0.960
C(24)	H(43)	0.960	C(26)	H(44)	0.980
C(27)	H(45)	0.980	C(28)	H(46)	0.980
C(29)	H(47)	0.980	C(31)	H(48)	0.980
C(32)	H(49)	0.980	C(33)	H(50)	0.980
C(34)	H(51)	0.980	C(36)	H(52)	0.930
C(37)	H(53)	0.930	C(39)	H(54)	0.930
C(40)	H(55)	0.930	C(42)	H(56)	0.960
C(42)	H(57)	0.960	C(42)	H(58)	0.960
C(44)	H(59)	0.960	C(44)	H(60)	0.960
C(44)	H(61)	0.960	C(45)	H(62)	0.960
C(45)	H(63)	0.960	C(45)	H(64)	0.960
C(46)	H(65)	0.960	C(46)	H(66)	0.960

C(46)	H(67)	0.960	C(48)	H(68)	0.960
C(48)	H(69)	0.960	C(48)	H(70)	0.960
C(49)	H(71)	0.960	C(49)	H(72)	0.960
C(49)	H(73)	0.960	C(50)	H(74)	0.960

Table 5. Bond lengths involving hydrogens (Å) (continued)

atom	atom	distance	atom	atom	distance
C(50)	H(75)	0.960	C(50)	H(76)	0.960
C(52)	H(77)	0.960	C(52)	H(78)	0.960
C(52)	H(79)	0.960	C(53)	H(80)	0.960
C(53)	H(81)	0.960	C(53)	H(82)	0.960
C(54)	H(83)	0.960	C(54)	H(84)	0.960
C(54)	H(85)	0.960	C(56)	H(86)	0.960
C(56)	H(87)	0.960	C(56)	H(88)	0.960
C(57)	H(89)	0.960	C(57)	H(90)	0.960
C(57)	H(91)	0.960	C(58)	H(92)	0.960
C(58)	H(93)	0.960	C(58)	H(94)	0.960
C(60)	H(95)	0.980	C(61)	H(96)	0.980
C(62)	H(97)	0.980	C(63)	H(98)	0.771
C(65)	H(99)	0.980	C(66)	H(100)	0.980
C(67)	H(101)	0.980	C(68)	H(102)	0.980

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	Pd(1)	P(2)	160.19(3)	P(1)	Pd(1)	C(1)	98.8(2)
P(2)	Pd(1)	C(1)	101.0(2)	P(3)	Pd(2)	P(4)	158.48(3)
P(3)	Pd(2)	C(35)	99.1(2)	P(4)	Pd(2)	C(35)	102.4(2)
C(25)	Fe(1)	C(26)	40.0(2)	C(25)	Fe(1)	C(27)	67.4(2)
C(25)	Fe(1)	C(28)	67.6(2)	C(25)	Fe(1)	C(29)	40.0(3)
C(25)	Fe(1)	C(30)	130.21(19)	C(25)	Fe(1)	C(31)	154.1(3)
C(25)	Fe(1)	C(32)	162.4(3)	C(25)	Fe(1)	C(33)	138.1(6)
C(25)	Fe(1)	C(34)	121.9(3)	C(26)	Fe(1)	C(27)	40.2(3)
C(26)	Fe(1)	C(28)	67.6(3)	C(26)	Fe(1)	C(29)	67.2(3)
C(26)	Fe(1)	C(30)	153.7(2)	C(26)	Fe(1)	C(31)	162.22(19)
C(26)	Fe(1)	C(32)	123.6(3)	C(26)	Fe(1)	C(33)	105.5(5)
C(26)	Fe(1)	C(34)	117.1(4)	C(27)	Fe(1)	C(28)	40.4(3)
C(27)	Fe(1)	C(29)	67.4(2)	C(27)	Fe(1)	C(30)	162.2(2)
C(27)	Fe(1)	C(31)	124.0(3)	C(27)	Fe(1)	C(32)	95.4(3)
C(27)	Fe(1)	C(33)	102.0(3)	C(27)	Fe(1)	C(34)	137.4(3)
C(28)	Fe(1)	C(29)	40.18(16)	C(28)	Fe(1)	C(30)	137.2(4)
C(28)	Fe(1)	C(31)	105.1(3)	C(28)	Fe(1)	C(32)	102.3(3)
C(28)	Fe(1)	C(33)	130.7(2)	C(28)	Fe(1)	C(34)	170.1(3)
C(29)	Fe(1)	C(30)	123.2(2)	C(29)	Fe(1)	C(31)	118.5(3)
C(29)	Fe(1)	C(32)	138.3(3)	C(29)	Fe(1)	C(33)	169.4(3)
C(29)	Fe(1)	C(34)	148.92(18)	C(30)	Fe(1)	C(31)	39.7(2)
C(30)	Fe(1)	C(32)	67.1(3)	C(30)	Fe(1)	C(33)	66.8(4)
C(30)	Fe(1)	C(34)	40.4(4)	C(31)	Fe(1)	C(32)	40.2(4)
C(31)	Fe(1)	C(33)	66.1(6)	C(31)	Fe(1)	C(34)	67.7(4)
C(32)	Fe(1)	C(33)	38.7(5)	C(32)	Fe(1)	C(34)	67.8(3)
C(33)	Fe(1)	C(34)	40.8(2)	C(59)	Fe(2)	C(60)	39.7(2)
C(59)	Fe(2)	C(61)	67.8(2)	C(59)	Fe(2)	C(62)	67.6(2)
C(59)	Fe(2)	C(63)	40.9(3)	C(59)	Fe(2)	C(64)	129.75(19)
C(59)	Fe(2)	C(65)	120.4(2)	C(59)	Fe(2)	C(66)	134.8(3)
C(59)	Fe(2)	C(67)	161.8(3)	C(59)	Fe(2)	C(68)	155.8(2)
C(60)	Fe(2)	C(61)	40.3(3)	C(60)	Fe(2)	C(62)	67.4(4)
C(60)	Fe(2)	C(63)	67.5(3)	C(60)	Fe(2)	C(64)	155.9(2)
C(60)	Fe(2)	C(65)	119.0(3)	C(60)	Fe(2)	C(66)	105.3(3)

C(60)	Fe(2)	C(67)	122.4(3)	C(60)	Fe(2)	C(68)	160.49(17)
C(61)	Fe(2)	C(62)	40.7(4)	C(61)	Fe(2)	C(63)	67.7(2)
C(61)	Fe(2)	C(64)	161.7(2)	C(61)	Fe(2)	C(65)	141.0(3)
C(61)	Fe(2)	C(66)	104.9(2)	C(61)	Fe(2)	C(67)	95.6(2)

Table 6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(61)	Fe(2)	C(68)	122.2(2)	C(62)	Fe(2)	C(63)	39.47(18)
C(62)	Fe(2)	C(64)	134.3(4)	C(62)	Fe(2)	C(65)	171.9(3)
C(62)	Fe(2)	C(66)	136.00(19)	C(62)	Fe(2)	C(67)	105.2(2)
C(62)	Fe(2)	C(68)	104.7(3)	C(63)	Fe(2)	C(64)	120.5(3)
C(63)	Fe(2)	C(65)	145.70(17)	C(63)	Fe(2)	C(66)	172.2(4)
C(63)	Fe(2)	C(67)	140.9(2)	C(63)	Fe(2)	C(68)	118.6(3)
C(64)	Fe(2)	C(65)	40.7(3)	C(64)	Fe(2)	C(66)	67.3(3)
C(64)	Fe(2)	C(67)	67.6(2)	C(64)	Fe(2)	C(68)	39.8(2)
C(65)	Fe(2)	C(66)	39.90(19)	C(65)	Fe(2)	C(67)	67.6(2)
C(65)	Fe(2)	C(68)	67.6(3)	C(66)	Fe(2)	C(67)	39.9(3)
C(66)	Fe(2)	C(68)	67.2(3)	C(67)	Fe(2)	C(68)	40.4(3)
Pd(1)	P(1)	C(17)	122.2(3)	Pd(1)	P(1)	C(21)	113.7(2)
Pd(1)	P(1)	C(30)	87.8(3)	C(17)	P(1)	C(21)	113.8(4)
C(17)	P(1)	C(30)	106.6(2)	C(21)	P(1)	C(30)	108.0(3)
Pd(1)	P(2)	C(9)	122.8(3)	Pd(1)	P(2)	C(13)	113.6(3)
Pd(1)	P(2)	C(25)	86.2(3)	C(9)	P(2)	C(13)	113.4(4)
C(9)	P(2)	C(25)	106.9(2)	C(13)	P(2)	C(25)	109.3(3)
Pd(2)	P(3)	C(43)	114.7(2)	Pd(2)	P(3)	C(47)	123.5(3)
Pd(2)	P(3)	C(64)	87.3(2)	C(43)	P(3)	C(47)	112.9(4)
C(43)	P(3)	C(64)	108.4(2)	C(47)	P(3)	C(64)	104.9(2)
Pd(2)	P(4)	C(51)	123.5(3)	Pd(2)	P(4)	C(55)	113.3(2)
Pd(2)	P(4)	C(59)	87.0(3)	C(51)	P(4)	C(55)	113.2(4)
C(51)	P(4)	C(59)	106.4(2)	C(55)	P(4)	C(59)	108.9(3)
C(7)	O(2)	C(8)	115.0(6)	C(41)	O(4)	C(42)	117.2(7)
Pd(1)	C(1)	C(2)	119.6(3)	Pd(1)	C(1)	C(6)	120.6(3)
C(2)	C(1)	C(6)	119.6(3)	C(1)	C(2)	C(3)	120.4(5)
C(2)	C(3)	C(4)	119.7(5)	C(3)	C(4)	C(5)	119.6(4)
C(3)	C(4)	C(7)	122.1(5)	C(5)	C(4)	C(7)	118.2(5)
C(4)	C(5)	C(6)	120.2(5)	C(1)	C(6)	C(5)	120.3(5)
O(1)	C(7)	O(2)	122.8(5)	O(1)	C(7)	C(4)	124.8(6)
O(2)	C(7)	C(4)	112.5(5)	P(2)	C(9)	C(10)	110.3(4)
P(2)	C(9)	C(11)	107.6(6)	P(2)	C(9)	C(12)	111.0(4)
C(10)	C(9)	C(11)	108.0(7)	C(10)	C(9)	C(12)	111.1(9)

C(11)	C(9)	C(12)	108.7(7)	P(2)	C(13)	C(14)	106.8(9)
P(2)	C(13)	C(15)	114.5(6)	P(2)	C(13)	C(16)	107.8(6)
C(14)	C(13)	C(15)	110.3(7)	C(14)	C(13)	C(16)	107.8(5)
C(15)	C(13)	C(16)	109.3(11)	P(1)	C(17)	C(18)	108.3(6)

Table 6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
P(1)	C(17)	C(19)	110.6(4)	P(1)	C(17)	C(20)	113.0(3)
C(18)	C(17)	C(19)	106.9(6)	C(18)	C(17)	C(20)	107.3(6)
C(19)	C(17)	C(20)	110.5(9)	P(1)	C(21)	C(22)	108.3(6)
P(1)	C(21)	C(23)	113.9(5)	P(1)	C(21)	C(24)	106.9(9)
C(22)	C(21)	C(23)	108.5(10)	C(22)	C(21)	C(24)	107.9(5)
C(23)	C(21)	C(24)	111.1(6)	Fe(1)	C(25)	P(2)	123.7(3)
Fe(1)	C(25)	C(26)	68.0(4)	Fe(1)	C(25)	C(29)	67.9(4)
P(2)	C(25)	C(26)	131.0(6)	P(2)	C(25)	C(29)	122.7(4)
C(26)	C(25)	C(29)	105.9(5)	Fe(1)	C(26)	C(25)	72.0(5)
Fe(1)	C(26)	C(27)	69.3(6)	C(25)	C(26)	C(27)	108.9(8)
Fe(1)	C(27)	C(26)	70.6(4)	Fe(1)	C(27)	C(28)	70.2(4)
C(26)	C(27)	C(28)	108.4(5)	Fe(1)	C(28)	C(27)	69.5(3)
Fe(1)	C(28)	C(29)	70.1(2)	C(27)	C(28)	C(29)	107.4(7)
Fe(1)	C(29)	C(25)	72.1(3)	Fe(1)	C(29)	C(28)	69.7(2)
C(25)	C(29)	C(28)	109.4(6)	Fe(1)	C(30)	P(1)	122.4(3)
Fe(1)	C(30)	C(31)	69.7(5)	Fe(1)	C(30)	C(34)	67.7(4)
P(1)	C(30)	C(31)	131.2(7)	P(1)	C(30)	C(34)	120.9(4)
C(31)	C(30)	C(34)	107.5(6)	Fe(1)	C(31)	C(30)	70.6(5)
Fe(1)	C(31)	C(32)	68.2(6)	C(30)	C(31)	C(32)	107.5(9)
Fe(1)	C(32)	C(31)	71.6(4)	Fe(1)	C(32)	C(33)	70.5(6)
C(31)	C(32)	C(33)	108.6(7)	Fe(1)	C(33)	C(32)	70.8(5)
Fe(1)	C(33)	C(34)	69.8(3)	C(32)	C(33)	C(34)	110.3(11)
Fe(1)	C(34)	C(30)	71.9(3)	Fe(1)	C(34)	C(33)	69.4(4)
C(30)	C(34)	C(33)	105.9(9)	Pd(2)	C(35)	C(36)	119.1(3)
Pd(2)	C(35)	C(40)	121.2(3)	C(36)	C(35)	C(40)	119.4(4)
C(35)	C(36)	C(37)	119.2(5)	C(36)	C(37)	C(38)	121.4(6)
C(37)	C(38)	C(39)	118.2(4)	C(37)	C(38)	C(41)	122.8(6)
C(39)	C(38)	C(41)	119.0(5)	C(38)	C(39)	C(40)	121.6(5)
C(35)	C(40)	C(39)	120.1(6)	O(3)	C(41)	O(4)	123.2(5)
O(3)	C(41)	C(38)	125.6(7)	O(4)	C(41)	C(38)	111.2(5)
P(3)	C(43)	C(44)	107.7(7)	P(3)	C(43)	C(45)	108.8(5)
P(3)	C(43)	C(46)	114.8(4)	C(44)	C(43)	C(45)	106.3(4)
C(44)	C(43)	C(46)	109.7(5)	C(45)	C(43)	C(46)	109.1(8)

P(3)	C(47)	C(48)	110.9(4)	P(3)	C(47)	C(49)	110.9(4)
P(3)	C(47)	C(50)	108.0(7)	C(48)	C(47)	C(49)	111.7(11)
C(48)	C(47)	C(50)	108.2(7)	C(49)	C(47)	C(50)	107.0(7)
P(4)	C(51)	C(52)	107.9(7)	P(4)	C(51)	C(53)	113.2(4)

Table 6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
P(4)	C(51)	C(54)	110.8(4)	C(52)	C(51)	C(53)	107.8(8)
C(52)	C(51)	C(54)	108.0(8)	C(53)	C(51)	C(54)	108.9(10)
P(4)	C(55)	C(56)	106.9(8)	P(4)	C(55)	C(57)	113.1(5)
P(4)	C(55)	C(58)	109.0(6)	C(56)	C(55)	C(57)	111.1(6)
C(56)	C(55)	C(58)	107.6(5)	C(57)	C(55)	C(58)	109.0(9)
Fe(2)	C(59)	P(4)	123.1(3)	Fe(2)	C(59)	C(60)	68.3(4)
Fe(2)	C(59)	C(63)	67.9(4)	P(4)	C(59)	C(60)	133.4(6)
P(4)	C(59)	C(63)	120.7(4)	C(60)	C(59)	C(63)	105.6(5)
Fe(2)	C(60)	C(59)	72.0(5)	Fe(2)	C(60)	C(61)	69.4(6)
C(59)	C(60)	C(61)	109.9(8)	Fe(2)	C(61)	C(60)	70.2(4)
Fe(2)	C(61)	C(62)	70.0(5)	C(60)	C(61)	C(62)	107.0(5)
Fe(2)	C(62)	C(61)	69.4(4)	Fe(2)	C(62)	C(63)	70.5(3)
C(61)	C(62)	C(63)	108.8(8)	Fe(2)	C(63)	C(59)	71.2(3)
Fe(2)	C(63)	C(62)	70.0(3)	C(59)	C(63)	C(62)	108.7(7)
Fe(2)	C(64)	P(3)	123.3(2)	Fe(2)	C(64)	C(65)	68.7(4)
Fe(2)	C(64)	C(68)	69.0(4)	P(3)	C(64)	C(65)	120.6(3)
P(3)	C(64)	C(68)	132.4(6)	C(65)	C(64)	C(68)	106.8(5)
Fe(2)	C(65)	C(64)	70.7(3)	Fe(2)	C(65)	C(66)	70.4(3)
C(64)	C(65)	C(66)	107.9(6)	Fe(2)	C(66)	C(65)	69.7(2)
Fe(2)	C(66)	C(67)	69.3(3)	C(65)	C(66)	C(67)	108.6(7)
Fe(2)	C(67)	C(66)	70.9(3)	Fe(2)	C(67)	C(68)	70.2(3)
C(66)	C(67)	C(68)	107.9(4)	Fe(2)	C(68)	C(64)	71.2(4)
Fe(2)	C(68)	C(67)	69.4(5)	C(64)	C(68)	C(67)	108.7(7)
F(1)	B(1)	F(2)	107.8(12)	F(1)	B(1)	F(3)	108.0(7)
F(1)	B(1)	F(4)	117.1(12)	F(2)	B(1)	F(3)	107.3(12)
F(2)	B(1)	F(4)	110.3(12)	F(3)	B(1)	F(4)	105.9(11)
F(5)	B(2)	F(6)	104.9(15)	F(5)	B(2)	F(7)	120(2)
F(5)	B(2)	F(8)	116.5(12)	F(6)	B(2)	F(7)	98.7(14)
F(6)	B(2)	F(8)	110(2)	F(7)	B(2)	F(8)	105.5(11)

Table 7. Bond angles involving hydrogens (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(2)	H(1)	119.8	C(3)	C(2)	H(1)	119.8
C(2)	C(3)	H(2)	120.1	C(4)	C(3)	H(2)	120.1
C(4)	C(5)	H(3)	119.9	C(6)	C(5)	H(3)	119.9
C(1)	C(6)	H(4)	119.9	C(5)	C(6)	H(4)	119.8
O(2)	C(8)	H(5)	109.5	O(2)	C(8)	H(6)	109.5
O(2)	C(8)	H(7)	109.5	H(5)	C(8)	H(6)	109.5
H(5)	C(8)	H(7)	109.5	H(6)	C(8)	H(7)	109.5
C(9)	C(10)	H(8)	109.5	C(9)	C(10)	H(9)	109.5
C(9)	C(10)	H(10)	109.5	H(8)	C(10)	H(9)	109.5
H(8)	C(10)	H(10)	109.5	H(9)	C(10)	H(10)	109.5
C(9)	C(11)	H(11)	109.5	C(9)	C(11)	H(12)	109.5
C(9)	C(11)	H(13)	109.5	H(11)	C(11)	H(12)	109.5
H(11)	C(11)	H(13)	109.5	H(12)	C(11)	H(13)	109.5
C(9)	C(12)	H(14)	109.5	C(9)	C(12)	H(15)	109.5
C(9)	C(12)	H(16)	109.5	H(14)	C(12)	H(15)	109.5
H(14)	C(12)	H(16)	109.5	H(15)	C(12)	H(16)	109.5
C(13)	C(14)	H(17)	109.5	C(13)	C(14)	H(18)	109.5
C(13)	C(14)	H(19)	109.5	H(17)	C(14)	H(18)	109.5
H(17)	C(14)	H(19)	109.5	H(18)	C(14)	H(19)	109.5
C(13)	C(15)	H(20)	109.5	C(13)	C(15)	H(21)	109.5
C(13)	C(15)	H(22)	109.5	H(20)	C(15)	H(21)	109.5
H(20)	C(15)	H(22)	109.5	H(21)	C(15)	H(22)	109.5
C(13)	C(16)	H(23)	109.5	C(13)	C(16)	H(24)	109.5
C(13)	C(16)	H(25)	109.5	H(23)	C(16)	H(24)	109.5
H(23)	C(16)	H(25)	109.5	H(24)	C(16)	H(25)	109.5
C(17)	C(18)	H(26)	109.5	C(17)	C(18)	H(27)	109.5
C(17)	C(18)	H(28)	109.5	H(26)	C(18)	H(27)	109.5
H(26)	C(18)	H(28)	109.5	H(27)	C(18)	H(28)	109.5
C(17)	C(19)	H(29)	109.5	C(17)	C(19)	H(30)	109.5
C(17)	C(19)	H(31)	109.5	H(29)	C(19)	H(30)	109.5
H(29)	C(19)	H(31)	109.4	H(30)	C(19)	H(31)	109.5
C(17)	C(20)	H(32)	109.5	C(17)	C(20)	H(33)	109.5
C(17)	C(20)	H(34)	109.5	H(32)	C(20)	H(33)	109.5

H(32)	C(20)	H(34)	109.5	H(33)	C(20)	H(34)	109.5
C(21)	C(22)	H(35)	109.5	C(21)	C(22)	H(36)	109.5
C(21)	C(22)	H(37)	109.5	H(35)	C(22)	H(36)	109.5
H(35)	C(22)	H(37)	109.5	H(36)	C(22)	H(37)	109.5

Table 7. Bond angles involving hydrogens (^{o}) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(21)	C(23)	H(38)	109.5	C(21)	C(23)	H(39)	109.5
C(21)	C(23)	H(40)	109.5	H(38)	C(23)	H(39)	109.5
H(38)	C(23)	H(40)	109.5	H(39)	C(23)	H(40)	109.4
C(21)	C(24)	H(41)	109.5	C(21)	C(24)	H(42)	109.5
C(21)	C(24)	H(43)	109.5	H(41)	C(24)	H(42)	109.4
H(41)	C(24)	H(43)	109.5	H(42)	C(24)	H(43)	109.5
Fe(1)	C(26)	H(44)	125.6	C(25)	C(26)	H(44)	125.6
C(27)	C(26)	H(44)	125.6	Fe(1)	C(27)	H(45)	125.8
C(26)	C(27)	H(45)	125.8	C(28)	C(27)	H(45)	125.8
Fe(1)	C(28)	H(46)	126.3	C(27)	C(28)	H(46)	126.3
C(29)	C(28)	H(46)	126.3	Fe(1)	C(29)	H(47)	125.3
C(25)	C(29)	H(47)	125.3	C(28)	C(29)	H(47)	125.3
Fe(1)	C(31)	H(48)	126.2	C(30)	C(31)	H(48)	126.2
C(32)	C(31)	H(48)	126.2	Fe(1)	C(32)	H(49)	125.7
C(31)	C(32)	H(49)	125.7	C(33)	C(32)	H(49)	125.7
Fe(1)	C(33)	H(50)	124.9	C(32)	C(33)	H(50)	124.9
C(34)	C(33)	H(50)	124.9	Fe(1)	C(34)	H(51)	127.0
C(30)	C(34)	H(51)	126.9	C(33)	C(34)	H(51)	127.0
C(35)	C(36)	H(52)	120.4	C(37)	C(36)	H(52)	120.4
C(36)	C(37)	H(53)	119.3	C(38)	C(37)	H(53)	119.3
C(38)	C(39)	H(54)	119.2	C(40)	C(39)	H(54)	119.2
C(35)	C(40)	H(55)	120.0	C(39)	C(40)	H(55)	119.9
O(4)	C(42)	H(56)	109.5	O(4)	C(42)	H(57)	109.5
O(4)	C(42)	H(58)	109.5	H(56)	C(42)	H(57)	109.5
H(56)	C(42)	H(58)	109.5	H(57)	C(42)	H(58)	109.5
C(43)	C(44)	H(59)	109.5	C(43)	C(44)	H(60)	109.5
C(43)	C(44)	H(61)	109.5	H(59)	C(44)	H(60)	109.5
H(59)	C(44)	H(61)	109.5	H(60)	C(44)	H(61)	109.5
C(43)	C(45)	H(62)	109.5	C(43)	C(45)	H(63)	109.5
C(43)	C(45)	H(64)	109.5	H(62)	C(45)	H(63)	109.5
H(62)	C(45)	H(64)	109.5	H(63)	C(45)	H(64)	109.5
C(43)	C(46)	H(65)	109.5	C(43)	C(46)	H(66)	109.5
C(43)	C(46)	H(67)	109.5	H(65)	C(46)	H(66)	109.5

H(65)	C(46)	H(67)	109.5	H(66)	C(46)	H(67)	109.5
C(47)	C(48)	H(68)	109.5	C(47)	C(48)	H(69)	109.5
C(47)	C(48)	H(70)	109.5	H(68)	C(48)	H(69)	109.5
H(68)	C(48)	H(70)	109.5	H(69)	C(48)	H(70)	109.5

Table 7. Bond angles involving hydrogens (^{o}) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(47)	C(49)	H(71)	109.5	C(47)	C(49)	H(72)	109.5
C(47)	C(49)	H(73)	109.5	H(71)	C(49)	H(72)	109.5
H(71)	C(49)	H(73)	109.5	H(72)	C(49)	H(73)	109.5
C(47)	C(50)	H(74)	109.5	C(47)	C(50)	H(75)	109.5
C(47)	C(50)	H(76)	109.5	H(74)	C(50)	H(75)	109.5
H(74)	C(50)	H(76)	109.5	H(75)	C(50)	H(76)	109.5
C(51)	C(52)	H(77)	109.5	C(51)	C(52)	H(78)	109.5
C(51)	C(52)	H(79)	109.5	H(77)	C(52)	H(78)	109.5
H(77)	C(52)	H(79)	109.5	H(78)	C(52)	H(79)	109.5
C(51)	C(53)	H(80)	109.5	C(51)	C(53)	H(81)	109.5
C(51)	C(53)	H(82)	109.5	H(80)	C(53)	H(81)	109.5
H(80)	C(53)	H(82)	109.5	H(81)	C(53)	H(82)	109.5
C(51)	C(54)	H(83)	109.5	C(51)	C(54)	H(84)	109.5
C(51)	C(54)	H(85)	109.5	H(83)	C(54)	H(84)	109.5
H(83)	C(54)	H(85)	109.5	H(84)	C(54)	H(85)	109.5
C(55)	C(56)	H(86)	109.5	C(55)	C(56)	H(87)	109.5
C(55)	C(56)	H(88)	109.5	H(86)	C(56)	H(87)	109.5
H(86)	C(56)	H(88)	109.4	H(87)	C(56)	H(88)	109.5
C(55)	C(57)	H(89)	109.5	C(55)	C(57)	H(90)	109.5
C(55)	C(57)	H(91)	109.5	H(89)	C(57)	H(90)	109.5
H(89)	C(57)	H(91)	109.5	H(90)	C(57)	H(91)	109.5
C(55)	C(58)	H(92)	109.5	C(55)	C(58)	H(93)	109.5
C(55)	C(58)	H(94)	109.5	H(92)	C(58)	H(93)	109.5
H(92)	C(58)	H(94)	109.5	H(93)	C(58)	H(94)	109.5
Fe(2)	C(60)	H(95)	125.0	C(59)	C(60)	H(95)	125.1
C(61)	C(60)	H(95)	125.0	Fe(2)	C(61)	H(96)	126.5
C(60)	C(61)	H(96)	126.5	C(62)	C(61)	H(96)	126.5
Fe(2)	C(62)	H(97)	125.6	C(61)	C(62)	H(97)	125.6
C(63)	C(62)	H(97)	125.6	Fe(2)	C(63)	H(98)	119.7
C(59)	C(63)	H(98)	118.5	C(62)	C(63)	H(98)	132.5
Fe(2)	C(65)	H(99)	126.0	C(64)	C(65)	H(99)	126.0
C(66)	C(65)	H(99)	126.0	Fe(2)	C(66)	H(100)	125.7
C(65)	C(66)	H(100)	125.7	C(67)	C(66)	H(100)	125.7

Fe(2)	C(67)	H(101)	126.0	C(66)	C(67)	H(101)	126.1
C(68)	C(67)	H(101)	126.0	Fe(2)	C(68)	H(102)	125.6
C(64)	C(68)	H(102)	125.6	C(67)	C(68)	H(102)	125.6

Table 8. Torsion Angles(°)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
P(1)	Pd(1)	P(2)	C(9)	121.1(2)	P(1)	Pd(1)	P(2)	C(13)	-96.0(2)
P(1)	Pd(1)	P(2)	C(25)	13.4(2)	P(2)	Pd(1)	P(1)	C(17)	121.8(2)
P(2)	Pd(1)	P(1)	C(21)	-95.2(2)	P(2)	Pd(1)	P(1)	C(30)	13.6(2)
P(1)	Pd(1)	C(1)	C(2)	-85.7(6)	P(1)	Pd(1)	C(1)	C(6)	89.0(7)
C(1)	Pd(1)	P(1)	C(17)	-58.6(2)	C(1)	Pd(1)	P(1)	C(21)	84.4(2)
C(1)	Pd(1)	P(1)	C(30)	-166.8(2)	P(2)	Pd(1)	C(1)	C(2)	94.2(6)
P(2)	Pd(1)	C(1)	C(6)	-91.1(7)	C(1)	Pd(1)	P(2)	C(9)	-58.5(2)
C(1)	Pd(1)	P(2)	C(13)	84.4(2)	C(1)	Pd(1)	P(2)	C(25)	-166.2(2)
P(3)	Pd(2)	P(4)	C(51)	-123.1(2)	P(3)	Pd(2)	P(4)	C(55)	93.9(2)
P(3)	Pd(2)	P(4)	C(59)	-15.4(2)	P(4)	Pd(2)	P(3)	C(43)	95.7(2)
P(4)	Pd(2)	P(3)	C(47)	-119.4(2)	P(4)	Pd(2)	P(3)	C(64)	-13.3(2)
P(3)	Pd(2)	C(35)	C(36)	85.6(6)	P(3)	Pd(2)	C(35)	C(40)	-88.0(7)
C(35)	Pd(2)	P(3)	C(43)	-86.3(2)	C(35)	Pd(2)	P(3)	C(47)	58.6(3)
C(35)	Pd(2)	P(3)	C(64)	164.7(2)	P(4)	Pd(2)	C(35)	C(36)	-95.1(7)
P(4)	Pd(2)	C(35)	C(40)	91.3(7)	C(35)	Pd(2)	P(4)	C(51)	58.9(2)
C(35)	Pd(2)	P(4)	C(55)	-84.1(2)	C(35)	Pd(2)	P(4)	C(59)	166.6(2)
C(25)	Fe(1)	C(26)	C(27)	-119.1(5)	C(26)	Fe(1)	C(25)	P(2)	-125.6(6)
C(26)	Fe(1)	C(25)	C(29)	118.9(4)	C(25)	Fe(1)	C(27)	C(26)	37.5(3)
C(25)	Fe(1)	C(27)	C(28)	-81.4(4)	C(27)	Fe(1)	C(25)	P(2)	-163.2(6)
C(27)	Fe(1)	C(25)	C(26)	-37.6(4)	C(27)	Fe(1)	C(25)	C(29)	81.3(4)
C(25)	Fe(1)	C(28)	C(27)	81.1(5)	C(25)	Fe(1)	C(28)	C(29)	-37.3(6)
C(28)	Fe(1)	C(25)	P(2)	153.0(6)	C(28)	Fe(1)	C(25)	C(26)	-81.5(4)
C(28)	Fe(1)	C(25)	C(29)	37.4(4)	C(25)	Fe(1)	C(29)	C(28)	119.4(7)
C(29)	Fe(1)	C(25)	P(2)	115.5(6)	C(29)	Fe(1)	C(25)	C(26)	-118.9(4)
C(25)	Fe(1)	C(30)	P(1)	19.0(6)	C(25)	Fe(1)	C(30)	C(31)	145.7(4)
C(25)	Fe(1)	C(30)	C(34)	-94.4(4)	C(30)	Fe(1)	C(25)	P(2)	19.3(7)
C(30)	Fe(1)	C(25)	C(26)	144.9(4)	C(30)	Fe(1)	C(25)	C(29)	-96.2(4)
C(25)	Fe(1)	C(31)	C(30)	-80.2(6)	C(25)	Fe(1)	C(31)	C(32)	160.8(5)
C(31)	Fe(1)	C(25)	P(2)	74.8(7)	C(31)	Fe(1)	C(25)	C(26)	-159.7(5)
C(31)	Fe(1)	C(25)	C(29)	-40.8(6)	C(25)	Fe(1)	C(32)	C(31)	-151.6(11)
C(25)	Fe(1)	C(32)	C(33)	90.1(13)	C(32)	Fe(1)	C(25)	P(2)	-149.9(12)
C(32)	Fe(1)	C(25)	C(26)	-24.3(14)	C(32)	Fe(1)	C(25)	C(29)	94.6(14)
C(25)	Fe(1)	C(33)	C(32)	-153.2(6)	C(25)	Fe(1)	C(33)	C(34)	85.5(10)

C(33)	Fe(1)	C(25)	P(2)	-80.4(6)	C(33)	Fe(1)	C(25)	C(26)	45.1(5)
C(33)	Fe(1)	C(25)	C(29)	164.0(4)	C(25)	Fe(1)	C(34)	C(30)	116.2(4)
C(25)	Fe(1)	C(34)	C(33)	-128.3(9)	C(34)	Fe(1)	C(25)	P(2)	-30.3(7)
C(34)	Fe(1)	C(25)	C(26)	95.3(4)	C(34)	Fe(1)	C(25)	C(29)	-145.8(4)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(26)	Fe(1)	C(27)	C(28)	-118.8(5)	C(27)	Fe(1)	C(26)	C(25)	119.1(5)
C(26)	Fe(1)	C(28)	C(27)	37.7(4)	C(26)	Fe(1)	C(28)	C(29)	-80.7(6)
C(28)	Fe(1)	C(26)	C(25)	81.3(3)	C(28)	Fe(1)	C(26)	C(27)	-37.9(3)
C(26)	Fe(1)	C(29)	C(25)	-37.6(3)	C(26)	Fe(1)	C(29)	C(28)	81.8(6)
C(29)	Fe(1)	C(26)	C(25)	37.6(3)	C(29)	Fe(1)	C(26)	C(27)	-81.5(3)
C(26)	Fe(1)	C(30)	P(1)	75.4(6)	C(26)	Fe(1)	C(30)	C(31)	-157.9(4)
C(26)	Fe(1)	C(30)	C(34)	-38.0(5)	C(30)	Fe(1)	C(26)	C(25)	-81.8(5)
C(30)	Fe(1)	C(26)	C(27)	159.1(3)	C(26)	Fe(1)	C(31)	C(30)	146.8(8)
C(26)	Fe(1)	C(31)	C(32)	27.8(11)	C(31)	Fe(1)	C(26)	C(25)	150.2(8)
C(31)	Fe(1)	C(26)	C(27)	31.1(10)	C(26)	Fe(1)	C(32)	C(31)	-170.2(4)
C(26)	Fe(1)	C(32)	C(33)	71.5(7)	C(32)	Fe(1)	C(26)	C(25)	171.4(4)
C(32)	Fe(1)	C(26)	C(27)	52.3(5)	C(26)	Fe(1)	C(33)	C(32)	-124.9(7)
C(26)	Fe(1)	C(33)	C(34)	113.7(8)	C(33)	Fe(1)	C(26)	C(25)	-150.6(4)
C(33)	Fe(1)	C(26)	C(27)	90.3(4)	C(26)	Fe(1)	C(34)	C(30)	162.1(3)
C(26)	Fe(1)	C(34)	C(33)	-82.3(10)	C(34)	Fe(1)	C(26)	C(25)	-108.4(3)
C(34)	Fe(1)	C(26)	C(27)	132.5(3)	C(27)	Fe(1)	C(28)	C(29)	-118.3(8)
C(28)	Fe(1)	C(27)	C(26)	118.8(5)	C(27)	Fe(1)	C(29)	C(25)	-81.3(5)
C(27)	Fe(1)	C(29)	C(28)	38.1(6)	C(29)	Fe(1)	C(27)	C(26)	80.9(4)
C(29)	Fe(1)	C(27)	C(28)	-37.9(4)	C(27)	Fe(1)	C(30)	P(1)	-153.4(8)
C(27)	Fe(1)	C(30)	C(31)	-26.7(12)	C(27)	Fe(1)	C(30)	C(34)	93.2(11)
C(30)	Fe(1)	C(27)	C(26)	-148.8(9)	C(30)	Fe(1)	C(27)	C(28)	92.3(10)
C(27)	Fe(1)	C(31)	C(30)	170.5(3)	C(27)	Fe(1)	C(31)	C(32)	51.5(6)
C(31)	Fe(1)	C(27)	C(26)	-169.0(3)	C(31)	Fe(1)	C(27)	C(28)	72.1(4)
C(27)	Fe(1)	C(32)	C(31)	-139.3(5)	C(27)	Fe(1)	C(32)	C(33)	102.4(7)
C(32)	Fe(1)	C(27)	C(26)	-138.6(4)	C(32)	Fe(1)	C(27)	C(28)	102.6(5)
C(27)	Fe(1)	C(33)	C(32)	-83.7(8)	C(27)	Fe(1)	C(33)	C(34)	155.0(8)
C(33)	Fe(1)	C(27)	C(26)	-99.9(6)	C(33)	Fe(1)	C(27)	C(28)	141.3(6)
C(27)	Fe(1)	C(34)	C(30)	-153.2(4)	C(27)	Fe(1)	C(34)	C(33)	-37.7(12)
C(34)	Fe(1)	C(27)	C(26)	-75.8(6)	C(34)	Fe(1)	C(27)	C(28)	165.4(5)
C(28)	Fe(1)	C(29)	C(25)	-119.4(7)	C(29)	Fe(1)	C(28)	C(27)	118.3(8)
C(28)	Fe(1)	C(30)	P(1)	-81.2(5)	C(28)	Fe(1)	C(30)	C(31)	45.6(4)
C(28)	Fe(1)	C(30)	C(34)	165.5(3)	C(30)	Fe(1)	C(28)	C(27)	-153.3(4)
C(30)	Fe(1)	C(28)	C(29)	88.3(6)	C(28)	Fe(1)	C(31)	C(30)	-149.8(3)

C(28)	Fe(1)	C(31)	C(32)	91.2(5)	C(31)	Fe(1)	C(28)	C(27)	-125.2(4)
C(31)	Fe(1)	C(28)	C(29)	116.5(6)	C(28)	Fe(1)	C(32)	C(31)	-99.0(5)
C(28)	Fe(1)	C(32)	C(33)	142.7(7)	C(32)	Fe(1)	C(28)	C(27)	-83.9(6)
C(32)	Fe(1)	C(28)	C(29)	157.8(7)	C(28)	Fe(1)	C(33)	C(32)	-51.4(11)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C(28)	Fe(1)	C(33)	C(34)	-172.7(7)
C(33)	Fe(1)	C(28)	C(29)	-172.2(8)
C(28)	Fe(1)	C(34)	C(33)	34(3)
C(34)	Fe(1)	C(28)	C(29)	159(2)
C(29)	Fe(1)	C(30)	C(31)	96.0(4)
C(30)	Fe(1)	C(29)	C(25)	114.9(4)
C(29)	Fe(1)	C(31)	C(30)	-108.7(3)
C(31)	Fe(1)	C(29)	C(25)	161.1(3)
C(29)	Fe(1)	C(32)	C(31)	-77.5(7)
C(32)	Fe(1)	C(29)	C(25)	-153.1(6)
C(29)	Fe(1)	C(33)	C(32)	-80(3)
C(33)	Fe(1)	C(29)	C(25)	-86(3)
C(29)	Fe(1)	C(34)	C(30)	71.8(10)
C(34)	Fe(1)	C(29)	C(25)	67.5(10)
C(30)	Fe(1)	C(31)	C(32)	-119.0(6)
C(31)	Fe(1)	C(30)	C(34)	119.9(5)
C(30)	Fe(1)	C(32)	C(33)	-81.0(7)
C(32)	Fe(1)	C(30)	C(31)	-37.8(5)
C(30)	Fe(1)	C(33)	C(32)	81.8(8)
C(33)	Fe(1)	C(30)	P(1)	153.3(7)
C(33)	Fe(1)	C(30)	C(34)	39.9(5)
C(34)	Fe(1)	C(30)	P(1)	113.4(6)
C(31)	Fe(1)	C(32)	C(33)	-118.3(9)
C(31)	Fe(1)	C(33)	C(32)	38.4(7)
C(33)	Fe(1)	C(31)	C(30)	81.9(4)
C(31)	Fe(1)	C(34)	C(30)	-36.7(3)
C(34)	Fe(1)	C(31)	C(30)	37.4(3)
C(32)	Fe(1)	C(33)	C(34)	-121.3(13)
C(32)	Fe(1)	C(34)	C(30)	-80.3(5)
C(34)	Fe(1)	C(32)	C(31)	81.2(5)
C(33)	Fe(1)	C(34)	C(30)	-115.6(11)
C(59)	Fe(2)	C(60)	C(61)	120.3(5)
C(60)	Fe(2)	C(59)	C(63)	-118.3(4)
C(33)	Fe(1)	C(28)	C(27)	-53.9(9)
C(28)	Fe(1)	C(34)	C(30)	-82(2)
C(34)	Fe(1)	C(28)	C(27)	-83(2)
C(29)	Fe(1)	C(30)	P(1)	-30.7(6)
C(29)	Fe(1)	C(30)	C(34)	-144.1(4)
C(30)	Fe(1)	C(29)	C(28)	-125.7(6)
C(29)	Fe(1)	C(31)	C(32)	132.3(5)
C(31)	Fe(1)	C(29)	C(28)	-79.5(6)
C(29)	Fe(1)	C(32)	C(33)	164.2(7)
C(32)	Fe(1)	C(29)	C(28)	-33.7(9)
C(29)	Fe(1)	C(33)	C(34)	159(2)
C(33)	Fe(1)	C(29)	C(28)	34(3)
C(29)	Fe(1)	C(34)	C(33)	-172.6(10)
C(34)	Fe(1)	C(29)	C(28)	-173.1(9)
C(31)	Fe(1)	C(30)	P(1)	-126.7(7)
C(30)	Fe(1)	C(32)	C(31)	37.3(4)
C(32)	Fe(1)	C(30)	P(1)	-164.5(6)
C(32)	Fe(1)	C(30)	C(34)	82.1(5)
C(30)	Fe(1)	C(33)	C(34)	-39.5(8)
C(33)	Fe(1)	C(30)	C(31)	-80.0(5)
C(30)	Fe(1)	C(34)	C(33)	115.6(11)
C(34)	Fe(1)	C(30)	C(31)	-119.9(5)
C(32)	Fe(1)	C(31)	C(30)	119.0(6)
C(31)	Fe(1)	C(33)	C(34)	-82.9(9)
C(33)	Fe(1)	C(31)	C(32)	-37.0(5)
C(31)	Fe(1)	C(34)	C(33)	78.8(9)
C(34)	Fe(1)	C(31)	C(32)	-81.6(5)
C(33)	Fe(1)	C(32)	C(31)	118.3(9)
C(32)	Fe(1)	C(34)	C(33)	35.3(10)
C(34)	Fe(1)	C(32)	C(33)	-37.1(7)
C(34)	Fe(1)	C(33)	C(32)	121.3(13)
C(60)	Fe(2)	C(59)	P(4)	128.6(7)
C(59)	Fe(2)	C(61)	C(60)	-36.6(3)

C(59)	Fe(2)	C(61)	C(62)	80.9(4)	C(61)	Fe(2)	C(59)	P(4)	165.7(6)
C(61)	Fe(2)	C(59)	C(60)	37.1(4)	C(61)	Fe(2)	C(59)	C(63)	-81.1(4)
C(59)	Fe(2)	C(62)	C(61)	-81.6(5)	C(59)	Fe(2)	C(62)	C(63)	38.3(6)
C(62)	Fe(2)	C(59)	P(4)	-150.1(6)	C(62)	Fe(2)	C(59)	C(60)	81.3(4)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(62)	Fe(2)	C(59)	C(63)	-37.0(4)	C(59)	Fe(2)	C(63)	C(62)	-118.9(8)
C(63)	Fe(2)	C(59)	P(4)	-113.1(7)	C(63)	Fe(2)	C(59)	C(60)	118.3(4)
C(59)	Fe(2)	C(64)	P(3)	-21.0(6)	C(59)	Fe(2)	C(64)	C(65)	92.5(3)
C(59)	Fe(2)	C(64)	C(68)	-148.7(3)	C(64)	Fe(2)	C(59)	P(4)	-20.4(7)
C(64)	Fe(2)	C(59)	C(60)	-149.0(4)	C(64)	Fe(2)	C(59)	C(63)	92.7(4)
C(59)	Fe(2)	C(65)	C(64)	-117.0(3)	C(59)	Fe(2)	C(65)	C(66)	124.9(6)
C(65)	Fe(2)	C(59)	P(4)	28.6(6)	C(65)	Fe(2)	C(59)	C(60)	-100.0(4)
C(65)	Fe(2)	C(59)	C(63)	141.7(4)	C(59)	Fe(2)	C(66)	C(65)	-85.7(6)
C(59)	Fe(2)	C(66)	C(67)	154.1(4)	C(66)	Fe(2)	C(59)	P(4)	76.5(6)
C(66)	Fe(2)	C(59)	C(60)	-52.1(4)	C(66)	Fe(2)	C(59)	C(63)	-170.4(3)
C(59)	Fe(2)	C(67)	C(66)	-83.1(9)	C(59)	Fe(2)	C(67)	C(68)	158.8(7)
C(67)	Fe(2)	C(59)	P(4)	140.3(7)	C(67)	Fe(2)	C(59)	C(60)	11.7(10)
C(67)	Fe(2)	C(59)	C(63)	-106.6(9)	C(59)	Fe(2)	C(68)	C(64)	76.6(5)
C(59)	Fe(2)	C(68)	C(67)	-164.0(4)	C(68)	Fe(2)	C(59)	P(4)	-74.6(7)
C(68)	Fe(2)	C(59)	C(60)	156.8(4)	C(68)	Fe(2)	C(59)	C(63)	38.6(6)
C(60)	Fe(2)	C(61)	C(62)	117.5(5)	C(61)	Fe(2)	C(60)	C(59)	-120.3(5)
C(60)	Fe(2)	C(62)	C(61)	-38.4(4)	C(60)	Fe(2)	C(62)	C(63)	81.5(7)
C(62)	Fe(2)	C(60)	C(59)	-81.5(3)	C(62)	Fe(2)	C(60)	C(61)	38.7(3)
C(60)	Fe(2)	C(63)	C(59)	37.5(3)	C(60)	Fe(2)	C(63)	C(62)	-81.4(7)
C(63)	Fe(2)	C(60)	C(59)	-38.7(3)	C(63)	Fe(2)	C(60)	C(61)	81.6(4)
C(60)	Fe(2)	C(64)	P(3)	-74.7(6)	C(60)	Fe(2)	C(64)	C(65)	38.7(5)
C(60)	Fe(2)	C(64)	C(68)	157.6(4)	C(64)	Fe(2)	C(60)	C(59)	76.0(6)
C(64)	Fe(2)	C(60)	C(61)	-163.7(4)	C(60)	Fe(2)	C(65)	C(64)	-163.0(2)
C(60)	Fe(2)	C(65)	C(66)	78.9(6)	C(65)	Fe(2)	C(60)	C(59)	103.8(3)
C(65)	Fe(2)	C(60)	C(61)	-135.9(3)	C(60)	Fe(2)	C(66)	C(65)	-117.2(5)
C(60)	Fe(2)	C(66)	C(67)	122.5(5)	C(66)	Fe(2)	C(60)	C(59)	144.5(3)
C(66)	Fe(2)	C(60)	C(61)	-95.2(4)	C(60)	Fe(2)	C(67)	C(66)	-74.3(5)
C(60)	Fe(2)	C(67)	C(68)	167.6(3)	C(67)	Fe(2)	C(60)	C(59)	-175.7(3)
C(67)	Fe(2)	C(60)	C(61)	-55.4(4)	C(60)	Fe(2)	C(68)	C(64)	-152.2(7)
C(60)	Fe(2)	C(68)	C(67)	-32.8(9)	C(68)	Fe(2)	C(60)	C(59)	-151.1(6)
C(68)	Fe(2)	C(60)	C(61)	-30.8(9)	C(61)	Fe(2)	C(62)	C(63)	119.9(9)
C(62)	Fe(2)	C(61)	C(60)	-117.5(5)	C(61)	Fe(2)	C(63)	C(59)	81.3(5)
C(61)	Fe(2)	C(63)	C(62)	-37.6(7)	C(63)	Fe(2)	C(61)	C(60)	-81.0(4)

C(63)	Fe(2)	C(61)	C(62)	36.5(4)	C(61)	Fe(2)	C(64)	P(3)	140.6(8)
C(61)	Fe(2)	C(64)	C(65)	-106.0(10)	C(61)	Fe(2)	C(64)	C(68)	12.8(11)
C(64)	Fe(2)	C(61)	C(60)	158.7(8)	C(64)	Fe(2)	C(61)	C(62)	-83.8(9)
C(61)	Fe(2)	C(65)	C(64)	151.4(4)	C(61)	Fe(2)	C(65)	C(66)	33.3(8)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(65)	Fe(2)	C(61)	C(60)	74.8(5)	C(65)	Fe(2)	C(61)	C(62)	-167.7(4)
C(61)	Fe(2)	C(66)	C(65)	-159.0(6)	C(61)	Fe(2)	C(66)	C(67)	80.7(6)
C(66)	Fe(2)	C(61)	C(60)	96.2(4)	C(66)	Fe(2)	C(61)	C(62)	-146.3(4)
C(61)	Fe(2)	C(67)	C(66)	-106.7(5)	C(61)	Fe(2)	C(67)	C(68)	135.2(4)
C(67)	Fe(2)	C(61)	C(60)	135.7(4)	C(67)	Fe(2)	C(61)	C(62)	-106.8(4)
C(61)	Fe(2)	C(68)	C(64)	-175.3(3)	C(61)	Fe(2)	C(68)	C(67)	-55.9(4)
C(68)	Fe(2)	C(61)	C(60)	168.3(3)	C(68)	Fe(2)	C(61)	C(62)	-74.2(4)
C(62)	Fe(2)	C(63)	C(59)	118.9(8)	C(63)	Fe(2)	C(62)	C(61)	-119.9(9)
C(62)	Fe(2)	C(64)	P(3)	75.8(4)	C(62)	Fe(2)	C(64)	C(65)	-170.8(2)
C(62)	Fe(2)	C(64)	C(68)	-52.0(3)	C(64)	Fe(2)	C(62)	C(61)	154.1(4)
C(64)	Fe(2)	C(62)	C(63)	-86.0(7)	C(62)	Fe(2)	C(65)	C(64)	55(2)
C(62)	Fe(2)	C(65)	C(66)	-63(2)	C(65)	Fe(2)	C(62)	C(61)	106(2)
C(65)	Fe(2)	C(62)	C(63)	-134(2)	C(62)	Fe(2)	C(66)	C(65)	169.6(7)
C(62)	Fe(2)	C(66)	C(67)	49.3(9)	C(66)	Fe(2)	C(62)	C(61)	50.5(8)
C(66)	Fe(2)	C(62)	C(63)	170.4(7)	C(62)	Fe(2)	C(67)	C(66)	-146.9(5)
C(62)	Fe(2)	C(67)	C(68)	95.0(4)	C(67)	Fe(2)	C(62)	C(61)	80.8(5)
C(67)	Fe(2)	C(62)	C(63)	-159.3(7)	C(62)	Fe(2)	C(68)	C(64)	144.3(3)
C(62)	Fe(2)	C(68)	C(67)	-96.3(3)	C(68)	Fe(2)	C(62)	C(61)	122.7(4)
C(68)	Fe(2)	C(62)	C(63)	-117.4(6)	C(63)	Fe(2)	C(64)	P(3)	28.4(5)
C(63)	Fe(2)	C(64)	C(65)	141.8(3)	C(63)	Fe(2)	C(64)	C(68)	-99.3(3)
C(64)	Fe(2)	C(63)	C(59)	-117.0(4)	C(64)	Fe(2)	C(63)	C(62)	124.1(7)
C(63)	Fe(2)	C(65)	C(64)	-70.9(8)	C(63)	Fe(2)	C(65)	C(66)	171.0(8)
C(65)	Fe(2)	C(63)	C(59)	-71.4(9)	C(65)	Fe(2)	C(63)	C(62)	169.7(8)
C(63)	Fe(2)	C(66)	C(65)	-139(2)	C(63)	Fe(2)	C(66)	C(67)	100(2)
C(66)	Fe(2)	C(63)	C(59)	61(2)	C(66)	Fe(2)	C(63)	C(62)	-58(2)
C(63)	Fe(2)	C(67)	C(66)	-167.8(6)	C(63)	Fe(2)	C(67)	C(68)	74.1(6)
C(67)	Fe(2)	C(63)	C(59)	151.6(5)	C(67)	Fe(2)	C(63)	C(62)	32.7(10)
C(63)	Fe(2)	C(68)	C(64)	104.3(3)	C(63)	Fe(2)	C(68)	C(67)	-136.3(3)
C(68)	Fe(2)	C(63)	C(59)	-163.1(3)	C(68)	Fe(2)	C(63)	C(62)	78.0(7)
C(64)	Fe(2)	C(65)	C(66)	-118.1(7)	C(65)	Fe(2)	C(64)	P(3)	-113.4(5)
C(65)	Fe(2)	C(64)	C(68)	118.8(3)	C(64)	Fe(2)	C(66)	C(65)	38.5(5)
C(64)	Fe(2)	C(66)	C(67)	-81.7(5)	C(66)	Fe(2)	C(64)	P(3)	-151.2(5)
C(66)	Fe(2)	C(64)	C(65)	-37.8(3)	C(66)	Fe(2)	C(64)	C(68)	81.0(3)

C(64)	Fe(2)	C(67)	C(66)	81.0(5)	C(64)	Fe(2)	C(67)	C(68)	-37.1(3)
C(67)	Fe(2)	C(64)	P(3)	165.4(5)	C(67)	Fe(2)	C(64)	C(65)	-81.1(3)
C(67)	Fe(2)	C(64)	C(68)	37.7(3)	C(64)	Fe(2)	C(68)	C(67)	119.4(5)
C(68)	Fe(2)	C(64)	P(3)	127.8(6)	C(68)	Fe(2)	C(64)	C(65)	-118.8(3)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(65)	Fe(2)	C(66)	C(67)	-120.3(8)	C(66)	Fe(2)	C(65)	C(64)	118.1(7)
C(65)	Fe(2)	C(67)	C(66)	36.8(5)	C(65)	Fe(2)	C(67)	C(68)	-81.3(4)
C(67)	Fe(2)	C(65)	C(64)	81.3(4)	C(67)	Fe(2)	C(65)	C(66)	-36.8(6)
C(65)	Fe(2)	C(68)	C(64)	-38.1(3)	C(65)	Fe(2)	C(68)	C(67)	81.2(3)
C(68)	Fe(2)	C(65)	C(64)	37.4(2)	C(68)	Fe(2)	C(65)	C(66)	-80.7(6)
C(66)	Fe(2)	C(67)	C(68)	-118.1(5)	C(67)	Fe(2)	C(66)	C(65)	120.3(8)
C(66)	Fe(2)	C(68)	C(64)	-81.5(3)	C(66)	Fe(2)	C(68)	C(67)	37.8(3)
C(68)	Fe(2)	C(66)	C(65)	81.9(6)	C(68)	Fe(2)	C(66)	C(67)	-38.4(4)
C(67)	Fe(2)	C(68)	C(64)	-119.4(5)	C(68)	Fe(2)	C(67)	C(66)	118.1(5)
Pd(1)	P(1)	C(17)	C(18)	-32.3(3)	Pd(1)	P(1)	C(17)	C(19)	84.6(8)
Pd(1)	P(1)	C(17)	C(20)	-150.9(7)	Pd(1)	P(1)	C(21)	C(22)	-83.5(6)
Pd(1)	P(1)	C(21)	C(23)	155.8(5)	Pd(1)	P(1)	C(21)	C(24)	32.6(3)
Pd(1)	P(1)	C(30)	Fe(1)	-23.0(4)	Pd(1)	P(1)	C(30)	C(31)	-113.6(7)
Pd(1)	P(1)	C(30)	C(34)	58.7(6)	C(17)	P(1)	C(21)	C(22)	62.7(6)
C(17)	P(1)	C(21)	C(23)	-58.1(5)	C(17)	P(1)	C(21)	C(24)	178.8(3)
C(21)	P(1)	C(17)	C(18)	-175.2(3)	C(21)	P(1)	C(17)	C(19)	-58.4(8)
C(21)	P(1)	C(17)	C(20)	66.1(8)	C(17)	P(1)	C(30)	Fe(1)	-146.0(4)
C(17)	P(1)	C(30)	C(31)	123.4(8)	C(17)	P(1)	C(30)	C(34)	-64.3(7)
C(30)	P(1)	C(17)	C(18)	65.8(4)	C(30)	P(1)	C(17)	C(19)	-177.3(8)
C(30)	P(1)	C(17)	C(20)	-52.9(9)	C(21)	P(1)	C(30)	Fe(1)	91.3(5)
C(21)	P(1)	C(30)	C(31)	0.7(9)	C(21)	P(1)	C(30)	C(34)	173.0(6)
C(30)	P(1)	C(21)	C(22)	-179.2(6)	C(30)	P(1)	C(21)	C(23)	60.1(6)
C(30)	P(1)	C(21)	C(24)	-63.1(4)	Pd(1)	P(2)	C(9)	C(10)	84.9(8)
Pd(1)	P(2)	C(9)	C(11)	-32.7(3)	Pd(1)	P(2)	C(9)	C(12)	-151.5(7)
Pd(1)	P(2)	C(13)	C(14)	32.3(4)	Pd(1)	P(2)	C(13)	C(15)	154.7(5)
Pd(1)	P(2)	C(13)	C(16)	-83.4(6)	Pd(1)	P(2)	C(25)	Fe(1)	-23.1(4)
Pd(1)	P(2)	C(25)	C(26)	-112.1(7)	Pd(1)	P(2)	C(25)	C(29)	60.6(5)
C(9)	P(2)	C(13)	C(14)	178.7(4)	C(9)	P(2)	C(13)	C(15)	-58.8(6)
C(9)	P(2)	C(13)	C(16)	63.1(7)	C(13)	P(2)	C(9)	C(10)	-58.0(9)
C(13)	P(2)	C(9)	C(11)	-175.7(3)	C(13)	P(2)	C(9)	C(12)	65.5(8)
C(9)	P(2)	C(25)	Fe(1)	-146.3(5)	C(9)	P(2)	C(25)	C(26)	124.6(8)
C(9)	P(2)	C(25)	C(29)	-62.6(7)	C(25)	P(2)	C(9)	C(10)	-178.5(8)
C(25)	P(2)	C(9)	C(11)	63.9(5)	C(25)	P(2)	C(9)	C(12)	-54.9(9)

C(13)	P(2)	C(25)	Fe(1)	90.6(6)	C(13)	P(2)	C(25)	C(26)	1.6(9)
C(13)	P(2)	C(25)	C(29)	174.4(6)	C(25)	P(2)	C(13)	C(14)	-62.1(5)
C(25)	P(2)	C(13)	C(15)	60.3(6)	C(25)	P(2)	C(13)	C(16)	-177.8(6)
Pd(2)	P(3)	C(43)	C(44)	-34.0(3)	Pd(2)	P(3)	C(43)	C(45)	80.8(5)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Pd(2)	P(3)	C(43)	C(46)	-156.6(4)	Pd(2)	P(3)	C(47)	C(48)	-91.4(9)
Pd(2)	P(3)	C(47)	C(49)	143.9(8)	Pd(2)	P(3)	C(47)	C(50)	27.0(4)
Pd(2)	P(3)	C(64)	Fe(2)	25.0(3)	Pd(2)	P(3)	C(64)	C(65)	-58.3(5)
Pd(2)	P(3)	C(64)	C(68)	116.1(6)	C(43)	P(3)	C(47)	C(48)	54.0(9)
C(43)	P(3)	C(47)	C(49)	-70.7(9)	C(43)	P(3)	C(47)	C(50)	172.4(3)
C(47)	P(3)	C(43)	C(44)	177.4(3)	C(47)	P(3)	C(43)	C(45)	-67.8(5)
C(47)	P(3)	C(43)	C(46)	54.8(5)	C(43)	P(3)	C(64)	Fe(2)	-90.1(5)
C(43)	P(3)	C(64)	C(65)	-173.4(5)	C(43)	P(3)	C(64)	C(68)	1.0(7)
C(64)	P(3)	C(43)	C(44)	61.6(4)	C(64)	P(3)	C(43)	C(45)	176.4(5)
C(64)	P(3)	C(43)	C(46)	-61.0(6)	C(47)	P(3)	C(64)	Fe(2)	149.0(4)
C(47)	P(3)	C(64)	C(65)	65.7(6)	C(47)	P(3)	C(64)	C(68)	-119.9(7)
C(64)	P(3)	C(47)	C(48)	171.9(8)	C(64)	P(3)	C(47)	C(49)	47.2(10)
C(64)	P(3)	C(47)	C(50)	-69.7(4)	Pd(2)	P(4)	C(51)	C(52)	33.3(5)
Pd(2)	P(4)	C(51)	C(53)	152.5(7)	Pd(2)	P(4)	C(51)	C(54)	-84.8(10)
Pd(2)	P(4)	C(55)	C(56)	-34.3(4)	Pd(2)	P(4)	C(55)	C(57)	-156.9(4)
Pd(2)	P(4)	C(55)	C(58)	81.7(6)	Pd(2)	P(4)	C(59)	Fe(2)	25.0(4)
Pd(2)	P(4)	C(59)	C(60)	115.5(8)	Pd(2)	P(4)	C(59)	C(63)	-57.2(5)
C(51)	P(4)	C(55)	C(56)	178.8(4)	C(51)	P(4)	C(55)	C(57)	56.2(4)
C(51)	P(4)	C(55)	C(58)	-65.2(7)	C(55)	P(4)	C(51)	C(52)	176.3(4)
C(55)	P(4)	C(51)	C(53)	-64.5(8)	C(55)	P(4)	C(51)	C(54)	58.2(10)
C(51)	P(4)	C(59)	Fe(2)	149.1(5)	C(51)	P(4)	C(59)	C(60)	-120.4(8)
C(51)	P(4)	C(59)	C(63)	66.9(7)	C(59)	P(4)	C(51)	C(52)	-64.2(6)
C(59)	P(4)	C(51)	C(53)	55.0(9)	C(59)	P(4)	C(51)	C(54)	177.8(9)
C(55)	P(4)	C(59)	Fe(2)	-88.6(6)	C(55)	P(4)	C(59)	C(60)	1.9(9)
C(55)	P(4)	C(59)	C(63)	-170.8(5)	C(59)	P(4)	C(55)	C(56)	60.7(5)
C(59)	P(4)	C(55)	C(57)	-61.9(5)	C(59)	P(4)	C(55)	C(58)	176.7(6)
C(8)	O(2)	C(7)	O(1)	2.5(15)	C(8)	O(2)	C(7)	C(4)	-177.1(9)
C(42)	O(4)	C(41)	O(3)	-0.1(17)	C(42)	O(4)	C(41)	C(38)	179.9(10)
Pd(1)	C(1)	C(2)	C(3)	173.8(6)	Pd(1)	C(1)	C(6)	C(5)	-173.3(6)
C(2)	C(1)	C(6)	C(5)	1.4(13)	C(6)	C(1)	C(2)	C(3)	-1.0(13)
C(1)	C(2)	C(3)	C(4)	-1.1(13)	C(2)	C(3)	C(4)	C(5)	3.0(13)
C(2)	C(3)	C(4)	C(7)	-178.3(8)	C(3)	C(4)	C(5)	C(6)	-2.6(13)
C(3)	C(4)	C(7)	O(1)	-179.4(9)	C(3)	C(4)	C(7)	O(2)	0.2(9)

C(5)	C(4)	C(7)	O(1)	-0.7(13)	C(5)	C(4)	C(7)	O(2)	178.9(8)
C(7)	C(4)	C(5)	C(6)	178.6(8)	C(4)	C(5)	C(6)	C(1)	0.5(11)
Fe(1)	C(25)	C(26)	C(27)	59.7(6)	Fe(1)	C(25)	C(29)	C(28)	-60.0(5)
P(2)	C(25)	C(26)	Fe(1)	116.2(6)	P(2)	C(25)	C(26)	C(27)	175.9(6)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
P(2)	C(25)	C(29)	Fe(1)	-116.8(5)	P(2)	C(25)	C(29)	C(28)	-176.8(5)
C(26)	C(25)	C(29)	Fe(1)	57.6(5)	C(26)	C(25)	C(29)	C(28)	-2.4(8)
C(29)	C(25)	C(26)	Fe(1)	-57.5(5)	C(29)	C(25)	C(26)	C(27)	2.2(9)
Fe(1)	C(26)	C(27)	C(28)	60.2(6)	C(25)	C(26)	C(27)	Fe(1)	-61.4(5)
C(25)	C(26)	C(27)	C(28)	-1.2(9)	Fe(1)	C(27)	C(28)	C(29)	60.1(5)
C(26)	C(27)	C(28)	Fe(1)	-60.5(5)	C(26)	C(27)	C(28)	C(29)	-0.4(9)
Fe(1)	C(28)	C(29)	C(25)	61.5(5)	C(27)	C(28)	C(29)	Fe(1)	-59.7(5)
C(27)	C(28)	C(29)	C(25)	1.8(9)	Fe(1)	C(30)	C(31)	C(32)	58.4(7)
Fe(1)	C(30)	C(34)	C(33)	-61.5(7)	P(1)	C(30)	C(31)	Fe(1)	115.8(6)
P(1)	C(30)	C(31)	C(32)	174.3(7)	P(1)	C(30)	C(34)	Fe(1)	-115.4(4)
P(1)	C(30)	C(34)	C(33)	-176.9(7)	C(31)	C(30)	C(34)	Fe(1)	58.5(5)
C(31)	C(30)	C(34)	C(33)	-2.9(10)	C(34)	C(30)	C(31)	Fe(1)	-57.3(5)
C(34)	C(30)	C(31)	C(32)	1.1(9)	Fe(1)	C(31)	C(32)	C(33)	61.1(9)
C(30)	C(31)	C(32)	Fe(1)	-59.9(5)	C(30)	C(31)	C(32)	C(33)	1.2(12)
Fe(1)	C(32)	C(33)	C(34)	58.7(8)	C(31)	C(32)	C(33)	Fe(1)	-61.8(7)
C(31)	C(32)	C(33)	C(34)	-3.1(14)	Fe(1)	C(33)	C(34)	C(30)	63.1(6)
C(32)	C(33)	C(34)	Fe(1)	-59.3(9)	C(32)	C(33)	C(34)	C(30)	3.8(13)
Pd(2)	C(35)	C(36)	C(37)	-171.8(7)	Pd(2)	C(35)	C(40)	C(39)	170.6(7)
C(36)	C(35)	C(40)	C(39)	-2.9(13)	C(40)	C(35)	C(36)	C(37)	1.9(13)
C(35)	C(36)	C(37)	C(38)	1.6(14)	C(36)	C(37)	C(38)	C(39)	-4.0(14)
C(36)	C(37)	C(38)	C(41)	176.5(9)	C(37)	C(38)	C(39)	C(40)	3.0(14)
C(37)	C(38)	C(41)	O(3)	-176.3(11)	C(37)	C(38)	C(41)	O(4)	3.7(15)
C(39)	C(38)	C(41)	O(3)	4.2(17)	C(39)	C(38)	C(41)	O(4)	-175.8(9)
C(41)	C(38)	C(39)	C(40)	-177.5(9)	C(38)	C(39)	C(40)	C(35)	0.4(11)
Fe(2)	C(59)	C(60)	C(61)	-59.3(6)	Fe(2)	C(59)	C(63)	C(62)	60.3(5)
P(4)	C(59)	C(60)	Fe(2)	-115.6(7)	P(4)	C(59)	C(60)	C(61)	-174.9(6)
P(4)	C(59)	C(63)	Fe(2)	116.4(5)	P(4)	C(59)	C(63)	C(62)	176.6(5)
C(60)	C(59)	C(63)	Fe(2)	-58.2(5)	C(60)	C(59)	C(63)	C(62)	2.1(8)
C(63)	C(59)	C(60)	Fe(2)	57.9(5)	C(63)	C(59)	C(60)	C(61)	-1.4(9)
Fe(2)	C(60)	C(61)	C(62)	-60.6(6)	C(59)	C(60)	C(61)	Fe(2)	60.9(6)
C(59)	C(60)	C(61)	C(62)	0.2(8)	Fe(2)	C(61)	C(62)	C(63)	-59.7(6)
C(60)	C(61)	C(62)	Fe(2)	60.8(5)	C(60)	C(61)	C(62)	C(63)	1.1(10)
Fe(2)	C(62)	C(63)	C(59)	-61.0(5)	C(61)	C(62)	C(63)	Fe(2)	59.0(6)

C(61)	C(62)	C(63)	C(59)	-2.0(9)	Fe(2)	C(64)	C(65)	C(66)	60.8(4)
Fe(2)	C(64)	C(68)	C(67)	-59.5(5)	P(3)	C(64)	C(65)	Fe(2)	117.0(4)
P(3)	C(64)	C(65)	C(66)	177.9(5)	P(3)	C(64)	C(68)	Fe(2)	-116.5(6)
P(3)	C(64)	C(68)	C(67)	-176.0(5)	C(65)	C(64)	C(68)	Fe(2)	58.5(4)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(65)	C(64)	C(68)	C(67)	-1.0(7)	C(68)	C(64)	C(65)	Fe(2)	-58.7(4)
C(68)	C(64)	C(65)	C(66)	2.1(7)	Fe(2)	C(65)	C(66)	C(67)	58.5(5)
C(64)	C(65)	C(66)	Fe(2)	-61.0(4)		C(64)	C(65)	C(66)	C(67) -2.5(8)
Fe(2)	C(66)	C(67)	C(68)	60.7(5)		C(65)	C(66)	C(67)	Fe(2) -58.7(5)
C(65)	C(66)	C(67)	C(68)	1.9(9)	Fe(2)	C(67)	C(68)	C(64)	60.5(4)
C(66)	C(67)	C(68)	Fe(2)	-61.1(5)		C(66)	C(67)	C(68)	C(64) -0.6(8)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 9. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	atom	atom	distance
F(1)	C(10)	3.481(17)	F(1)	C(14)[1)]	3.412(17)
F(2)	C(26)[1)]	3.55(2)	F(3)	C(61)[2)]	3.338(10)
F(4)	C(67)[2)]	3.547(10)	F(6)	C(8)[2)]	3.32(2)
F(7)	C(23)[3)]	3.534(11)	F(8)	C(32)[1)]	3.230(11)
F(8)	C(44)[4)]	3.446(15)	O(1)	C(18)[5)]	3.484(12)
O(1)	C(19)[5)]	3.425(9)	O(1)	C(20)[5)]	3.511(7)
O(1)	C(57)	3.590(14)	O(3)	C(14)[1)]	3.589(8)
C(7)	C(57)	3.517(17)	C(8)	F(6)[6)]	3.32(2)
C(8)	C(45)[7)]	3.415(9)	C(10)	F(1)	3.481(17)
C(10)	C(58)	3.510(9)	C(14)	F(1)[8)]	3.412(17)
C(14)	O(3)[8)]	3.589(8)	C(18)	O(1)[5)]	3.484(12)
C(19)	O(1)[5)]	3.425(9)	C(20)	O(1)[5)]	3.511(7)
C(23)	F(7)[9)]	3.534(11)	C(26)	F(2)[8)]	3.55(2)
C(26)	C(52)[1)]	3.444(18)	C(27)	C(52)[1)]	3.45(2)
C(32)	F(8)[8)]	3.230(11)	C(32)	C(46)[10)]	3.550(16)
C(44)	F(8)[11)]	3.446(15)	C(45)	C(8)[12)]	3.415(9)
C(46)	C(32)[13)]	3.550(16)	C(52)	C(26)[8)]	3.444(18)
C(52)	C(27)[8)]	3.45(2)	C(57)	O(1)	3.590(14)
C(57)	C(7)	3.517(17)	C(58)	C(10)	3.510(9)
C(61)	F(3)[6)]	3.338(10)	C(67)	F(4)[6)]	3.547(10)

Symmetry Operators:

(1) -X+2,Y+1/2-1,-Z+1/2
(2) -X+1,Y+1/2-1,-Z+1/2+1
(3) X-1,-Y+1/2-1,Z+1/2
(4) X,Y-1,Z
(5) -X+2,-Y+1,-Z+1
(6) -X+1,Y+1/2,-Z+1/2+1
(7) X,-Y+1/2,Z+1/2
(8) -X+2,Y+1/2,-Z+1/2
(9) X+1,-Y+1/2-1,Z+1/2-1
(10) X+1,-Y+1/2,Z+1/2-1
(11) X,Y+1,Z
(12) X,-Y+1/2,Z+1/2-1
(13) X-1,-Y+1/2,Z+1/2

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
F(1)	H(10)	2.537	F(1)	H(19)[1)]	2.475
F(1)	H(20)[1)]	3.306	F(1)	H(54)	3.135
F(1)	H(55)	2.963	F(2)	H(17)[1)]	3.473
F(2)	H(19)[1)]	3.142	F(2)	H(20)[1)]	3.236
F(2)	H(44)[1)]	2.660	F(2)	H(50)[1)]	3.353
F(2)	H(75)	3.424	F(2)	H(77)[2)]	2.987
F(2)	H(96)[3)]	3.498	F(2)	H(101)[3)]	3.520
F(3)	H(39)[4)]	2.818	F(3)	H(55)	3.269
F(3)	H(74)	3.405	F(3)	H(75)	3.316
F(3)	H(86)	3.041	F(3)	H(87)	3.427
F(3)	H(94)	3.525	F(3)	H(96)[3)]	2.503
F(3)	H(101)[3)]	2.757	F(4)	H(36)[4)]	2.776
F(4)	H(39)[4)]	3.086	F(4)	H(40)[4)]	3.546
F(4)	H(56)[1)]	3.593	F(4)	H(77)[2)]	3.254
F(4)	H(80)[2)]	3.446	F(4)	H(81)[2)]	3.412
F(4)	H(101)[3)]	2.606	F(5)	H(49)[1)]	3.416
F(5)	H(71)	3.497	F(5)	H(73)	3.510
F(5)	H(76)	3.450	F(5)	H(88)[3)]	3.358
F(5)	H(89)[3)]	3.072	F(5)	H(90)[3)]	3.301
F(5)	H(95)[3)]	2.800	F(6)	H(6)[3)]	2.532
F(6)	H(7)[3)]	3.312	F(6)	H(41)[5)]	3.523
F(6)	H(43)[5)]	3.334	F(6)	H(46)[5)]	2.875
F(6)	H(48)[5)]	2.918	F(6)	H(62)[6)]	3.517
F(6)	H(63)[6)]	2.996	F(6)	H(89)[3)]	2.826
F(7)	H(38)[5)]	2.596	F(7)	H(43)[5)]	3.404
F(7)	H(48)[5)]	2.773	F(7)	H(60)[2)]	2.993
F(7)	H(86)[3)]	3.405	F(7)	H(88)[3)]	3.001
F(7)	H(89)[3)]	3.009	F(7)	H(97)[2)]	2.930
F(8)	H(45)[1)]	3.509	F(8)	H(48)[5)]	3.364
F(8)	H(49)[1)]	2.265	F(8)	H(60)[2)]	3.192
F(8)	H(61)[2)]	2.874	O(1)	H(28)[7)]	2.752
O(1)	H(30)[7)]	3.550	O(1)	H(31)[7)]	2.719
O(1)	H(34)[7)]	2.815	O(1)	H(81)	3.419

O(1)	H(82)	3.157	O(1)	H(91)	2.774
O(2)	H(13)[4)]	3.440	O(2)	H(42)[4)]	3.459
O(2)	H(43)[4)]	3.488	O(2)	H(47)[4)]	3.103
O(2)	H(89)	3.489	O(2)	H(91)	3.006

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
O(3)	H(4)[1)]	2.825	O(3)	H(14)	3.538
O(3)	H(18)[1)]	2.670	O(3)	H(21)	3.244
O(3)	H(22)	3.247	O(3)	H(23)[1)]	3.510
O(3)	H(26)[1)]	3.135	O(3)	H(28)[1)]	3.528
O(4)	H(11)[8)]	3.574	O(4)	H(13)[8)]	3.158
O(4)	H(15)[8)]	3.261	O(4)	H(21)	3.098
O(4)	H(28)[1)]	3.521	C(2)	H(1)[4)]	3.362
C(3)	H(1)[4)]	3.597	C(3)	H(11)[4)]	3.594
C(3)	H(12)[4)]	3.333	C(3)	H(42)[4)]	2.976
C(3)	H(92)	3.475	C(4)	H(57)[9)]	3.503
C(4)	H(91)	3.132	C(4)	H(92)	3.486
C(5)	H(58)[8)]	3.394	C(5)	H(85)	2.885
C(6)	H(58)[8)]	3.431	C(6)	H(85)	3.343
C(7)	H(28)[7)]	3.460	C(7)	H(91)	2.645
C(8)	H(46)[4)]	3.226	C(8)	H(47)[4)]	3.366
C(8)	H(53)[9)]	3.489	C(8)	H(62)[9)]	3.113
C(8)	H(63)[9)]	3.250	C(8)	H(64)[9)]	3.316
C(8)	H(89)	3.560	C(8)	H(91)	3.435
C(10)	H(37)[4)]	3.350	C(10)	H(92)	3.443
C(10)	H(93)	3.406	C(10)	H(94)	3.113
C(11)	H(2)[4)]	3.139	C(11)	H(53)[1)]	3.492
C(12)	H(23)[1)]	3.027	C(12)	H(53)[1)]	3.352
C(14)	H(54)[8)]	3.150	C(16)	H(15)[8)]	3.549
C(16)	H(84)	3.163	C(19)	H(56)[9)]	3.561
C(19)	H(57)[9)]	3.214	C(20)	H(66)[10)]	3.445
C(20)	H(102)[10)]	3.379	C(22)	H(9)[4)]	3.421
C(22)	H(11)[4)]	3.185	C(23)	H(86)[4)]	3.287
C(23)	H(101)[10)]	3.247	C(23)	H(102)[10)]	2.975
C(24)	H(2)[4)]	3.088	C(24)	H(89)[4)]	3.596
C(24)	H(92)[4)]	3.490	C(26)	H(77)[1)]	3.315
C(26)	H(79)[1)]	2.848	C(27)	H(52)[1)]	3.118
C(27)	H(59)[1)]	3.540	C(27)	H(61)[1)]	3.430

C(27)	H(77)[1)]	3.569	C(27)	H(78)[1)]	3.320
C(27)	H(79)[1)]	2.922	C(28)	H(6)[4)]	3.034
C(28)	H(52)[1)]	2.961	C(28)	H(61)[1)]	3.372
C(28)	H(62)[1)]	2.989	C(29)	H(6)[4)]	3.295
C(29)	H(52)[1)]	3.477	C(29)	H(53)[1)]	3.505

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(30)	H(65)[10)]	3.575	C(31)	H(65)[10)]	2.863
C(32)	H(65)[10)]	2.657	C(33)	H(65)[10)]	3.249
C(33)	H(68)[8)]	2.726	C(34)	H(68)[8)]	2.942
C(36)	H(5)[11)]	3.534	C(37)	H(5)[11)]	3.043
C(37)	H(13)[8)]	3.484	C(37)	H(15)[8)]	3.383
C(37)	H(16)[8)]	3.491	C(38)	H(21)	3.397
C(38)	H(25)	3.292	C(39)	H(10)	3.595
C(39)	H(18)[1)]	3.579	C(39)	H(25)	3.256
C(41)	H(21)	2.963	C(41)	H(22)	3.494
C(41)	H(26)[1)]	3.525	C(41)	H(28)[1)]	3.453
C(42)	H(21)	3.573	C(42)	H(29)[11)]	3.347
C(42)	H(30)[11)]	3.551	C(42)	H(31)[11)]	3.583
C(44)	H(45)[8)]	3.343	C(44)	H(46)[8)]	3.492
C(45)	H(5)[11)]	3.183	C(45)	H(6)[11)]	3.058
C(45)	H(7)[11)]	3.452	C(45)	H(46)[8)]	3.100
C(45)	H(71)[6)]	3.569	C(46)	H(32)[12)]	3.413
C(46)	H(70)[6)]	3.246	C(46)	H(71)[6)]	3.193
C(48)	H(50)[1)]	3.407	C(48)	H(67)[6)]	3.183
C(49)	H(67)[6)]	3.144	C(50)	H(50)[1)]	3.290
C(50)	H(96)[3)]	2.972	C(52)	H(44)[8)]	3.149
C(52)	H(45)[8)]	3.143	C(54)	H(3)	3.456
C(54)	H(23)	3.483	C(54)	H(24)	3.357
C(56)	H(39)[4)]	3.597	C(56)	H(97)[3)]	3.094
C(57)	H(7)	3.380	C(57)	H(43)[4)]	3.367
C(58)	H(8)	3.255	C(58)	H(9)	3.117
C(61)	H(74)[13)]	3.100	C(61)	H(76)[13)]	3.293
C(61)	H(99)[13)]	2.977	C(62)	H(88)[13)]	3.508
C(62)	H(99)[13)]	3.101	C(62)	H(100)[13)]	3.110
C(63)	H(100)[13)]	3.115	C(66)	H(80)[3)]	3.104
C(67)	H(33)[12)]	3.306	C(67)	H(40)[12)]	3.139
C(67)	H(80)[3)]	3.218	C(68)	H(32)[12)]	3.352
C(68)	H(33)[12)]	3.287	C(68)	H(40)[12)]	2.964

B(1)	H(19)[1)]	3.341	B(1)	H(20)[1)]	3.535
B(1)	H(36)[4)]	3.576	B(1)	H(39)[4)]	3.479
B(1)	H(96)[3)]	3.540	B(1)	H(101)[3)]	3.143
B(2)	H(48)[5)]	3.306	B(2)	H(49)[1)]	3.262
B(2)	H(89)[3)]	3.189	H(1)	C(2)[4)]	3.362

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(1)	C(3)[4)]	3.597	H(1)	H(1)[4)]	2.615
H(1)	H(2)[4)]	3.098	H(1)	H(42)[4)]	3.541
H(2)	C(11)[4)]	3.139	H(2)	C(24)[4)]	3.088
H(2)	H(1)[4)]	3.098	H(2)	H(11)[4)]	3.180
H(2)	H(12)[4)]	2.597	H(2)	H(13)[4)]	3.147
H(2)	H(41)[4)]	3.388	H(2)	H(42)[4)]	2.260
H(2)	H(43)[4)]	3.262	H(2)	H(47)[4)]	3.278
H(3)	C(54)	3.456	H(3)	H(31)[7)]	2.987
H(3)	H(58)[8)]	2.804	H(3)	H(81)	3.148
H(3)	H(83)	3.583	H(3)	H(85)	2.580
H(4)	O(3)[8)]	2.825	H(4)	H(58)[8)]	2.876
H(4)	H(85)	3.382	H(5)	C(36)[9)]	3.534
H(5)	C(37)[9)]	3.043	H(5)	C(45)[9)]	3.183
H(5)	H(28)[7)]	3.478	H(5)	H(46)[4)]	3.342
H(5)	H(47)[4)]	3.536	H(5)	H(52)[9)]	3.574
H(5)	H(53)[9)]	2.738	H(5)	H(62)[9)]	2.853
H(5)	H(63)[9)]	3.280	H(5)	H(64)[9)]	2.900
H(6)	F(6)[13)]	2.532	H(6)	C(28)[4)]	3.034
H(6)	C(29)[4)]	3.295	H(6)	C(45)[9)]	3.058
H(6)	H(41)[4)]	3.496	H(6)	H(46)[4)]	2.367
H(6)	H(47)[4)]	2.923	H(6)	H(62)[9)]	2.626
H(6)	H(63)[9)]	2.836	H(6)	H(64)[9)]	3.232
H(6)	H(89)	3.415	H(7)	F(6)[13)]	3.312
H(7)	C(45)[9)]	3.452	H(7)	C(57)	3.380
H(7)	H(34)[7)]	3.207	H(7)	H(62)[9)]	3.411
H(7)	H(63)[9)]	3.105	H(7)	H(64)[9)]	3.274
H(7)	H(89)	3.236	H(7)	H(90)	3.324
H(7)	H(91)	3.023	H(8)	C(58)	3.255
H(8)	H(54)	3.554	H(8)	H(92)	3.365
H(8)	H(93)	2.910	H(8)	H(94)	2.967
H(9)	C(22)[4)]	3.421	H(9)	C(58)	3.117
H(9)	H(37)[4)]	2.555	H(9)	H(92)	2.813

H(9)	H(93)	3.153	H(9)	H(94)	2.868
H(10)	F(1)	2.537	H(10)	C(39)	3.595
H(10)	H(37)[4)]	3.352	H(10)	H(54)	3.162
H(10)	H(55)	3.390	H(10)	H(94)	2.976
H(11)	O(4)[1)]	3.574	H(11)	C(3)[4)]	3.594

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(11)	C(22)[4)]	3.185	H(11)	H(2)[4)]	3.180
H(11)	H(35)[4)]	2.936	H(11)	H(36)[4)]	3.263
H(11)	H(37)[4)]	2.838	H(11)	H(56)[1)]	3.499
H(11)	H(57)[1)]	3.211	H(12)	C(3)[4)]	3.333
H(12)	H(2)[4)]	2.597	H(13)	O(2)[4)]	3.440
H(13)	O(4)[1)]	3.158	H(13)	C(37)[1)]	3.484
H(13)	H(2)[4)]	3.147	H(13)	H(53)[1)]	2.572
H(13)	H(57)[1)]	3.505	H(14)	O(3)	3.538
H(14)	H(18)[1)]	3.462	H(14)	H(19)[1)]	3.225
H(14)	H(23)[1)]	2.703	H(14)	H(54)	3.067
H(15)	O(4)[1)]	3.261	H(15)	C(16)[1)]	3.549
H(15)	C(37)[1)]	3.383	H(15)	H(19)[1)]	3.540
H(15)	H(21)[1)]	2.877	H(15)	H(23)[1)]	2.840
H(15)	H(25)[1)]	3.575	H(15)	H(53)[1)]	2.863
H(16)	C(37)[1)]	3.491	H(16)	H(23)[1)]	3.030
H(16)	H(53)[1)]	3.036	H(16)	H(83)[1)]	3.584
H(17)	F(2)[8)]	3.473	H(17)	H(54)[8)]	3.511
H(18)	O(3)[8)]	2.670	H(18)	C(39)[8)]	3.579
H(18)	H(14)[8)]	3.462	H(18)	H(54)[8)]	2.768
H(19)	F(1)[8)]	2.475	H(19)	F(2)[8)]	3.142
H(19)	B(1)[8)]	3.341	H(19)	H(14)[8)]	3.225
H(19)	H(15)[8)]	3.540	H(19)	H(54)[8)]	2.740
H(20)	F(1)[8)]	3.306	H(20)	F(2)[8)]	3.236
H(20)	B(1)[8)]	3.535	H(20)	H(56)	3.539
H(20)	H(77)[1)]	3.460	H(20)	H(83)[1)]	3.470
H(21)	O(3)	3.244	H(21)	O(4)	3.098
H(21)	C(38)	3.397	H(21)	C(41)	2.963
H(21)	C(42)	3.573	H(21)	H(15)[8)]	2.877
H(21)	H(56)	3.089	H(22)	O(3)	3.247
H(22)	C(41)	3.494	H(22)	H(83)[1)]	3.365
H(23)	O(3)[8)]	3.510	H(23)	C(12)[8)]	3.027
H(23)	C(54)	3.483	H(23)	H(14)[8)]	2.703

H(23)	H(15)[8)]	2.840	H(23)	H(16)[8)]	3.030
H(23)	H(83)	3.240	H(23)	H(84)	3.024
H(24)	C(54)	3.357	H(24)	H(83)	3.467
H(24)	H(84)	2.916	H(24)	H(85)	3.158
H(24)	H(93)	3.164	H(25)	C(38)	3.292

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(25)	C(39)	3.256	H(25)	H(15)[8)]	3.575
H(25)	H(54)	3.486	H(25)	H(84)	3.013
H(25)	H(93)	3.472	H(26)	O(3)[8)]	3.135
H(26)	C(41)[8)]	3.525	H(26)	H(58)[8)]	3.594
H(27)	H(68)[8)]	3.369	H(27)	H(69)[8)]	3.328
H(28)	O(1)[7)]	2.752	H(28)	O(3)[8)]	3.528
H(28)	O(4)[8)]	3.521	H(28)	C(7)[7)]	3.460
H(28)	C(41)[8)]	3.453	H(28)	H(5)[7)]	3.478
H(28)	H(58)[8)]	3.256	H(29)	C(42)[9)]	3.347
H(29)	H(56)[9)]	3.096	H(29)	H(57)[9)]	2.840
H(30)	O(1)[7)]	3.550	H(30)	C(42)[9)]	3.551
H(30)	H(57)[9)]	2.944	H(30)	H(58)[9)]	3.513
H(31)	O(1)[7)]	2.719	H(31)	C(42)[9)]	3.583
H(31)	H(3)[7)]	2.987	H(31)	H(56)[9)]	3.365
H(31)	H(57)[9)]	3.344	H(31)	H(58)[9)]	3.450
H(31)	H(81)[7)]	3.004	H(32)	C(46)[10)]	3.413
H(32)	C(68)[10)]	3.352	H(32)	H(65)[10)]	3.423
H(32)	H(66)[10)]	2.621	H(32)	H(72)[10)]	3.513
H(32)	H(102)[10)]	2.809	H(33)	C(67)[10)]	3.306
H(33)	C(68)[10)]	3.287	H(33)	H(80)[7)]	3.481
H(33)	H(81)[7)]	3.365	H(33)	H(101)[10)]	3.104
H(33)	H(102)[10)]	3.076	H(34)	O(1)[7)]	2.815
H(34)	H(7)[7)]	3.207	H(34)	H(66)[10)]	3.574
H(34)	H(72)[10)]	3.570	H(35)	H(11)[4)]	2.936
H(35)	H(57)[9)]	3.465	H(36)	F(4)[4)]	2.776
H(36)	B(1)[4)]	3.576	H(36)	H(11)[4)]	3.263
H(36)	H(56)[9)]	3.496	H(37)	C(10)[4)]	3.350
H(37)	H(9)[4)]	2.555	H(37)	H(10)[4)]	3.352
H(37)	H(11)[4)]	2.838	H(37)	H(92)[4)]	3.038
H(37)	H(94)[4)]	3.488	H(38)	F(7)[14)]	2.596
H(38)	H(60)[10)]	3.546	H(38)	H(86)[4)]	3.093
H(38)	H(97)[10)]	3.277	H(38)	H(102)[10)]	2.836

H(39)	F(3)[4)]	2.818	H(39)	F(4)[4)]	3.086
H(39)	C(56)[4)]	3.597	H(39)	B(1)[4)]	3.479
H(39)	H(86)[4)]	2.643	H(39)	H(97)[10)]	3.430
H(39)	H(101)[10)]	2.933	H(39)	H(102)[10)]	3.348
H(40)	F(4)[4)]	3.546	H(40)	C(67)[10)]	3.139

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(40)	C(68)[10)]	2.964	H(40)	H(101)[10)]	2.735
H(40)	H(102)[10)]	2.352	H(41)	F(6)[14)]	3.523
H(41)	H(2)[4)]	3.388	H(41)	H(6)[4)]	3.496
H(42)	O(2)[4)]	3.459	H(42)	C(3)[4)]	2.976
H(42)	H(1)[4)]	3.541	H(42)	H(2)[4)]	2.260
H(42)	H(92)[4)]	3.350	H(43)	F(6)[14)]	3.334
H(43)	F(7)[14)]	3.404	H(43)	O(2)[4)]	3.488
H(43)	C(57)[4)]	3.367	H(43)	H(2)[4)]	3.262
H(43)	H(86)[4)]	3.252	H(43)	H(89)[4)]	2.661
H(43)	H(91)[4)]	3.394	H(43)	H(92)[4)]	2.843
H(44)	F(2)[8)]	2.660	H(44)	C(52)[1)]	3.149
H(44)	H(77)[1)]	2.766	H(44)	H(78)[1)]	3.508
H(44)	H(79)[1)]	2.741	H(45)	F(8)[8)]	3.509
H(45)	C(44)[1)]	3.343	H(45)	C(52)[1)]	3.143
H(45)	H(52)[1)]	3.350	H(45)	H(59)[1)]	2.908
H(45)	H(61)[1)]	2.905	H(45)	H(77)[1)]	3.286
H(45)	H(78)[1)]	2.776	H(45)	H(79)[1)]	2.867
H(45)	H(98)[1)]	3.416	H(46)	F(6)[14)]	2.875
H(46)	C(8)[4)]	3.226	H(46)	C(44)[1)]	3.492
H(46)	C(45)[1)]	3.100	H(46)	H(5)[4)]	3.342
H(46)	H(6)[4)]	2.367	H(46)	H(52)[1)]	3.080
H(46)	H(59)[1)]	3.497	H(46)	H(61)[1)]	2.785
H(46)	H(62)[1)]	2.252	H(46)	H(63)[1)]	3.194
H(47)	O(2)[4)]	3.103	H(47)	C(8)[4)]	3.366
H(47)	H(2)[4)]	3.278	H(47)	H(5)[4)]	3.536
H(47)	H(6)[4)]	2.923	H(47)	H(53)[1)]	3.426
H(48)	F(6)[14)]	2.918	H(48)	F(7)[14)]	2.773
H(48)	F(8)[14)]	3.364	H(48)	B(2)[14)]	3.306
H(48)	H(60)[10)]	3.377	H(48)	H(65)[10)]	3.084
H(49)	F(5)[8)]	3.416	H(49)	F(8)[8)]	2.265
H(49)	B(2)[8)]	3.262	H(49)	H(61)[1)]	3.567
H(49)	H(65)[10)]	2.709	H(50)	F(2)[8)]	3.353

H(50)	C(48)[8)]	3.407	H(50)	C(50)[8)]	3.290
H(50)	H(68)[8)]	2.488	H(50)	H(75)[8)]	3.004
H(50)	H(76)[8)]	2.814	H(51)	H(68)[8)]	2.893
H(52)	C(27)[8)]	3.118	H(52)	C(28)[8)]	2.961
H(52)	C(29)[8)]	3.477	H(52)	H(5)[11)]	3.574

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(52)	H(45)[8)]	3.350	H(52)	H(46)[8)]	3.080
H(53)	C(8)[11)]	3.489	H(53)	C(11)[8)]	3.492
H(53)	C(12)[8)]	3.352	H(53)	C(29)[8)]	3.505
H(53)	H(5)[11)]	2.738	H(53)	H(13)[8)]	2.572
H(53)	H(15)[8)]	2.863	H(53)	H(16)[8)]	3.036
H(53)	H(47)[8)]	3.426	H(54)	F(1)	3.135
H(54)	C(14)[1)]	3.150	H(54)	H(8)	3.554
H(54)	H(10)	3.162	H(54)	H(14)	3.067
H(54)	H(17)[1)]	3.511	H(54)	H(18)[1)]	2.768
H(54)	H(19)[1)]	2.740	H(54)	H(25)	3.486
H(55)	F(1)	2.963	H(55)	F(3)	3.269
H(55)	H(10)	3.390	H(56)	F(4)[8)]	3.593
H(56)	C(19)[11)]	3.561	H(56)	H(11)[8)]	3.499
H(56)	H(20)	3.539	H(56)	H(21)	3.089
H(56)	H(29)[11)]	3.096	H(56)	H(31)[11)]	3.365
H(56)	H(36)[11)]	3.496	H(57)	C(4)[11)]	3.503
H(57)	C(19)[11)]	3.214	H(57)	H(11)[8)]	3.211
H(57)	H(13)[8)]	3.505	H(57)	H(29)[11)]	2.840
H(57)	H(30)[11)]	2.944	H(57)	H(31)[11)]	3.344
H(57)	H(35)[11)]	3.465	H(58)	C(5)[1)]	3.394
H(58)	C(6)[1)]	3.431	H(58)	H(3)[1)]	2.804
H(58)	H(4)[1)]	2.876	H(58)	H(26)[1)]	3.594
H(58)	H(28)[1)]	3.256	H(58)	H(30)[11)]	3.513
H(58)	H(31)[11)]	3.450	H(59)	C(27)[8)]	3.540
H(59)	H(45)[8)]	2.908	H(59)	H(46)[8)]	3.497
H(60)	F(7)[15)]	2.993	H(60)	F(8)[15)]	3.192
H(60)	H(38)[12)]	3.546	H(60)	H(48)[12)]	3.377
H(61)	F(8)[15)]	2.874	H(61)	C(27)[8)]	3.430
H(61)	C(28)[8)]	3.372	H(61)	H(45)[8)]	2.905
H(61)	H(46)[8)]	2.785	H(61)	H(49)[8)]	3.567
H(62)	F(6)[6)]	3.517	H(62)	C(8)[11)]	3.113
H(62)	C(28)[8)]	2.989	H(62)	H(5)[11)]	2.853

H(62)	H(6)[11)]	2.626	H(62)	H(7)[11)]	3.411
H(62)	H(46)[8)]	2.252	H(63)	F(6)[6)]	2.996
H(63)	C(8)[11)]	3.250	H(63)	H(5)[11)]	3.280
H(63)	H(6)[11)]	2.836	H(63)	H(7)[11)]	3.105
H(63)	H(46)[8)]	3.194	H(63)	H(71)[6)]	2.869

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(64)	C(8)[11)]	3.316	H(64)	H(5)[11)]	2.900
H(64)	H(6)[11)]	3.232	H(64)	H(7)[11)]	3.274
H(64)	H(71)[6)]	3.580	H(65)	C(30)[12)]	3.575
H(65)	C(31)[12)]	2.863	H(65)	C(32)[12)]	2.657
H(65)	C(33)[12)]	3.249	H(65)	H(32)[12)]	3.423
H(65)	H(48)[12)]	3.084	H(65)	H(49)[12)]	2.709
H(65)	H(71)[6)]	3.407	H(66)	C(20)[12)]	3.445
H(66)	H(32)[12)]	2.621	H(66)	H(34)[12)]	3.574
H(66)	H(70)[6)]	3.194	H(67)	C(48)[6)]	3.183
H(67)	C(49)[6)]	3.144	H(67)	H(68)[6)]	3.104
H(67)	H(70)[6)]	2.531	H(67)	H(71)[6)]	2.284
H(67)	H(72)[6)]	3.359	H(68)	C(33)[1)]	2.726
H(68)	C(34)[1)]	2.942	H(68)	H(27)[1)]	3.369
H(68)	H(50)[1)]	2.488	H(68)	H(51)[1)]	2.893
H(68)	H(67)[6)]	3.104	H(69)	H(27)[1)]	3.328
H(70)	C(46)[6)]	3.246	H(70)	H(66)[6)]	3.194
H(70)	H(67)[6)]	2.531	H(70)	H(71)[6)]	3.360
H(70)	H(72)[6)]	3.039	H(71)	F(5)	3.497
H(71)	C(45)[6)]	3.569	H(71)	C(46)[6)]	3.193
H(71)	H(63)[6)]	2.869	H(71)	H(64)[6)]	3.580
H(71)	H(65)[6)]	3.407	H(71)	H(67)[6)]	2.284
H(71)	H(70)[6)]	3.360	H(72)	H(32)[12)]	3.513
H(72)	H(34)[12)]	3.570	H(72)	H(67)[6)]	3.359
H(72)	H(70)[6)]	3.039	H(73)	F(5)	3.510
H(73)	H(95)[3)]	3.580	H(74)	F(3)	3.405
H(74)	C(61)[3)]	3.100	H(74)	H(96)[3)]	2.527
H(75)	F(2)	3.424	H(75)	F(3)	3.316
H(75)	H(50)[1)]	3.004	H(75)	H(96)[3)]	3.308
H(76)	F(5)	3.450	H(76)	C(61)[3)]	3.293
H(76)	H(50)[1)]	2.814	H(76)	H(95)[3)]	3.414
H(76)	H(96)[3)]	2.661	H(77)	F(2)[15)]	2.987
H(77)	F(4)[15)]	3.254	H(77)	C(26)[8)]	3.315

H(77)	C(27)[8)]	3.569	H(77)	H(20)[8)]	3.460
H(77)	H(44)[8)]	2.766	H(77)	H(45)[8)]	3.286
H(77)	H(100)[13)]	3.509	H(78)	C(27)[8)]	3.320
H(78)	H(44)[8)]	3.508	H(78)	H(45)[8)]	2.776
H(78)	H(100)[13)]	3.346	H(79)	C(26)[8)]	2.848

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(79)	C(27)[8)]	2.922	H(79)	H(44)[8)]	2.741
H(79)	H(45)[8)]	2.867	H(80)	F(4)[15)]	3.446
H(80)	C(66)[13)]	3.104	H(80)	C(67)[13)]	3.218
H(80)	H(33)[7)]	3.481	H(80)	H(100)[13)]	2.902
H(80)	H(101)[13)]	3.107	H(81)	F(4)[15)]	3.412
H(81)	O(1)	3.419	H(81)	H(3)	3.148
H(81)	H(31)[7)]	3.004	H(81)	H(33)[7)]	3.365
H(82)	O(1)	3.157	H(83)	H(3)	3.583
H(83)	H(16)[8)]	3.584	H(83)	H(20)[8)]	3.470
H(83)	H(22)[8)]	3.365	H(83)	H(23)	3.240
H(83)	H(24)	3.467	H(84)	C(16)	3.163
H(84)	H(23)	3.024	H(84)	H(24)	2.916
H(84)	H(25)	3.013	H(85)	C(5)	2.885
H(85)	C(6)	3.343	H(85)	H(3)	2.580
H(85)	H(4)	3.382	H(85)	H(24)	3.158
H(86)	F(3)	3.041	H(86)	F(7)[13)]	3.405
H(86)	C(23)[4)]	3.287	H(86)	H(38)[4)]	3.093
H(86)	H(39)[4)]	2.643	H(86)	H(43)[4)]	3.252
H(86)	H(97)[3)]	2.828	H(87)	F(3)	3.427
H(87)	H(97)[3)]	3.230	H(88)	F(5)[13)]	3.358
H(88)	F(7)[13)]	3.001	H(88)	C(62)[3)]	3.508
H(88)	H(97)[3)]	2.726	H(89)	F(5)[13)]	3.072
H(89)	F(6)[13)]	2.826	H(89)	F(7)[13)]	3.009
H(89)	O(2)	3.489	H(89)	C(8)	3.560
H(89)	C(24)[4)]	3.596	H(89)	B(2)[13)]	3.189
H(89)	H(6)	3.415	H(89)	H(7)	3.236
H(89)	H(43)[4)]	2.661	H(90)	F(5)[13)]	3.301
H(90)	H(7)	3.324	H(91)	O(1)	2.774
H(91)	O(2)	3.006	H(91)	C(4)	3.132
H(91)	C(7)	2.645	H(91)	C(8)	3.435
H(91)	H(7)	3.023	H(91)	H(43)[4)]	3.394
H(92)	C(3)	3.475	H(92)	C(4)	3.486

H(92)	C(10)	3.443	H(92)	C(24)[4)]	3.490
H(92)	H(8)	3.365	H(92)	H(9)	2.813
H(92)	H(37)[4)]	3.038	H(92)	H(42)[4)]	3.350
H(92)	H(43)[4)]	2.843	H(93)	C(10)	3.406
H(93)	H(8)	2.910	H(93)	H(9)	3.153

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(93)	H(24)	3.164	H(93)	H(25)	3.472
H(94)	F(3)	3.525	H(94)	C(10)	3.113
H(94)	H(8)	2.967	H(94)	H(9)	2.868
H(94)	H(10)	2.976	H(94)	H(37)[4)]	3.488
H(95)	F(5)[13)]	2.800	H(95)	H(73)[13)]	3.580
H(95)	H(76)[13)]	3.414	H(96)	F(2)[13)]	3.498
H(96)	F(3)[13)]	2.503	H(96)	C(50)[13)]	2.972
H(96)	B(1)[13)]	3.540	H(96)	H(74)[13)]	2.527
H(96)	H(75)[13)]	3.308	H(96)	H(76)[13)]	2.661
H(96)	H(99)[13)]	2.870	H(97)	F(7)[15)]	2.930
H(97)	C(56)[13)]	3.094	H(97)	H(38)[12)]	3.277
H(97)	H(39)[12)]	3.430	H(97)	H(86)[13)]	2.828
H(97)	H(87)[13)]	3.230	H(97)	H(88)[13)]	2.726
H(97)	H(99)[13)]	3.109	H(97)	H(100)[13)]	3.214
H(98)	H(45)[8)]	3.416	H(98)	H(100)[13)]	3.276
H(99)	C(61)[3)]	2.977	H(99)	C(62)[3)]	3.101
H(99)	H(96)[3)]	2.870	H(99)	H(97)[3)]	3.109
H(100)	C(62)[3)]	3.110	H(100)	C(63)[3)]	3.115
H(100)	H(77)[3)]	3.509	H(100)	H(78)[3)]	3.346
H(100)	H(80)[3)]	2.902	H(100)	H(97)[3)]	3.214
H(100)	H(98)[3)]	3.276	H(101)	F(2)[13)]	3.520
H(101)	F(3)[13)]	2.757	H(101)	F(4)[13)]	2.606
H(101)	C(23)[12)]	3.247	H(101)	B(1)[13)]	3.143
H(101)	H(33)[12)]	3.104	H(101)	H(39)[12)]	2.933
H(101)	H(40)[12)]	2.735	H(101)	H(80)[3)]	3.107
H(102)	C(20)[12)]	3.379	H(102)	C(23)[12)]	2.975
H(102)	H(32)[12)]	2.809	H(102)	H(33)[12)]	3.076
H(102)	H(38)[12)]	2.836	H(102)	H(39)[12)]	3.348
H(102)	H(40)[12)]	2.352			

Symmetry Operators:

(1) -X+2,Y+1/2-1,-Z+1/2
(2) X,Y-1,Z
(3) -X+1,Y+1/2-1,-Z+1/2+1
(4) -X+2,-Y,-Z+1
(5) X-1,-Y+1/2-1,Z+1/2
(6) -X+1,-Y,-Z+1
(7) -X+2,-Y+1,-Z+1
(8) -X+2,Y+1/2,-Z+1/2
(9) X,-Y+1/2,Z+1/2
(10) X+1,-Y+1/2,Z+1/2-1
(11) X,-Y+1/2,Z+1/2-1
(12) X-1,-Y+1/2,Z+1/2
(13) -X+1,Y+1/2,-Z+1/2+1
(14) X+1,-Y+1/2-1,Z+1/2-1
(15) X,Y+1,Z

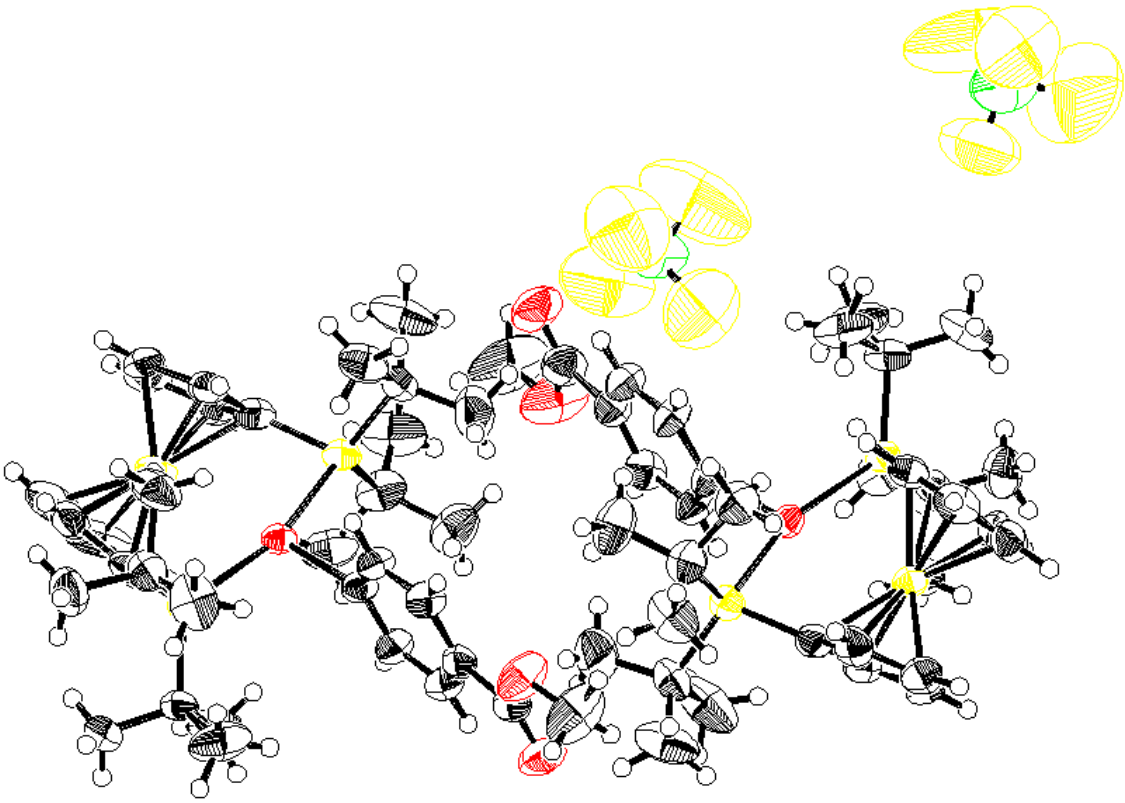


Table S7. The total energies and relative energies calculated at the B3LYP/LANL2DZ level of reaction species in gas-phase, and in solution where THF is considered using the CPCM continuum model. Pd(PH3)2 is used in the calculations.

	E (a.u.)	ΔE (a.u.)	ΔE (kcal/mol)	E in THF (a.u.)	ΔE in THF (a.u.)	ΔE in THF (kcal/mol)
a	-143.3313337			-143.33742075		
b	-244.7694105			-244.77633182		
a+b	-388.1007443		0	-388.11375257		0.0
TS_oa	-388.0870887	0.01365555	8.6	-388.09755192	0.016200650	10.2
c	-388.1344494	-0.03370519	-21.2	-388.15543042	-0.041677850	-26.2
d	-451.1505169			-451.22138930		
d2				-374.76490447		
e	-481.2576629			-481.34220027		
d+e	-932.4081798	0.1262476	79.2	-932.56358957	-0.02012884	-12.6
d2+e				-856.10710474	0.00789877	5.0
f(cyclic)	-856.1035468	0.01656427	10.4	-856.13251046	-0.01750695	-11.0
g(open)	-856.0908430	0.02926811	18.4	-856.13566352	-0.02066001	-13.0
TS_tm	-932.4889705	0.04545691	28.5	-932.51634050	0.02712023	17.0
h	-531.4996020	0.02805186	17.6	-531.50991381	-0.00615547	-3.9
TS_re	-531.4699109	0.05774300	36.2	-531.47775187	0.02600647	16.3
i	-531.5561420	-0.02848813	-17.9	-531.56386789	-0.06010955	-37.7
H_2O	-76.4143163			-76.42845722		
BF_3H_2O	-401.0067735			-401.03970239		
KBr	-41.3866273			-41.45655080		
RBF_3K	-509.4059941			-509.45780174		

(**a**) $Pd(PH_3)_2$

E(RB+HF-LYP) = -143.331333733 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.000000	0.000000	0.000000
2	15	0	-0.000082	0.000000	2.374791
3	1	0	1.240170	0.000000	3.104176
4	1	0	-0.620117	1.073917	3.104496
5	1	0	-0.620117	-1.073918	3.104496
6	15	0	0.000082	0.000000	-2.374791
7	1	0	-1.240170	0.000000	-3.104176
8	1	0	0.620117	1.073918	-3.104496
9	1	0	0.620117	-1.073917	-3.104496

(**a**) $Pd(PH_3)_2(THF)$

E(RB+HF-LYP) = -143.337420749 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.000000	0.000000	0.000000
2	15	0	0.000000	0.000000	2.374791
3	1	0	1.240277	0.000000	3.104133
4	1	0	-0.620010	1.073917	3.104517
5	1	0	-0.620010	-1.073918	3.104517
6	15	0	0.000000	0.000000	-2.374791
7	1	0	-1.240277	0.000000	-3.104133
8	1	0	0.620010	1.073918	-3.104517
9	1	0	0.620010	-1.073917	-3.104517

(**b**) Ph-Br

E(RB+HF-LYP) = -244.769410522 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.218692	1.218214	0.000001
2	6	0	0.809361	1.226438	0.000004
3	6	0	0.125135	0.000022	-0.000012
4	6	0	0.809347	-1.226425	-0.000005
5	6	0	2.218656	-1.218237	0.000010
6	6	0	2.925066	-0.000010	-0.000005
7	1	0	2.755989	2.163351	0.000005
8	1	0	0.263391	2.164904	0.000004
9	1	0	0.263323	-2.164860	-0.000005
10	1	0	2.755967	-2.163365	0.000014
11	1	0	4.012017	-0.000040	-0.000008
12	35	0	-1.848235	0.000000	0.000001

(**b**) Ph-Br(THF)

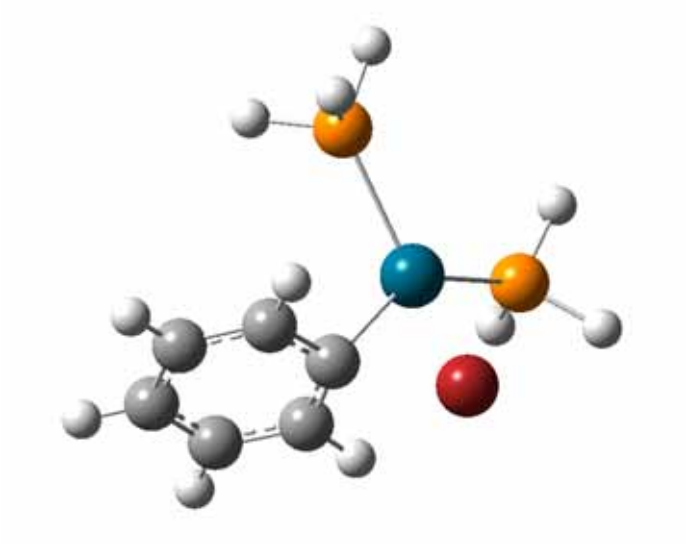
E(RB+HF-LYP) = -244.776331821 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.131439	0.000017	0.000002
2	6	0	-0.810349	-1.229605	-0.000028
3	6	0	-2.221492	-1.220110	0.000030
4	6	0	-2.927595	-0.000009	-0.000002
5	6	0	-2.221523	1.220096	-0.000028
6	6	0	-0.810362	1.229611	0.000031
7	1	0	-0.265568	-2.171921	-0.000030
8	1	0	-2.759634	-2.167346	0.000032

9	1	0	-4.016826	-0.000034	-0.000004
10	1	0	-2.759650	2.167340	-0.000041
11	1	0	-0.265625	2.171953	0.000039
12	35	0	1.851539	0.000000	-0.000001

TS_oa



E(RB+HF-LYP) = -388.087088702 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.822517	-0.327490	0.046403
2	6	0	-1.219114	0.301358	0.071506
3	6	0	-1.432251	0.382673	1.471068
4	6	0	-2.530713	-0.305001	2.036080
5	6	0	-3.437797	-0.999242	1.216955
6	6	0	-3.255101	-1.003415	-0.186665
7	6	0	-2.165078	-0.338906	-0.770345
8	1	0	-0.779742	0.989072	2.091489
9	1	0	-2.682938	-0.265921	3.112545
10	1	0	-4.291812	-1.509014	1.655919
11	1	0	-3.967685	-1.519979	-0.826498
12	1	0	-2.036289	-0.317773	-1.848315
13	35	0	-0.217226	2.095050	-0.817110
14	15	0	0.717499	-2.394504	-1.353952
15	1	0	1.842383	-3.233465	-1.688827
16	15	0	2.959105	0.037282	1.316867

17	1	0	3.007969	-0.155118	2.743478
18	1	0	-0.137210	-3.461045	-0.901273
19	1	0	0.180295	-2.327381	-2.689758
20	1	0	4.175620	-0.678351	1.028951
21	1	0	3.547752	1.350306	1.311291

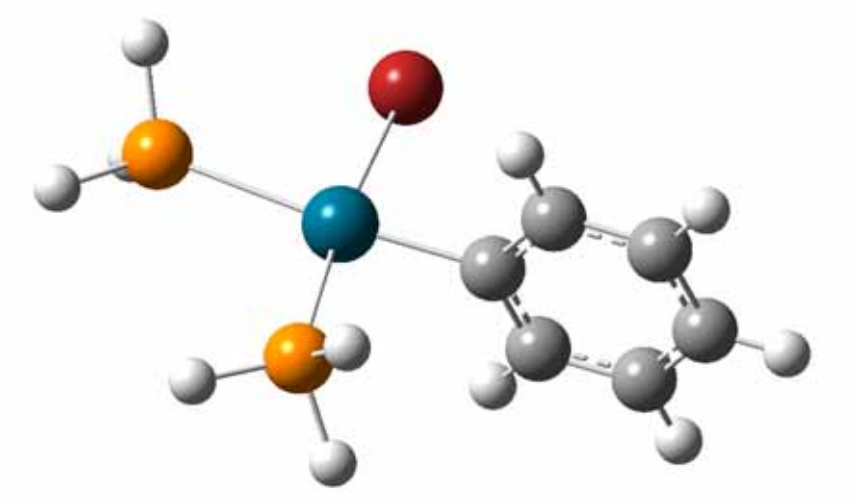
TS_oa (THF)

E(RB+HF-LYP) = -388.097551917 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.822517	-0.327490	0.046403
2	6	0	-1.219114	0.301358	0.071506
3	6	0	-1.432251	0.382673	1.471068
4	6	0	-2.530713	-0.305001	2.036080
5	6	0	-3.437797	-0.999242	1.216955
6	6	0	-3.255101	-1.003415	-0.186665
7	6	0	-2.165078	-0.338906	-0.770345
8	1	0	-0.779742	0.989072	2.091489
9	1	0	-2.682938	-0.265921	3.112545
10	1	0	-4.291812	-1.509014	1.655919
11	1	0	-3.967685	-1.519979	-0.826498
12	1	0	-2.036289	-0.317773	-1.848315
13	35	0	-0.217226	2.095050	-0.817110
14	15	0	0.717499	-2.394504	-1.353952
15	1	0	1.842383	-3.233465	-1.688827
16	15	0	2.959105	0.037282	1.316867
17	1	0	3.007969	-0.155118	2.743478
18	1	0	-0.137210	-3.461045	-0.901273
19	1	0	0.180295	-2.327381	-2.689758
20	1	0	4.175620	-0.678351	1.028951
21	1	0	3.547752	1.350306	1.311291

(**c**) $Pd(PH_3)_2(Ph)(Br)$



E(RB+HF-LYP) = -388.134449441 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.585407	0.419251	-0.000101
2	15	0	-0.034417	2.743448	-0.000123
3	1	0	-0.853605	3.181949	1.086466
4	1	0	0.931435	3.805153	0.000691
5	1	0	-0.852065	3.182279	-1.087751
6	6	0	-1.416645	0.073390	-0.000007
7	6	0	-2.114290	-0.050333	-1.220298
8	6	0	-3.504891	-0.291267	-1.216844
9	6	0	-4.203779	-0.408896	0.000234
10	6	0	-3.504672	-0.291353	1.217198
11	6	0	-2.114066	-0.050425	1.220411
12	1	0	-1.584139	0.011984	-2.168114
13	1	0	-4.033602	-0.395850	-2.162502
14	1	0	-5.274443	-0.600596	0.000322
15	1	0	-4.033208	-0.396016	2.162946
16	1	0	-1.583745	0.011827	2.168138

17	15	0	3.118936	0.579986	0.000303
18	1	0	3.933543	1.769375	0.000186
19	1	0	3.753820	-0.101381	1.085059
20	1	0	3.754615	-0.102171	-1.083484
21	35	0	0.965570	-2.096865	-0.000120

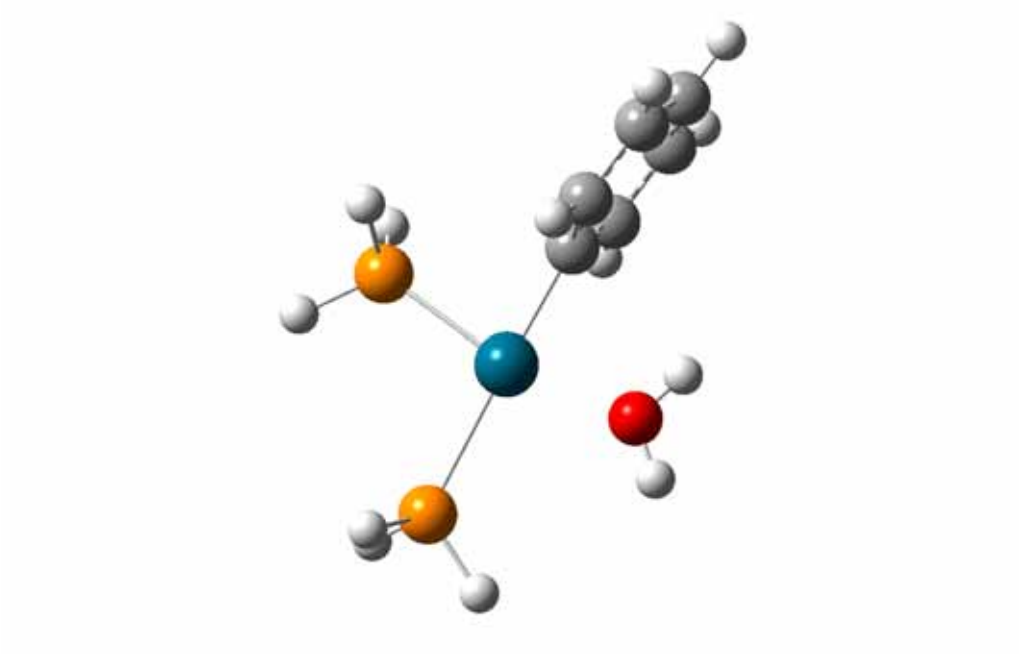
(**c**) $Pd(PH_3)_2(Ph)(Br)$ (THF)

E(RB+HF-LYP) = -388.155430420 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.585407	0.419251	-0.000101
2	15	0	-0.034416	2.743448	-0.000123
3	1	0	-0.853604	3.181949	1.086466
4	1	0	0.931436	3.805153	0.000691
5	1	0	-0.852064	3.182279	-1.087751
6	6	0	-1.416645	0.073390	-0.000007
7	6	0	-2.114290	-0.050333	-1.220298
8	6	0	-3.504891	-0.291266	-1.216844
9	6	0	-4.203779	-0.408895	0.000234
10	6	0	-3.504672	-0.291352	1.217198
11	6	0	-2.114066	-0.050424	1.220411
12	1	0	-1.584139	0.011984	-2.168114
13	1	0	-4.033602	-0.395849	-2.162502
14	1	0	-5.274443	-0.600595	0.000322
15	1	0	-4.033208	-0.396015	2.162946
16	1	0	-1.583745	0.011828	2.168138
17	15	0	3.118936	0.579985	0.000303
18	1	0	3.933543	1.769374	0.000186
19	1	0	3.753820	-0.101382	1.085059
20	1	0	3.754615	-0.102172	-1.083484
21	35	0	0.965569	-2.096865	-0.000120

(**d'**) $(PH_3)_2Pd(Ph)(H_2O)$



E(RB+HF-LYP) = -451.150516931 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.764287	-0.145887	-0.003961
2	15	0	-3.317352	-0.404870	0.002561
3	1	0	-4.033788	-0.033799	1.183638
4	1	0	-4.087867	0.315094	-0.963818
5	15	0	-0.631137	2.214640	0.008796
6	1	0	0.041308	2.805439	-1.098291
7	1	0	-1.845085	2.965949	0.030900
8	1	0	-3.884373	-1.704445	-0.195997
9	1	0	0.072364	2.788977	1.105067
10	6	0	1.260621	-0.006179	-0.001284
11	6	0	1.951627	-0.055606	1.227408
12	6	0	1.957179	-0.026355	-1.227478
13	6	0	3.361328	-0.146320	1.222062

14	1	0	1.419318	-0.029085	2.175905
15	6	0	3.366781	-0.117489	-1.217801
16	1	0	1.429171	0.021509	-2.177487
17	6	0	4.066589	-0.175932	0.003188
18	1	0	3.898797	-0.188987	2.166048
19	1	0	3.908535	-0.138092	-2.160074
20	1	0	5.151191	-0.239915	0.004865
21	8	0	-0.380860	-2.281672	-0.004441
22	1	0	-0.984871	-3.042569	-0.071849
23	1	0	0.561990	-2.535164	0.011930

(**d**) $(PH_3)_2Pd(Ph)(H_2O)$ (THF)

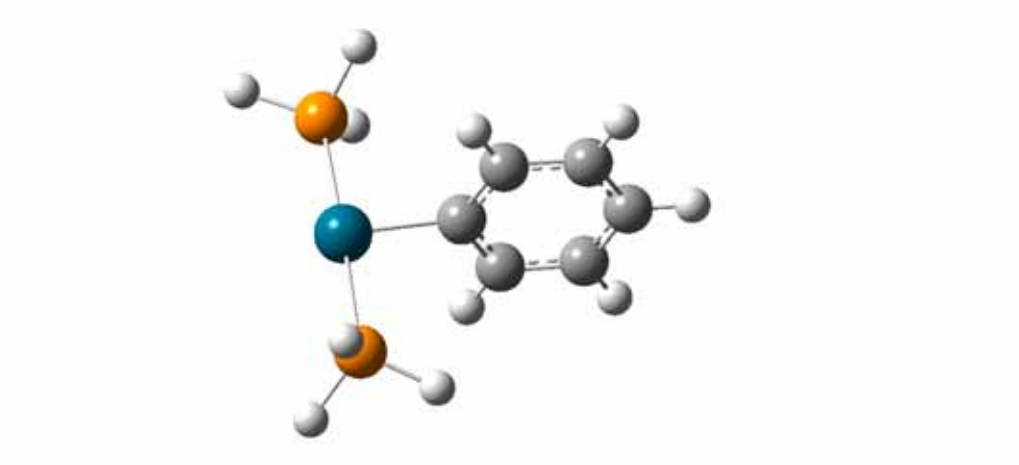
E(RB+HF-LYP) = -451.221389297 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.764287	-0.145887	-0.003961
2	15	0	-3.317352	-0.404870	0.002560
3	1	0	-4.033788	-0.033799	1.183637
4	1	0	-4.087867	0.315094	-0.963819
5	15	0	-0.631137	2.214640	0.008796
6	1	0	0.041308	2.805439	-1.098291
7	1	0	-1.845085	2.965949	0.030900
8	1	0	-3.884373	-1.704445	-0.195998
9	1	0	0.072364	2.788977	1.105067
10	6	0	1.260621	-0.006179	-0.001284
11	6	0	1.951627	-0.055606	1.227408
12	6	0	1.957179	-0.026355	-1.227478
13	6	0	3.361328	-0.146320	1.222062
14	1	0	1.419318	-0.029085	2.175905
15	6	0	3.366781	-0.117489	-1.217801
16	1	0	1.429171	0.021509	-2.177487

17	6	0	4.066589	-0.175932	0.003188
18	1	0	3.898797	-0.188987	2.166048
19	1	0	3.908535	-0.138092	-2.160074
20	1	0	5.151191	-0.239915	0.004865
21	8	0	-0.380860	-2.281672	-0.004441
22	1	0	-0.984871	-3.042569	-0.071849
23	1	0	0.561990	-2.535164	0.011930

(**d2**) (PH3)2Pd(Ph)(THF)



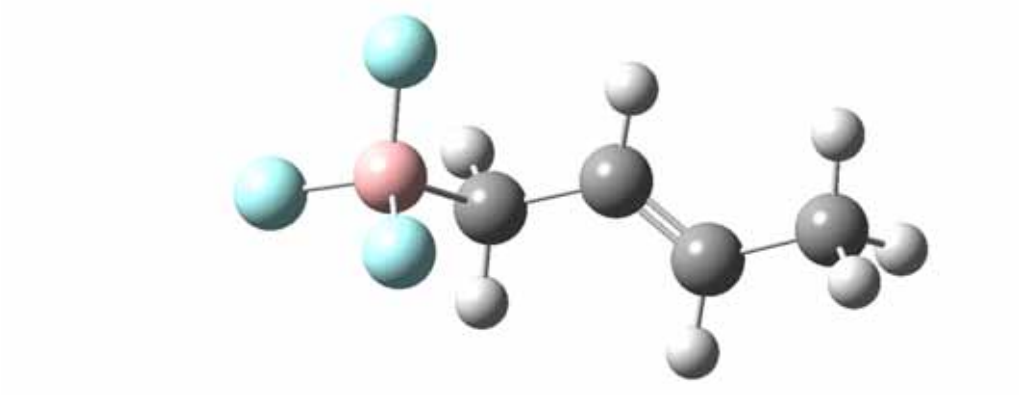
E(RB+HF-LYP) = -374.764904468 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.141984	-0.012733	0.000219
2	15	0	1.207228	2.454692	0.076189
3	1	0	1.574509	3.060539	1.316771
4	1	0	2.107788	3.112051	-0.818442
5	15	0	1.164742	-2.431626	-0.071597
6	1	0	0.521601	-3.000974	-1.210230
7	1	0	2.405940	-3.137793	-0.068091
8	1	0	-0.009749	3.142731	-0.208387
9	1	0	0.467933	-3.074179	0.992886
10	6	0	-0.868671	-0.054874	0.008484
11	6	0	-1.566548	-0.184854	1.223840
12	6	0	-1.534752	0.134014	-1.216217
13	6	0	-2.979429	-0.129245	1.203687
14	1	0	-1.044883	-0.327787	2.169903
15	6	0	-2.947177	0.184509	-1.217101
16	1	0	-0.987276	0.232476	-2.153608
17	6	0	-3.668049	0.056257	-0.012163

18	1	0	-3.529244	-0.231078	2.138997
19	1	0	-3.473423	0.326989	-2.160765
20	1	0	-4.756245	0.101938	-0.021190

(**e'**) $CH_3CH=CHCH^2BF_3^-$



E(RB+HF-LYP) = -481.257662872 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.160066	-0.154934	-0.506846
2	1	0	1.157068	0.740208	-1.137162
3	6	0	2.296782	-0.462659	0.161648
4	1	0	2.301208	-1.340780	0.813435
5	6	0	3.578904	0.347059	0.116053
6	1	0	3.841474	0.746409	1.109417
7	1	0	4.436716	-0.257153	-0.224145
8	1	0	3.473457	1.199986	-0.568231
9	6	0	-0.149705	-0.891489	-0.440224
10	1	0	-0.070277	-1.768633	0.220583
11	1	0	-0.425215	-1.253064	-1.446699
12	5	0	-1.397011	0.030195	0.043498
13	9	0	-2.650872	-0.729025	-0.060580
14	9	0	-1.268715	0.479662	1.426642
15	9	0	-1.529930	1.222051	-0.807003

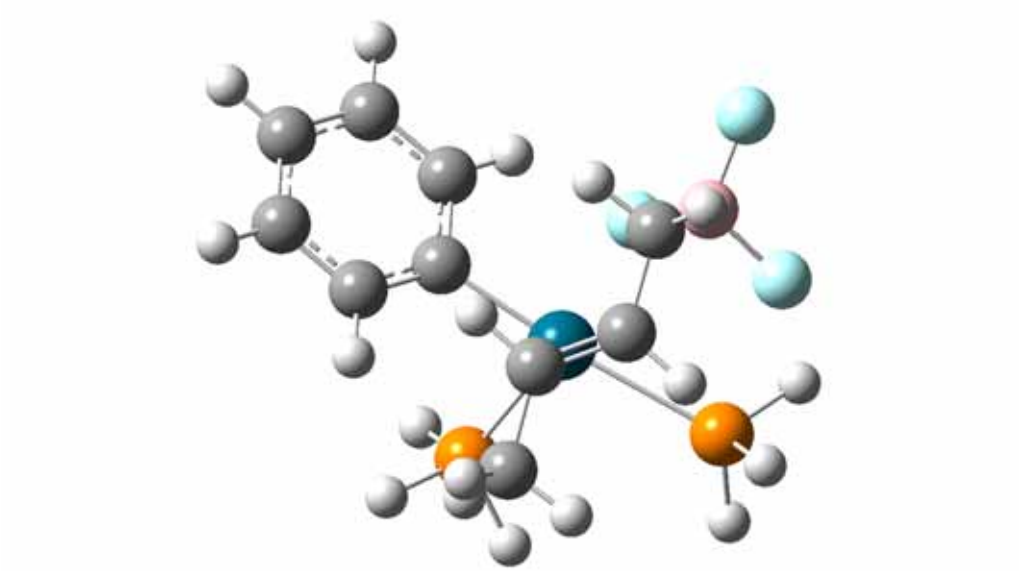
(**e**) $CH_3CH{=}CHCH^2BF_3^-$ (THF)

E(RB+HF-LYP) = -481.342200275 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.160066	-0.154933	-0.506846
2	1	0	1.157068	0.740210	-1.137161
3	6	0	2.296782	-0.462659	0.161647
4	1	0	2.301208	-1.340782	0.813432
5	6	0	3.578904	0.347059	0.116054
6	1	0	3.841474	0.746407	1.109419
7	1	0	4.436716	-0.257153	-0.224146
8	1	0	3.473457	1.199987	-0.568229
9	6	0	-0.149705	-0.891488	-0.440226
10	1	0	-0.070277	-1.768633	0.220579
11	1	0	-0.425215	-1.253061	-1.446702
12	5	0	-1.397011	0.030195	0.043498
13	9	0	-2.650872	-0.729025	-0.060582
14	9	0	-1.268715	0.479659	1.426643
15	9	0	-1.529930	1.222053	-0.807001

(**f'**) $(H_3P)_2Pd(Ph)+CH_3CH=CHCH_2BF_3^-$ (Cyclic)



E(RB+HF-LYP) = -856.103546793 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.048526	0.774161	-0.435018
2	15	0	-2.226046	1.873213	-0.844532
3	1	0	-2.308257	3.302904	-0.976889
4	1	0	-2.889333	1.494345	-2.046633
5	15	0	1.334062	2.719942	-0.149293
6	1	0	2.415943	2.909674	-1.059107
7	1	0	0.694952	3.995938	-0.247252
8	1	0	-3.278811	1.674882	0.094014
9	1	0	2.021256	2.877067	1.091775
10	6	0	1.809288	-0.208351	-0.230347
11	6	0	2.561685	-0.227663	0.960770
12	6	0	2.198154	-0.995312	-1.332900
13	6	0	3.711819	-1.043684	1.046730
14	1	0	2.256047	0.350991	1.830118

15	6	0	3.350441	-1.801699	-1.239762
16	1	0	1.595383	-1.016005	-2.236984
17	6	0	4.110426	-1.825156	-0.053209
18	1	0	4.283521	-1.069044	1.972276
19	1	0	3.640664	-2.419059	-2.087036
20	1	0	4.995179	-2.453633	0.015445
21	6	0	-1.917374	-1.038434	1.968496
22	1	0	-2.854745	-0.479783	2.053782
23	6	0	-0.852058	-0.617118	2.690732
24	1	0	0.080236	-1.182504	2.624000
25	6	0	-0.854302	0.567204	3.636090
26	1	0	-0.631614	0.254829	4.667396
27	1	0	-0.090588	1.312622	3.361161
28	1	0	-1.830734	1.069229	3.642408
29	6	0	-1.943938	-2.222852	1.033632
30	1	0	-2.801723	-2.868414	1.282539
31	1	0	-1.035293	-2.830446	1.146893
32	5	0	-2.103680	-1.828427	-0.510174
33	9	0	-3.125164	-0.821848	-0.766025
34	9	0	-0.794907	-1.121815	-1.004016
35	9	0	-2.262255	-2.924313	-1.401095

(**f**) $(H_3P)_2Pd(Ph)+CH_3CH=CHCH_2BF_3^-$ (Cyclic, THF)

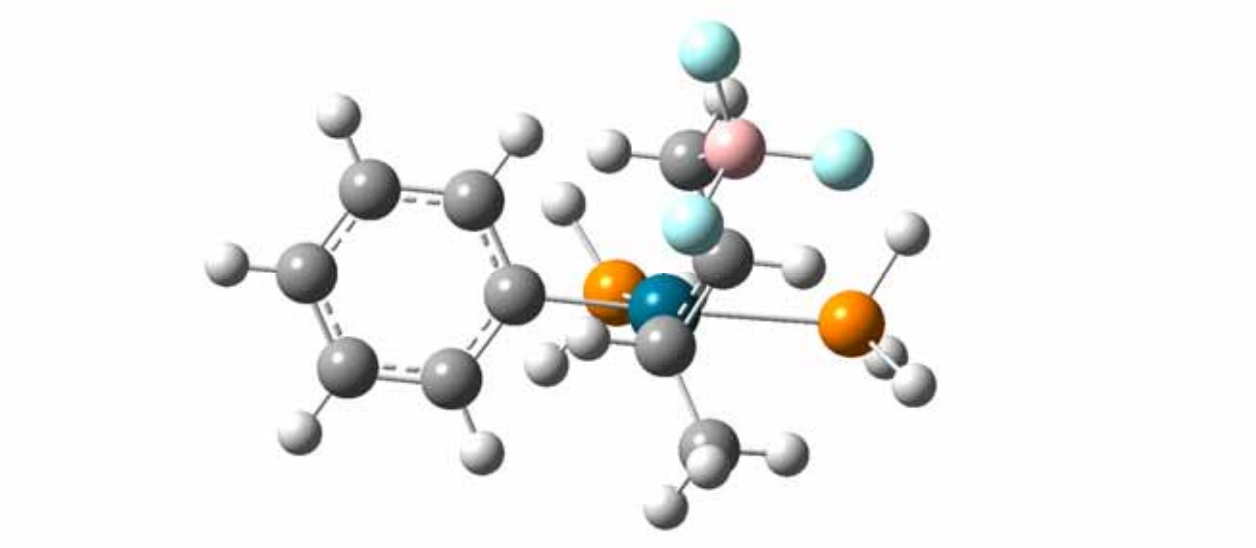
E(RB+HF-LYP) = -856.132510462 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.048526	0.774161	-0.435018
2	15	0	-2.226046	1.873213	-0.844532
3	1	0	-2.308257	3.302904	-0.976889
4	1	0	-2.889333	1.494345	-2.046633
5	15	0	1.334062	2.719942	-0.149293

6	1	0	2.415943	2.909674	-1.059107
7	1	0	0.694952	3.995938	-0.247252
8	1	0	-3.278811	1.674882	0.094014
9	1	0	2.021256	2.877067	1.091775
10	6	0	1.809288	-0.208351	-0.230347
11	6	0	2.561685	-0.227663	0.960770
12	6	0	2.198154	-0.995312	-1.332900
13	6	0	3.711819	-1.043684	1.046730
14	1	0	2.256047	0.350991	1.830118
15	6	0	3.350441	-1.801699	-1.239762
16	1	0	1.595383	-1.016005	-2.236984
17	6	0	4.110426	-1.825156	-0.053209
18	1	0	4.283521	-1.069044	1.972276
19	1	0	3.640664	-2.419059	-2.087036
20	1	0	4.995179	-2.453633	0.015445
21	6	0	-1.917374	-1.038434	1.968496
22	1	0	-2.854745	-0.479783	2.053782
23	6	0	-0.852058	-0.617118	2.690732
24	1	0	0.080236	-1.182504	2.624000
25	6	0	-0.854302	0.567204	3.636090
26	1	0	-0.631614	0.254829	4.667396
27	1	0	-0.090588	1.312622	3.361161
28	1	0	-1.830734	1.069229	3.642408
29	6	0	-1.943938	-2.222852	1.033632
30	1	0	-2.801723	-2.868414	1.282539
31	1	0	-1.035293	-2.830446	1.146893
32	5	0	-2.103680	-1.828427	-0.510174
33	9	0	-3.125164	-0.821848	-0.766025
34	9	0	-0.794907	-1.121815	-1.004016
35	9	0	-2.262255	-2.924313	-1.401095

(**g'**) $(H_3P)_2Pd(Ph)+CH_3CH=CHCH_2BF_3^-$ (Open)



E(RB+HF-LYP) = -856.090842957 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.771834	-0.866999	0.031100
2	15	0	0.146423	-3.256104	-0.114373
3	1	0	-0.749651	-4.371883	-0.213965
4	1	0	0.971522	-3.554354	-1.246299
5	15	0	-2.913340	-1.408102	-1.052104
6	1	0	-3.197006	-0.668097	-2.240247
7	1	0	-3.286088	-2.720415	-1.499594
8	1	0	1.002935	-3.774719	0.909263
9	1	0	-4.079926	-1.085094	-0.293555
10	6	0	-1.546863	1.023057	0.064248
11	6	0	-2.393643	1.421420	1.122131
12	6	0	-1.274007	1.918920	-0.990257
13	6	0	-2.959452	2.714619	1.124237
14	1	0	-2.604437	0.746935	1.950221
15	6	0	-1.846191	3.209431	-0.983756

16	1	0	-0.613231	1.632750	-1.805246
17	6	0	-2.688470	3.609735	0.071243
18	1	0	-3.601360	3.018820	1.948523
19	1	0	-1.622808	3.897768	-1.795953
20	1	0	-3.120173	4.607508	0.077156
21	6	0	1.633646	-0.273081	0.203504
22	1	0	2.110764	-1.255801	0.217361
23	6	0	0.857028	0.078605	1.325236
24	1	0	0.580170	1.127107	1.405161
25	6	0	0.921547	-0.667657	2.647818
26	1	0	1.694744	-0.199017	3.274614
27	1	0	-0.025125	-0.613184	3.199369
28	1	0	1.198331	-1.721916	2.524886
29	6	0	2.129056	0.631087	-0.832267
30	1	0	1.624195	1.600074	-0.866803
31	1	0	2.204134	0.173521	-1.826146
32	5	0	3.737000	0.916140	-0.414857
33	9	0	4.321939	1.759727	-1.414461
34	9	0	3.794247	1.543419	0.884648
35	9	0	4.421617	-0.366756	-0.369157

(**g**) $(H_3P)_2Pd(Ph)+CH_3CH=CHCH_2BF_3^-$ (Open, THF)

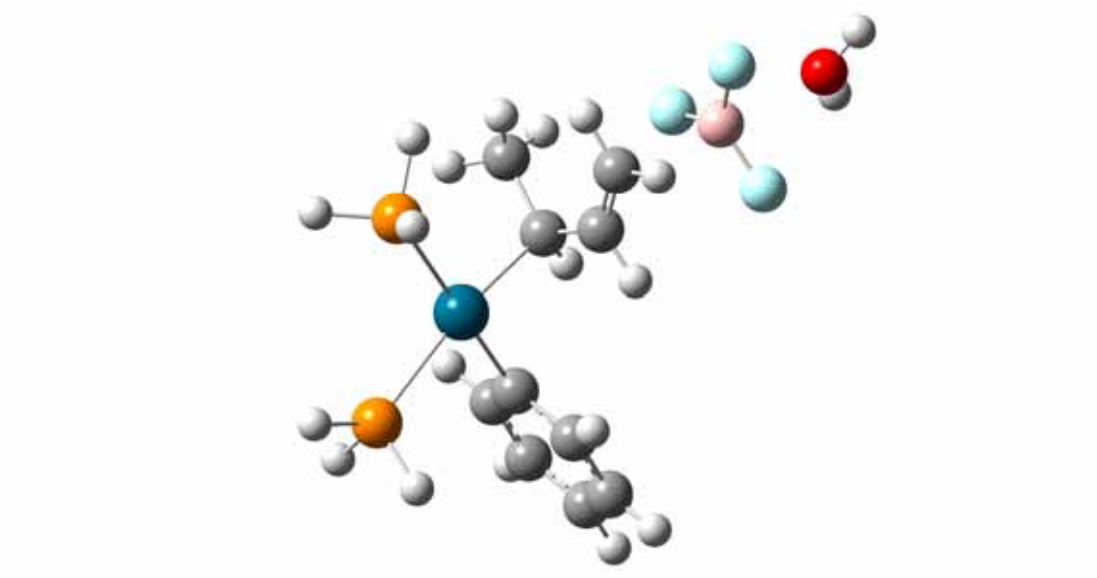
E(RB+HF-LYP) = -856.135663523 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.771834	-0.866999	0.031100
2	15	0	0.146423	-3.256104	-0.114373
3	1	0	-0.749651	-4.371883	-0.213965
4	1	0	0.971522	-3.554354	-1.246299
5	15	0	-2.913340	-1.408102	-1.052104
6	1	0	-3.197006	-0.668097	-2.240247

7	1	0	-3.286088	-2.720415	-1.499594
8	1	0	1.002935	-3.774719	0.909263
9	1	0	-4.079926	-1.085094	-0.293555
10	6	0	-1.546863	1.023057	0.064248
11	6	0	-2.393643	1.421420	1.122131
12	6	0	-1.274007	1.918920	-0.990257
13	6	0	-2.959452	2.714619	1.124237
14	1	0	-2.604437	0.746935	1.950221
15	6	0	-1.846191	3.209431	-0.983756
16	1	0	-0.613231	1.632750	-1.805246
17	6	0	-2.688470	3.609735	0.071243
18	1	0	-3.601360	3.018820	1.948523
19	1	0	-1.622808	3.897768	-1.795953
20	1	0	-3.120173	4.607508	0.077156
21	6	0	1.633646	-0.273081	0.203504
22	1	0	2.110764	-1.255801	0.217361
23	6	0	0.857028	0.078605	1.325236
24	1	0	0.580170	1.127107	1.405161
25	6	0	0.921547	-0.667657	2.647818
26	1	0	1.694744	-0.199017	3.274614
27	1	0	-0.025125	-0.613184	3.199369
28	1	0	1.198331	-1.721916	2.524886
29	6	0	2.129056	0.631087	-0.832267
30	1	0	1.624195	1.600074	-0.866803
31	1	0	2.204134	0.173521	-1.826146
32	5	0	3.737000	0.916140	-0.414857
33	9	0	4.321939	1.759727	-1.414461
34	9	0	3.794247	1.543419	0.884648
35	9	0	4.421617	-0.366756	-0.369157

TS_tm



E(RB+HF-LYP) = -932.488970450 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.434346	-0.715524	0.112317
2	15	0	-3.877317	-0.793597	-0.521597
3	1	0	-4.752158	-0.122597	0.394507
4	1	0	-4.220958	-0.048088	-1.696429
5	1	0	-4.716213	-1.941293	-0.773000
6	6	0	-1.671346	1.318280	0.071027
7	6	0	-2.006123	2.045300	1.241079
8	6	0	-2.225105	3.438476	1.193540
9	6	0	-2.108475	4.135990	-0.024957
10	6	0	-1.773182	3.427547	-1.195009
11	6	0	-1.559016	2.033165	-1.147770
12	1	0	-2.087999	1.530844	2.197154
13	1	0	-2.478566	3.975511	2.106405
14	1	0	-2.270877	5.211122	-0.060785

15	1	0	-1.673474	3.955959	-2.141909
16	1	0	-1.298108	1.509802	-2.066443
17	6	0	1.291773	-0.413087	-0.647547
18	6	0	0.594156	-0.252242	0.646518
19	1	0	1.076660	0.371119	-1.377334
20	1	0	0.551612	0.801843	0.931507
21	15	0	-1.159234	-3.239035	0.023435
22	1	0	-2.105825	-4.126008	0.642940
23	1	0	-1.151372	-3.863066	-1.269293
24	1	0	0.031339	-3.858427	0.531930
25	5	0	4.117036	0.084565	-0.288479
26	6	0	2.177761	-1.382573	-1.030937
27	1	0	2.574285	-1.406735	-2.042923
28	1	0	2.463462	-2.209590	-0.386293
29	8	0	6.112881	1.427977	0.397017
30	9	0	4.915571	-0.952046	-0.705781
31	9	0	3.736717	0.155347	1.026240
32	9	0	3.833972	1.101289	-1.160584
33	1	0	6.024846	2.273919	0.866785
34	1	0	7.028124	1.173654	0.193111
35	6	0	1.103443	-1.100099	1.836041
36	1	0	1.509664	-2.069274	1.522063
37	1	0	1.912326	-0.558805	2.344530
38	1	0	0.303537	-1.288801	2.564805

TS_tm (THF)

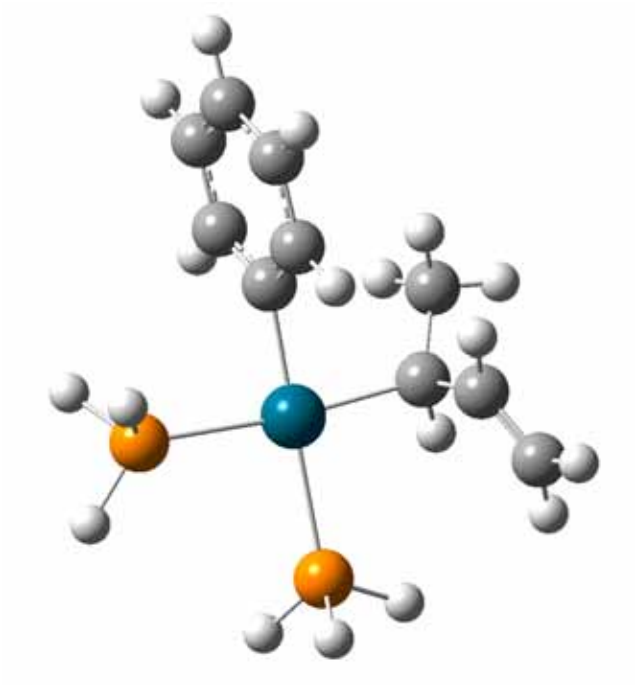
E(RB+HF-LYP) = -932.516340503 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.434346	-0.715524	0.112317
2	15	0	-3.877317	-0.793597	-0.521597
3	1	0	-4.752158	-0.122597	0.394507

4	1	0	-4.220958	-0.048088	-1.696429
5	1	0	-4.716213	-1.941293	-0.773000
6	6	0	-1.671346	1.318280	0.071027
7	6	0	-2.006123	2.045300	1.241079
8	6	0	-2.225105	3.438476	1.193540
9	6	0	-2.108475	4.135990	-0.024957
10	6	0	-1.773182	3.427547	-1.195009
11	6	0	-1.559016	2.033165	-1.147770
12	1	0	-2.087999	1.530844	2.197154
13	1	0	-2.478566	3.975511	2.106405
14	1	0	-2.270877	5.211122	-0.060785
15	1	0	-1.673474	3.955959	-2.141909
16	1	0	-1.298108	1.509802	-2.066443
17	6	0	1.291773	-0.413087	-0.647547
18	6	0	0.594156	-0.252242	0.646518
19	1	0	1.076660	0.371119	-1.377334
20	1	0	0.551612	0.801843	0.931507
21	15	0	-1.159234	-3.239035	0.023435
22	1	0	-2.105825	-4.126008	0.642940
23	1	0	-1.151372	-3.863066	-1.269293
24	1	0	0.031339	-3.858427	0.531930
25	5	0	4.117036	0.084565	-0.288479
26	6	0	2.177761	-1.382573	-1.030937
27	1	0	2.574285	-1.406735	-2.042923
28	1	0	2.463462	-2.209590	-0.386293
29	8	0	6.112881	1.427977	0.397017
30	9	0	4.915571	-0.952046	-0.705781
31	9	0	3.736717	0.155347	1.026240
32	9	0	3.833972	1.101289	-1.160584
33	1	0	6.024846	2.273919	0.866785
34	1	0	7.028124	1.173654	0.193111
35	6	0	1.103443	-1.100099	1.836041
36	1	0	1.509664	-2.069274	1.522063
37	1	0	1.912326	-0.558805	2.344530
38	1	0	0.303537	-1.288801	2.564805

(**h**) $(H_3P)_2Pd(Ph)(CH(CH_3)CH=CH_2)$



E(RB+HF-LYP) = -531.499602019 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.618932	-0.342812	-0.150023
2	15	0	3.104971	-0.771550	-0.250115
3	1	0	3.794116	-1.101936	0.966189
4	1	0	3.676319	-1.811586	-1.063182
5	1	0	3.970842	0.292778	-0.671251
6	15	0	0.001192	-2.726118	0.457419
7	1	0	0.844805	-3.880604	0.657120
8	1	0	-0.770238	-2.852455	1.659143
9	1	0	-0.938835	-3.339152	-0.435199
10	6	0	-1.395756	0.007645	-0.023961
11	6	0	-1.981714	0.448326	1.190205
12	6	0	-2.261628	-0.264036	-1.113853

13	6	0	-3.377912	0.619744	1.308151
14	1	0	-1.351857	0.664604	2.052020
15	6	0	-3.657705	-0.093005	-0.998566
16	1	0	-1.849464	-0.597351	-2.065171
17	6	0	-4.222761	0.351144	0.213359
18	1	0	-3.801241	0.964428	2.250715
19	1	0	-4.299389	-0.302646	-1.853389
20	1	0	-5.298616	0.487148	0.301823
21	6	0	0.918787	1.731898	-0.587321
22	1	0	1.845510	1.709570	-1.181242
23	6	0	1.174137	2.329118	0.756583
24	1	0	0.285713	2.476950	1.377034
25	6	0	2.378301	2.710905	1.259561
26	1	0	3.295290	2.631331	0.675222
27	1	0	2.472815	3.129175	2.259214
28	6	0	-0.173129	2.459133	-1.392808
29	1	0	0.175163	3.468757	-1.670199
30	1	0	-0.418792	1.920868	-2.316100
31	1	0	-1.099170	2.569278	-0.819336

(h) $(H_3P)_2Pd(Ph)(CH(CH_3)CH=CH_2)$ (THF)

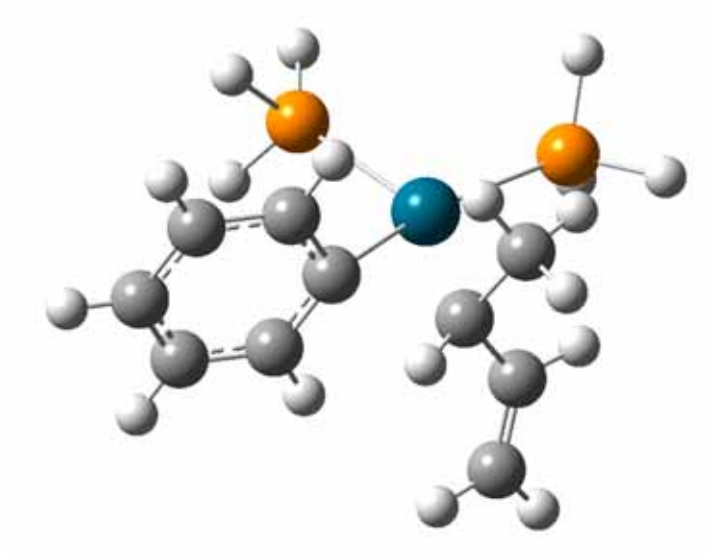
E(RB+HF-LYP) = -531.509913813 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.618932	-0.342812	-0.150023
2	15	0	3.104971	-0.771550	-0.250115
3	1	0	3.794116	-1.101936	0.966189
4	1	0	3.676319	-1.811586	-1.063182
5	1	0	3.970842	0.292778	-0.671251
6	15	0	0.001192	-2.726118	0.457419
7	1	0	0.844805	-3.880604	0.657120
8	1	0	-0.770238	-2.852455	1.659143

9	1	0	-0.938835	-3.339152	-0.435199
10	6	0	-1.395756	0.007645	-0.023961
11	6	0	-1.981714	0.448326	1.190205
12	6	0	-2.261628	-0.264036	-1.113853
13	6	0	-3.377912	0.619744	1.308151
14	1	0	-1.351857	0.664604	2.052020
15	6	0	-3.657705	-0.093006	-0.998566
16	1	0	-1.849464	-0.597352	-2.065171
17	6	0	-4.222761	0.351143	0.213359
18	1	0	-3.801241	0.964428	2.250715
19	1	0	-4.299389	-0.302647	-1.853389
20	1	0	-5.298616	0.487147	0.301823
21	6	0	0.918787	1.731898	-0.587321
22	1	0	1.845510	1.709570	-1.181242
23	6	0	1.174137	2.329118	0.756583
24	1	0	0.285713	2.476950	1.377034
25	6	0	2.378301	2.710905	1.259560
26	1	0	3.295290	2.631331	0.675221
27	1	0	2.472815	3.129175	2.259213
28	6	0	-0.173129	2.459133	-1.392808
29	1	0	0.175162	3.468757	-1.670199
30	1	0	-0.418792	1.920868	-2.316100
31	1	0	-1.099170	2.569278	-0.819336

TS_re



E(RB+HF-LYP) = -531.469910877 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.741675	-0.303912	0.048821
2	6	0	1.245287	0.343407	0.164715
3	6	0	1.929974	0.413152	-1.082389
4	6	0	1.990700	-0.047813	1.311637
5	6	0	3.291142	0.072753	-1.179923
6	1	0	1.390653	0.742615	-1.968713
7	6	0	3.354488	-0.384502	1.207499
8	1	0	1.505790	-0.093857	2.284949
9	6	0	4.015405	-0.327748	-0.036484
10	1	0	3.788736	0.124032	-2.147303
11	1	0	3.900297	-0.689829	2.099084
12	1	0	5.069634	-0.583592	-0.113075
13	6	0	0.018221	1.923590	0.478078
14	1	0	0.970472	2.456920	0.428469
15	6	0	-0.554449	2.088477	1.898506

16	1	0	0.040696	1.540904	2.638726
17	1	0	-0.538051	3.151722	2.188089
18	1	0	-1.590143	1.735930	1.970850
19	6	0	-0.859008	2.420441	-0.627835
20	1	0	-1.933471	2.284032	-0.484659
21	6	0	-0.429172	3.053897	-1.750936
22	1	0	0.627143	3.244785	-1.932179
23	1	0	-1.127224	3.391382	-2.513372
24	15	0	-0.129173	-2.725112	-0.428895
25	1	0	0.593087	-2.913319	-1.659397
26	1	0	0.901597	-3.225690	0.440353
27	15	0	-3.248778	-0.519178	0.067256
28	1	0	-4.175862	0.537648	0.400146
29	1	0	-3.910023	-0.913894	-1.150176
30	1	0	-0.881635	-3.960723	-0.504762
31	1	0	-3.860912	-1.518709	0.904569

TS_re (THF)

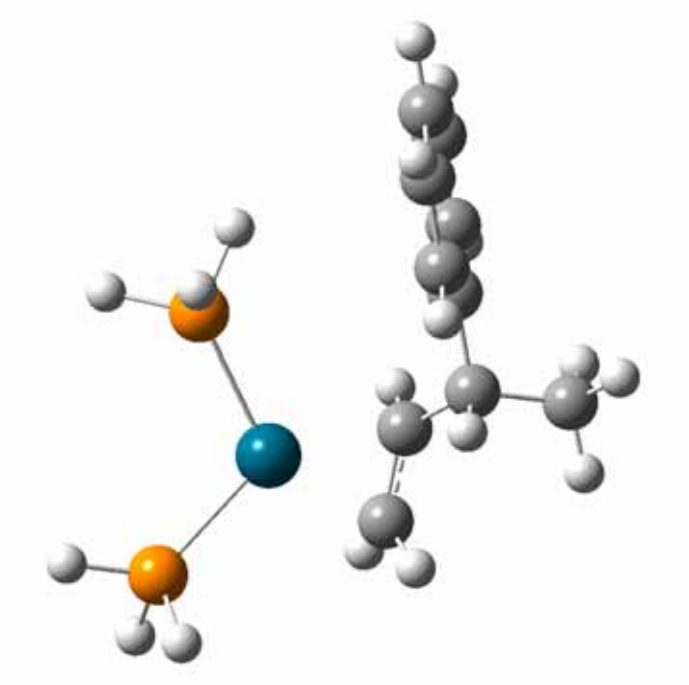
E(RB+HF-LYP) = -531.477751867 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.741675	-0.303912	0.048821
2	6	0	1.245287	0.343407	0.164715
3	6	0	1.929974	0.413152	-1.082389
4	6	0	1.990700	-0.047813	1.311637
5	6	0	3.291142	0.072753	-1.179923
6	1	0	1.390653	0.742615	-1.968713
7	6	0	3.354488	-0.384502	1.207499
8	1	0	1.505790	-0.093857	2.284949
9	6	0	4.015405	-0.327748	-0.036484
10	1	0	3.788736	0.124032	-2.147303
11	1	0	3.900297	-0.689829	2.099084

12	1	0	5.069634	-0.583592	-0.113075
13	6	0	0.018221	1.923590	0.478078
14	1	0	0.970472	2.456920	0.428469
15	6	0	-0.554449	2.088477	1.898506
16	1	0	0.040696	1.540904	2.638726
17	1	0	-0.538051	3.151722	2.188089
18	1	0	-1.590143	1.735930	1.970850
19	6	0	-0.859008	2.420441	-0.627835
20	1	0	-1.933471	2.284032	-0.484659
21	6	0	-0.429172	3.053897	-1.750936
22	1	0	0.627143	3.244785	-1.932179
23	1	0	-1.127224	3.391382	-2.513372
24	15	0	-0.129173	-2.725112	-0.428895
25	1	0	0.593087	-2.913319	-1.659397
26	1	0	0.901597	-3.225690	0.440353
27	15	0	-3.248778	-0.519178	0.067256
28	1	0	-4.175862	0.537648	0.400146
29	1	0	-3.910023	-0.913894	-1.150176
30	1	0	-0.881635	-3.960723	-0.504762
31	1	0	-3.860912	-1.518709	0.904569

(i) $(H_3P)_2Pd$-$(PhCH(CH_3)CH=CH_2)$



E(RB+HF-LYP) = -531.556141978 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.480488	-0.000714	-0.158540
2	15	0	0.366905	-2.189638	-0.361914
3	1	0	1.004615	-3.323595	-0.986687
4	1	0	-0.032659	-2.884230	0.834243
5	15	0	3.833831	-0.439041	0.451696
6	1	0	4.479126	-1.728990	0.547967
7	1	0	4.309057	0.049442	1.721623
8	6	0	-1.150667	1.704863	0.424014
9	1	0	-0.731495	1.653907	1.438623
10	6	0	-1.848646	3.092336	0.278864
11	1	0	-2.671472	3.197064	0.998749
12	1	0	-1.124781	3.898475	0.449687

13	1	0	-2.263841	3.220623	-0.729631
14	6	0	0.014056	1.596853	-0.570110
15	1	0	-0.282376	1.470614	-1.614297
16	6	0	1.280782	2.172794	-0.306402
17	6	0	-2.174332	0.578962	0.278697
18	6	0	-2.500216	-0.246351	1.376609
19	6	0	-2.844323	0.352474	-0.946347
20	6	0	-3.464059	-1.267712	1.261101
21	1	0	-1.996732	-0.086883	2.328807
22	6	0	-3.805695	-0.666506	-1.069360
23	1	0	-2.617742	0.975460	-1.809276
24	6	0	-4.121607	-1.483195	0.035374
25	1	0	-3.701123	-1.888370	2.122818
26	1	0	-4.310522	-0.821907	-2.020649
27	1	0	-4.868392	-2.268486	-0.057686
28	1	0	1.923700	2.496118	-1.124228
29	1	0	1.481081	2.642027	0.657770
30	1	0	4.869292	0.174982	-0.340649
31	1	0	-0.890999	-2.320310	-1.045708

(i) $(H_3P)_2Pd$-$(PhCH(CH_3)CH=CH_2)$ (THF)

E(RB+HF-LYP) = -531.563867890 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.480482	-0.000581	-0.158569
2	15	0	0.366940	-2.189523	-0.361873
3	1	0	1.004696	-3.323534	-0.986506
4	1	0	-0.033227	-2.884173	0.834050
5	15	0	3.833899	-0.439231	0.451624
6	1	0	4.479785	-1.729125	0.544538
7	1	0	4.308309	0.045922	1.723133
8	6	0	-1.150716	1.704813	0.424175

9	1	0	-0.731489	1.653721	1.438758
10	6	0	-1.848666	3.092316	0.279259
11	1	0	-2.671453	3.196955	0.999203
12	1	0	-1.124764	3.898402	0.450178
13	1	0	-2.263898	3.220790	-0.729193
14	6	0	0.013928	1.596852	-0.570063
15	1	0	-0.282655	1.470562	-1.614201
16	6	0	1.280645	2.172899	-0.306566
17	6	0	-2.174359	0.578895	0.278773
18	6	0	-2.500055	-0.246682	1.376548
19	6	0	-2.844492	0.352637	-0.946238
20	6	0	-3.463833	-1.268105	1.260919
21	1	0	-1.996488	-0.087377	2.328734
22	6	0	-3.805786	-0.666386	-1.069364
23	1	0	-2.618077	0.975861	-1.809035
24	6	0	-4.121502	-1.483355	0.035216
25	1	0	-3.700752	-1.888968	2.122531
26	1	0	-4.310721	-0.821613	-2.020622
27	1	0	-4.868229	-2.268689	-0.057934
28	1	0	1.923419	2.496126	-1.124540
29	1	0	1.481086	2.642208	0.657536
30	1	0	4.869415	0.177548	-0.338520
31	1	0	-0.890718	-2.319882	-1.046177

H_2O

E(RB+HF-LYP) = -76.4143162919 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.111982
2	1	0	0.000000	0.800544	-0.447929
3	1	0	0.000000	-0.800544	-0.447929

H_2O(THF)

E(RB+HF-LYP) = -76.4284572211 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.114344
2	1	0	0.000000	0.801460	-0.457374
3	1	0	0.000000	-0.801460	-0.457374

K-Br

E(RB+HF-LYP) = -41.3866272542 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	19	0	0.000000	0.000000	-1.932835
2	35	0	0.000000	0.000000	1.049253

K-Br(THF)

E(RB+HF-LYP) = -41.4565507982 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	19	0	0.000000	0.000000	-2.105459
2	35	0	0.000000	0.000000	1.142963

$CH_3CH=CHCH_2BF_3K$

E(RB+HF-LYP) = -509.405994055 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.310562	-0.961553	0.023535
2	1	0	-4.360242	-1.820270	-0.663250
3	1	0	-5.294151	-0.468661	-0.008683
4	1	0	-4.158887	-1.349629	1.039007
5	6	0	-3.200979	-0.008363	-0.367416
6	1	0	-3.271105	0.430427	-1.366378
7	6	0	-2.148500	0.320977	0.412957
8	1	0	-2.073071	-0.125187	1.408381
9	6	0	-1.020046	1.249626	0.023142
10	1	0	-0.950048	2.079287	0.746257
11	1	0	-1.213607	1.694866	-0.963681
12	5	0	0.395289	0.539411	-0.004019
13	9	0	0.595918	-0.502638	-1.043249
14	9	0	1.549989	1.457389	-0.233577
15	9	0	0.782557	-0.163347	1.255012
16	19	0	3.003632	-0.729719	-0.027818

$CH_3CH=CHCH_2BF_3K$ (THF)

E(RB+HF-LYP) = -509.457801744 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.355634	-1.021196	0.012716
2	1	0	-4.409930	-1.851137	-0.708125
3	1	0	-5.343904	-0.537114	0.012979
4	1	0	-4.186176	-1.448853	1.009362
5	6	0	-3.261553	-0.041032	-0.357806
6	1	0	-3.355321	0.440005	-1.337282
7	6	0	-2.199364	0.269649	0.420487
8	1	0	-2.109080	-0.213806	1.399328
9	6	0	-1.091601	1.233742	0.053647
10	1	0	-1.039810	2.042895	0.803098
11	1	0	-1.306707	1.707817	-0.916388
12	5	0	0.351220	0.564706	-0.004067
13	9	0	0.546553	-0.445079	-1.064708
14	9	0	1.447338	1.539458	-0.233616
15	9	0	0.753293	-0.135588	1.241939
16	19	0	3.195741	-0.749444	-0.026813

$BF_3\_H_2O$

E(RB+HF-LYP) = -401.006773477 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.229552	0.036439	-0.011760
2	9	0	-0.213154	1.412555	-0.260624
3	9	0	-0.650357	-0.782752	-1.058805
4	9	0	-0.699084	-0.346292	1.245698
5	8	0	1.421542	-0.258382	0.062965
6	1	0	1.791922	-1.154693	0.144738
7	1	0	2.046859	0.487958	0.073924

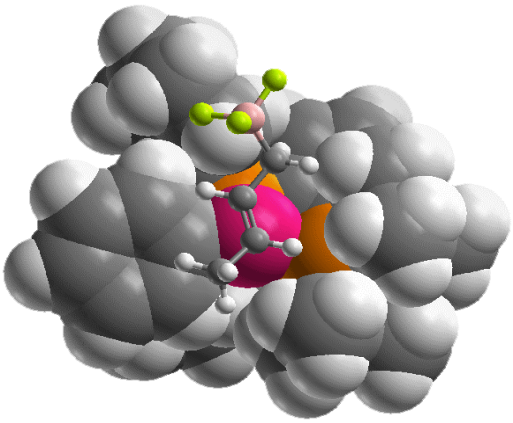
$BF_3\_H_2O$ (THF)

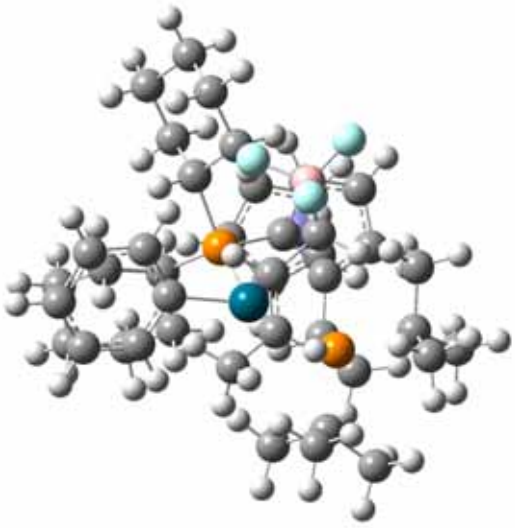
E(RB+HF-LYP) = -401.039702389 A.U.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.229552	0.036439	-0.011760
2	9	0	-0.213153	1.412556	-0.260621
3	9	0	-0.650356	-0.782749	-1.058808
4	9	0	-0.699086	-0.346294	1.245696
5	8	0	1.421542	-0.258383	0.062966
6	1	0	1.791921	-1.154695	0.144738
7	1	0	2.046859	0.487956	0.073928

(CyPF-*t*-Bu)Pd(Ph)((*E*)-$CH_3CH{=}CHCH_2BF_3$), *re*, 3.5 kcal/mol (**28**)





E(RB+HF-LYP) = -2226.49332420 A.U.

Standard orientation:

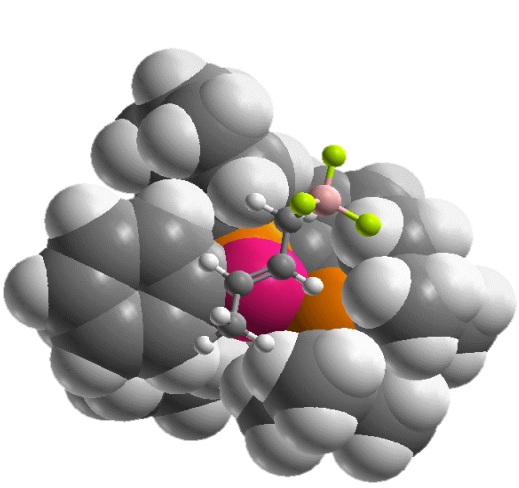
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.242679	-4.425239	-3.364745
2	6	0	1.658286	-0.059911	-1.000524
3	6	0	2.031294	1.326560	-0.749088
4	6	0	2.737325	1.809697	-1.910968
5	6	0	2.776016	0.761822	-2.894820
6	6	0	2.126120	-0.388632	-2.335424
7	6	0	4.935556	-1.167286	0.084213
8	6	0	5.253530	0.203962	0.397553
9	6	0	5.775566	0.821806	-0.796527
10	6	0	5.774934	-0.167284	-1.846415
11	6	0	5.253063	-1.396766	-1.301683
12	6	0	1.577273	-1.916666	1.448654
13	6	0	2.128449	-0.909749	2.485819
14	6	0	3.012724	-1.609915	3.549047
15	6	0	2.268482	-2.772020	4.239826
16	6	0	1.734889	-3.774894	3.194584
17	6	0	0.826164	-3.075764	2.153851

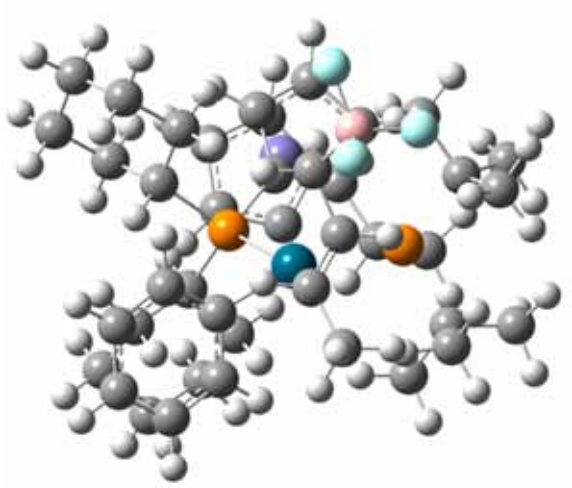
18	6	0	-0.018651	-2.595276	-1.018156
19	6	0	1.123322	-3.587136	-1.367767
20	6	0	0.555582	-4.827541	-2.104849
21	6	0	-1.373660	-3.437557	-3.008914
22	6	0	-0.836827	-2.188116	-2.269928
23	6	0	1.681328	2.148126	0.466501
24	6	0	2.741430	3.234007	0.767112
25	6	0	-0.467863	3.628401	2.121849
26	6	0	-1.982521	3.688187	2.448406
27	6	0	0.200474	2.767902	3.229492
28	6	0	0.093319	5.072277	2.173258
29	6	0	-0.485710	3.935303	-1.114371
30	6	0	-0.546613	3.093651	-2.417316
31	6	0	-1.858405	4.636281	-0.930320
32	6	0	0.613798	5.015300	-1.279786
33	6	0	-2.265249	-1.340735	1.549073
34	6	0	-2.895431	-2.451350	0.948581
35	6	0	-3.438223	-3.474987	1.755905
36	6	0	-3.363315	-3.399137	3.159853
37	6	0	-2.744505	-2.285120	3.760140
38	6	0	-2.194187	-1.263759	2.958310
39	26	0	3.798560	0.150271	-1.165947
40	1	0	6.095955	-0.009929	-2.866755
41	1	0	3.159751	2.797013	-2.026304
42	1	0	3.225334	0.821460	-3.875791
43	1	0	1.997622	-1.327824	-2.844464
44	1	0	4.552524	-1.903168	0.774093
45	1	0	5.147104	0.675649	1.364326
46	1	0	6.107264	1.846376	-0.892664
47	1	0	5.127298	-2.326732	-1.838318
48	1	0	2.426238	-2.333775	0.890532
49	1	0	1.290588	-0.410489	2.995404
50	1	0	2.720625	-0.136708	1.982255
51	1	0	3.923233	-2.002183	3.068726
52	1	0	3.343003	-0.870062	4.292213
53	1	0	1.423636	-2.371074	4.821414

54	1	0	2.935412	-3.278537	4.951249
55	1	0	1.166173	-4.574275	3.689219
56	1	0	2.584208	-4.257261	2.684236
57	1	0	-0.062899	-2.688163	2.662305
58	1	0	0.476198	-3.818151	1.427866
59	1	0	-0.708454	-3.118575	-0.343268
60	1	0	1.873765	-3.112457	-2.011481
61	1	0	1.649612	-3.918893	-0.464072
62	1	0	-0.105016	-5.384661	-1.421765
63	1	0	1.382869	-5.502298	-2.369215
64	1	0	0.438948	-3.958900	-4.095260
65	1	0	-0.659259	-5.320070	-3.847838
66	1	0	-2.116962	-3.941389	-2.373299
67	1	0	-1.914478	-3.110204	-3.904270
68	1	0	-0.220323	-1.599003	-2.962229
69	1	0	-1.689788	-1.564773	-1.989962
70	1	0	1.646055	1.480491	1.331216
71	1	0	3.734269	2.766903	0.762874
72	1	0	2.592356	3.683879	1.751855
73	1	0	2.751088	4.038855	0.029989
74	1	0	-2.114356	4.193241	3.416487
75	1	0	-2.408506	2.685934	2.529647
76	1	0	-2.556673	4.246832	1.703967
77	1	0	-0.088691	3.169157	4.211170
78	1	0	1.294123	2.781032	3.181429
79	1	0	-0.136851	1.724155	3.184774
80	1	0	-0.026895	5.455737	3.197476
81	1	0	-0.456672	5.747232	1.509339
82	1	0	1.154750	5.135393	1.921621
83	1	0	-0.713692	3.774114	-3.264979
84	1	0	-1.370655	2.378576	-2.402249
85	1	0	0.381298	2.548553	-2.607245
86	1	0	-2.091097	5.189139	-1.851105
87	1	0	-1.856740	5.357960	-0.106138
88	1	0	-2.670921	3.919260	-0.771171
89	1	0	0.287090	5.719502	-2.059122

90	1	0	1.558592	4.579357	-1.619493
91	1	0	0.796801	5.592011	-0.369364
92	1	0	-3.934273	-4.317877	1.279242
93	1	0	-3.791631	-4.186593	3.775413
94	1	0	-2.691256	-2.206133	4.844430
95	15	0	0.499533	-1.079566	0.066163
96	15	0	-0.220108	2.671522	0.393385
97	46	0	-1.514060	0.302062	0.604793
98	1	0	-3.011905	-2.518079	-0.129883
99	6	0	-3.673872	0.430212	-0.435274
100	1	0	-4.043421	-0.579648	-0.278571
101	6	0	-3.393539	0.773836	-1.867296
102	6	0	-4.559915	0.993474	1.898857
103	1	0	-5.527425	1.514652	1.836824
104	1	0	-4.761869	-0.076958	1.992906
105	1	0	-4.068060	1.330925	2.819625
106	1	0	-1.726680	-0.407460	3.441734
107	6	0	-3.756987	1.301442	0.647169
108	1	0	-3.542336	2.353937	0.469430
109	1	0	-3.532670	1.844650	-2.063728
110	5	0	-4.345160	-0.143839	-2.827692
111	9	0	-3.989532	0.041439	-4.216063
112	9	0	-4.101374	-1.560646	-2.464882
113	9	0	-5.746430	0.136724	-2.627776
114	1	0	-2.373344	0.496202	-2.170723

(CyPF-*t*-Bu)Pd(Ph)((*E*)-$CH_3CH{=}CHCH_2BF_3$), *si*, 6.1 kcal/mol (**29**)





E(RB+HF-LYP) = -2226.48918359 A.U.

Standard orientation:

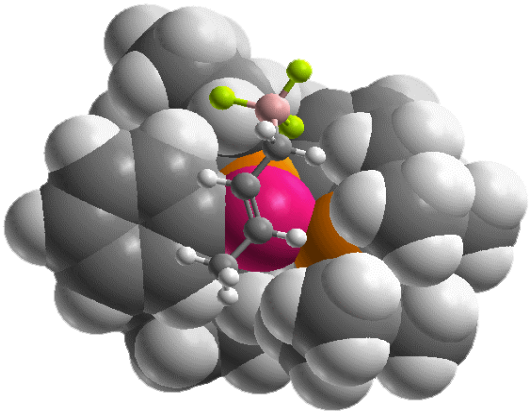
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.995772	3.502462	4.335394
2	6	0	1.662592	-0.540726	0.954124
3	6	0	1.597419	-1.880548	0.388005
4	6	0	2.114105	-2.799190	1.372624
5	6	0	2.462181	-2.059608	2.554846
6	6	0	2.199638	-0.672551	2.297297
7	6	0	5.142154	-0.231790	-0.030085
8	6	0	5.011576	-1.507542	-0.690209
9	6	0	5.303331	-2.537522	0.275866
10	6	0	5.608368	-1.897363	1.531733
11	6	0	5.505787	-0.471043	1.342529
12	6	0	2.186590	1.762869	-1.004134
13	6	0	2.421696	0.901978	-2.267321
14	6	0	3.499239	1.523253	-3.191147
15	6	0	3.165282	2.984045	-3.561828
16	6	0	2.940009	3.832734	-2.292162

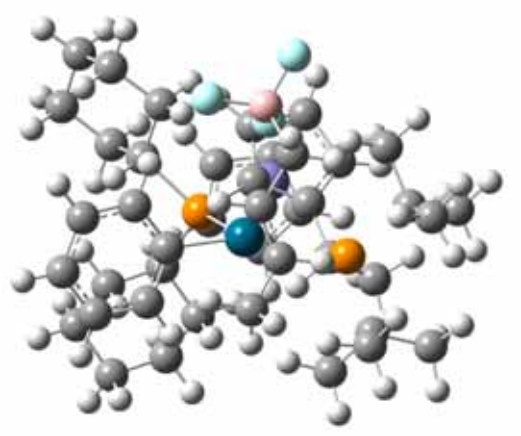
17	6	0	1.838776	3.223393	-1.390456
18	6	0	0.785300	2.278351	1.622469
19	6	0	2.144152	2.807856	2.153548
20	6	0	1.911223	3.950887	3.174359
21	6	0	-0.348791	2.959739	3.802401
22	6	0	-0.141136	1.818829	2.776872
23	6	0	1.018920	-2.255064	-0.953005
24	6	0	1.705786	-3.499736	-1.562640
25	6	0	-1.473345	-2.597540	-2.732545
26	6	0	-2.929141	-2.106824	-2.929816
27	6	0	-0.578591	-1.747238	-3.675933
28	6	0	-1.393275	-4.090182	-3.143670
29	6	0	-1.597167	-3.618154	0.354101
30	6	0	-1.479561	-3.077670	1.805476
31	6	0	-3.093634	-3.924319	0.080744
32	6	0	-0.788603	-4.936026	0.242759
33	6	0	-1.641702	2.433552	-1.047428
34	6	0	-1.874313	3.497915	-0.149880
35	6	0	-2.038854	4.815816	-0.627581
36	6	0	-1.978895	5.088296	-2.008082
37	6	0	-1.763716	4.028423	-2.910410
38	6	0	-1.596392	2.711090	-2.433689
39	26	0	3.636752	-1.407628	0.941450
40	1	0	5.856961	-2.399399	2.456444
41	1	0	2.215240	-3.866948	1.248382
42	1	0	2.863097	-2.469759	3.470600
43	1	0	2.362139	0.121873	3.004516
44	1	0	5.012890	0.736247	-0.489550
45	1	0	4.767829	-1.663106	-1.731874
46	1	0	5.291900	-3.603370	0.094801
47	1	0	5.675790	0.284297	2.097169
48	1	0	3.110317	1.762187	-0.409475
49	1	0	1.479292	0.811685	-2.828275
50	1	0	2.735284	-0.107997	-1.978796
51	1	0	4.477240	1.495099	-2.685056
52	1	0	3.597442	0.910747	-4.098757

53	1	0	2.253370	3.005368	-4.178942
54	1	0	3.972985	3.413868	-4.170358
55	1	0	2.655026	4.858000	-2.565520
56	1	0	3.884673	3.904586	-1.728830
57	1	0	0.883356	3.248921	-1.924965
58	1	0	1.718165	3.849468	-0.498826
59	1	0	0.286184	3.118476	1.123117
60	1	0	2.715749	2.010185	2.642622
61	1	0	2.767373	3.182757	1.332813
62	1	0	1.448914	4.807935	2.659761
63	1	0	2.880164	4.297027	3.561608
64	1	0	1.502601	2.716198	4.917721
65	1	0	0.819409	4.341516	5.022424
66	1	0	-0.906438	3.782642	3.327567
67	1	0	-0.971314	2.593226	4.629001
68	1	0	0.287476	0.949153	3.291424
69	1	0	-1.110556	1.497358	2.380374
70	1	0	1.193674	-1.425204	-1.643195
71	1	0	2.791215	-3.336584	-1.559059
72	1	0	1.400590	-3.661579	-2.598955
73	1	0	1.507388	-4.418474	-1.008013
74	1	0	-3.245526	-2.322381	-3.961113
75	1	0	-2.990946	-1.026815	-2.776264
76	1	0	-3.638909	-2.594192	-2.255069
77	1	0	-0.982234	-1.810359	-4.696612
78	1	0	0.458795	-2.095419	-3.713631
79	1	0	-0.581572	-0.689300	-3.380988
80	1	0	-1.654871	-4.170271	-4.209574
81	1	0	-2.106480	-4.706636	-2.588278
82	1	0	-0.397410	-4.522405	-3.017219
83	1	0	-1.719567	-3.896268	2.498847
84	1	0	-2.204722	-2.285373	1.998040
85	1	0	-0.473428	-2.719946	2.044412
86	1	0	-3.427745	-4.653639	0.831362
87	1	0	-3.263871	-4.366128	-0.906544
88	1	0	-3.736514	-3.051659	0.216489

89	1	0	-1.284271	-5.691145	0.869535
90	1	0	0.230168	-4.820006	0.624275
91	1	0	-0.743819	-5.331497	-0.776178
92	1	0	-2.229705	5.620971	0.079500
93	1	0	-2.113369	6.103197	-2.374291
94	1	0	-1.730950	4.220548	-3.981365
95	15	0	0.876871	0.982970	0.194209
96	15	0	-0.952312	-2.182207	-0.865213
97	46	0	-1.433852	0.453307	-0.558735
98	1	0	-1.972418	3.308979	0.916058
99	6	0	-3.695562	-0.017166	0.205789
100	1	0	-1.441519	1.907524	-3.152087
101	6	0	-4.036724	0.993802	-0.676437
102	1	0	-4.023174	2.008121	-0.286570
103	6	0	-4.743424	0.842098	-2.001546
104	1	0	-4.867892	-0.202162	-2.298930
105	1	0	-5.748891	1.277255	-1.902649
106	1	0	-4.236387	1.395043	-2.804257
107	1	0	-3.842816	-1.044288	-0.120203
108	6	0	-3.515768	0.187770	1.676866
109	1	0	-2.606312	-0.283713	2.070649
110	1	0	-3.511009	1.254092	1.939549
111	5	0	-4.754678	-0.540876	2.469294
112	9	0	-6.023745	0.045856	2.105046
113	9	0	-4.549142	-0.434119	3.896296
114	9	0	-4.771473	-1.965464	2.097224

(CyPF-*t*-Bu)Pd(Ph)((*E*)-$CH_3CH{=}CHCH_2BF_3$), re, 0 kcal/mol (**30**)





E(RB+HF-LYP) = -2226.49897596 A.U.

Standard orientation:

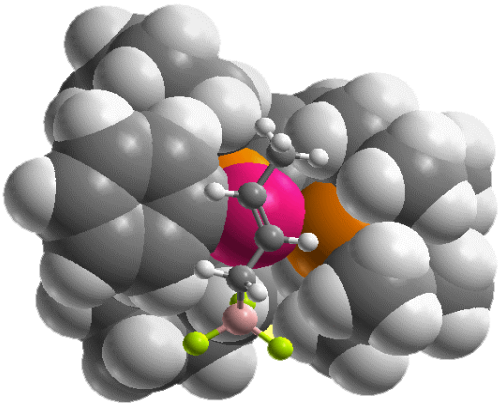
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.775323	-4.810265	-3.010545
2	6	0	1.615093	0.044244	-0.880275
3	6	0	1.827682	1.467382	-0.649164
4	6	0	2.572571	1.985609	-1.771224
5	6	0	2.793239	0.920596	-2.710500
6	6	0	2.219109	-0.272489	-2.160150
7	6	0	4.901241	-0.761388	0.423886
8	6	0	5.020910	0.623049	0.810988
9	6	0	5.572637	1.349279	-0.305990
10	6	0	5.789091	0.414106	-1.382585
11	6	0	5.372044	-0.891093	-0.931079
12	6	0	1.505196	-1.668180	1.658155
13	6	0	1.842949	-0.549510	2.668200
14	6	0	2.715592	-1.076830	3.836090
15	6	0	2.070336	-2.287297	4.542757
16	6	0	1.737766	-3.398182	3.523970
17	6	0	0.837797	-2.865045	2.382947
18	6	0	0.367907	-2.744435	-0.888047
19	6	0	1.697001	-3.543604	-0.979070

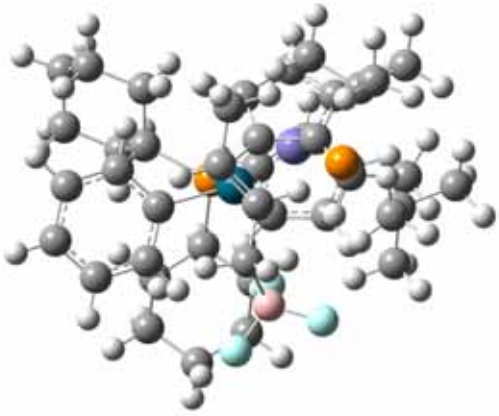
20	6	0	1.454526	-4.930918	-1.629062
21	6	0	-0.533537	-3.998686	-2.907312
22	6	0	-0.297762	-2.604992	-2.278955
23	6	0	1.333688	2.287647	0.517513
24	6	0	2.295564	3.454997	0.847003
25	6	0	-0.971995	3.661090	2.027639
26	6	0	-2.498976	3.661784	2.299306
27	6	0	-0.313487	2.876998	3.196048
28	6	0	-0.494076	5.136183	2.050309
29	6	0	-0.874795	3.862987	-1.210133
30	6	0	-0.776542	2.987917	-2.487323
31	6	0	-2.313202	4.438775	-1.117057
32	6	0	0.125365	5.039323	-1.350428
33	6	0	-2.432390	-1.706658	1.046442
34	6	0	-2.929078	-2.715392	0.192161
35	6	0	-3.485082	-3.891571	0.741104
36	6	0	-3.553288	-4.073820	2.136275
37	6	0	-3.065082	-3.064388	2.987923
38	6	0	-2.503935	-1.888745	2.445081
39	26	0	3.732619	0.464400	-0.889016
40	1	0	6.182093	0.652511	-2.361162
41	1	0	2.902314	3.007414	-1.889581
42	1	0	3.307764	0.998930	-3.657397
43	1	0	2.226300	-1.234853	-2.640610
44	1	0	4.546667	-1.567129	1.048407
45	1	0	4.767793	1.037258	1.777212
46	1	0	5.785289	2.409035	-0.336306
47	1	0	5.404009	-1.804139	-1.509137
48	1	0	2.447559	-2.011094	1.212318
49	1	0	0.911870	-0.127675	3.076019
50	1	0	2.385097	0.257668	2.164711
51	1	0	3.702996	-1.372283	3.446968
52	1	0	2.891537	-0.263388	4.554894
53	1	0	1.143699	-1.966904	5.044981
54	1	0	2.740682	-2.671257	5.324494
55	1	0	1.230694	-4.235169	4.024061

56	1	0	2.673709	-3.799893	3.102927
57	1	0	-0.123483	-2.553823	2.804020
58	1	0	0.620708	-3.680859	1.684448
59	1	0	-0.326951	-3.319206	-0.260350
60	1	0	2.436386	-2.994627	-1.576386
61	1	0	2.142064	-3.696770	0.010886
62	1	0	0.813837	-5.532231	-0.964625
63	1	0	2.413159	-5.463615	-1.714427
64	1	0	1.461455	-4.309117	-3.712815
65	1	0	0.576496	-5.810783	-3.420599
66	1	0	-1.260960	-4.557017	-2.296920
67	1	0	-0.989292	-3.868337	-3.897320
68	1	0	0.329596	-2.012378	-2.955478
69	1	0	-1.240327	-2.065384	-2.211346
70	1	0	1.303343	1.640413	1.395565
71	1	0	3.319164	3.062294	0.885448
72	1	0	2.075328	3.898558	1.820807
73	1	0	2.274983	4.253772	0.103008
74	1	0	-2.690581	4.239161	3.215830
75	1	0	-2.871871	2.649284	2.460520
76	1	0	-3.076927	4.122949	1.493551
77	1	0	-0.654763	3.308003	4.148423
78	1	0	0.779826	2.930096	3.187711
79	1	0	-0.610837	1.820446	3.184712
80	1	0	-0.649751	5.536583	3.063678
81	1	0	-1.077025	5.760106	1.364350
82	1	0	0.563178	5.258057	1.806642
83	1	0	-1.095707	3.591122	-3.350169
84	1	0	-1.400777	2.094258	-2.446839
85	1	0	0.248694	2.656766	-2.674696
86	1	0	-2.541197	4.956045	-2.059451
87	1	0	-2.424651	5.167551	-0.306482
88	1	0	-3.064917	3.652050	-0.990298
89	1	0	-0.200571	5.662605	-2.196760
90	1	0	1.132555	4.683286	-1.588659
91	1	0	0.177750	5.682332	-0.467753

92	1	0	-3.877488	-4.653423	0.070228
93	1	0	-3.987559	-4.980407	2.551689
94	1	0	-3.118487	-3.185498	4.068623
95	15	0	0.480925	-1.076790	0.109203
96	15	0	-0.593916	2.657386	0.341455
97	46	0	-1.728743	0.092834	0.396835
98	1	0	-2.931728	-2.579873	-0.885072
99	6	0	-4.221430	0.280556	-0.514956
100	1	0	-4.600368	-0.733734	-0.384727
101	6	0	-4.181427	0.752038	-1.928097
102	6	0	-4.553621	0.623015	1.990434
103	1	0	-5.453490	1.226942	2.186027
104	1	0	-4.842192	-0.431505	2.011438
105	1	0	-3.862059	0.794358	2.823766
106	1	0	-2.142820	-1.116375	3.121826
107	6	0	-3.978760	1.014638	0.635673
108	1	0	-3.733085	2.066265	0.509537
109	1	0	-5.195089	0.620700	-2.344670
110	5	0	-3.229049	-0.128501	-2.906861
111	9	0	-3.531126	-1.556691	-2.785813
112	9	0	-3.368543	0.276876	-4.278851
113	9	0	-1.814823	0.040429	-2.514942
114	1	0	-3.913994	1.812880	-2.006514

(CyPF-*t*-Bu)Pd(Ph)((*E*)-$CH_3CH{=}CHCH_2BF_3$), re, 0.3 kcal/mol (**31**)





E(RB+HF-LYP) = -2226.49857824 A.U.

Standard orientation:

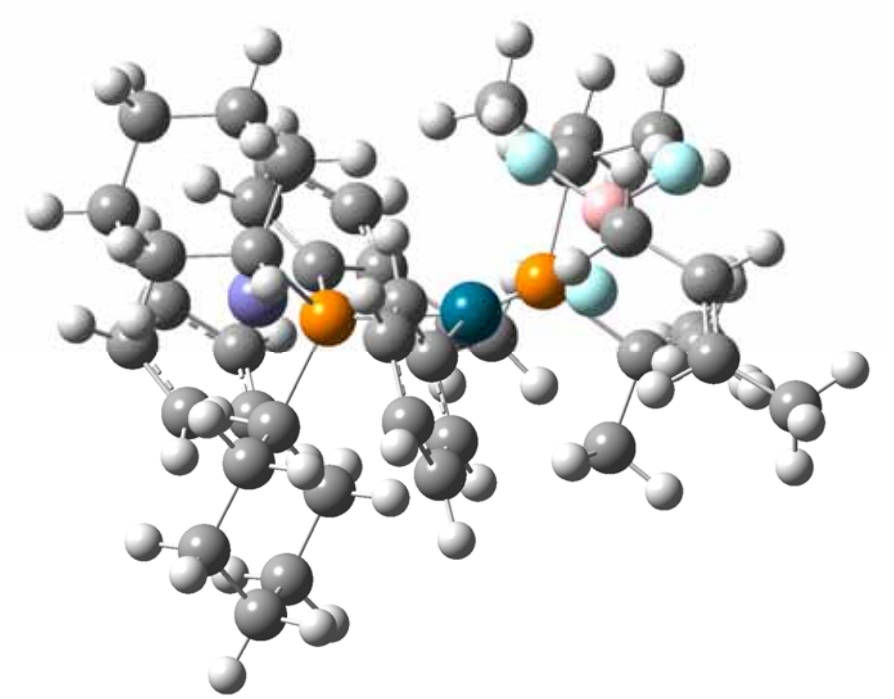
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.242010	4.636995	-3.047863
2	6	0	-2.026207	-0.091919	-0.653202
3	6	0	-2.037728	-1.539660	-0.487494
4	6	0	-3.152094	-2.054986	-1.253032
5	6	0	-3.812863	-0.963487	-1.910332
6	6	0	-3.137624	0.242820	-1.529550
7	6	0	-4.456396	0.216998	2.026635
8	6	0	-4.381942	-1.212436	2.194807
9	6	0	-5.341439	-1.813473	1.301699
10	6	0	-6.001764	-0.754321	0.578254
11	6	0	-5.451929	0.502099	1.026003
12	6	0	-1.051599	1.610048	1.694644
13	6	0	-0.812025	0.456227	2.698954
14	6	0	-1.181073	0.875266	4.145270
15	6	0	-0.453767	2.165649	4.580434
16	6	0	-0.702032	3.301975	3.564697
17	6	0	-0.275299	2.873950	2.139885
18	6	0	-1.015167	2.703054	-1.137918

19	6	0	-2.285224	3.504398	-0.747010
20	6	0	-2.326987	4.848511	-1.519663
21	6	0	-0.984621	3.822839	-3.428251
22	6	0	-0.937622	2.473473	-2.670431
23	6	0	-1.088470	-2.401927	0.314952
24	6	0	-1.781769	-3.725131	0.727966
25	6	0	1.617545	-3.902403	0.577435
26	6	0	3.149041	-3.891375	0.315436
27	6	0	1.416503	-3.513362	2.069295
28	6	0	1.120927	-5.351567	0.318566
29	6	0	0.442042	-3.209814	-2.364233
30	6	0	0.034457	-1.999171	-3.248789
31	6	0	1.786872	-3.778610	-2.890288
32	6	0	-0.635736	-4.313452	-2.516940
33	6	0	2.280225	2.146973	-0.405991
34	6	0	2.286240	3.028624	-1.509601
35	6	0	2.838957	4.321706	-1.393666
36	6	0	3.397642	4.748487	-0.173282
37	6	0	3.407364	3.865258	0.922544
38	6	0	2.856172	2.570448	0.810514
39	26	0	-3.927064	-0.713338	0.169306
40	1	0	-6.767266	-0.881582	-0.174801
41	1	0	-3.452505	-3.090119	-1.308328
42	1	0	-4.676167	-1.032479	-2.556551
43	1	0	-3.418989	1.226677	-1.859164
44	1	0	-3.880628	0.946816	2.573630
45	1	0	-3.735083	-1.736549	2.884378
46	1	0	-5.531946	-2.871833	1.187935
47	1	0	-5.741966	1.483517	0.677214
48	1	0	-2.124333	1.845784	1.667511
49	1	0	0.244160	0.156937	2.664368
50	1	0	-1.419562	-0.413874	2.422266
51	1	0	-2.269621	1.033389	4.221658
52	1	0	-0.932799	0.052206	4.829696
53	1	0	0.626387	1.968827	4.646106
54	1	0	-0.787793	2.468371	5.582913

55	1	0	-0.140239	4.200817	3.854895
56	1	0	-1.769963	3.576986	3.569945
57	1	0	0.796353	2.661224	2.147549
58	1	0	-0.428177	3.706935	1.442939
59	1	0	-0.150897	3.321649	-0.867092
60	1	0	-3.198989	2.939692	-0.967992
61	1	0	-2.299810	3.711005	0.329452
62	1	0	-1.483674	5.477554	-1.194927
63	1	0	-3.247430	5.391279	-1.260977
64	1	0	-3.141672	4.102431	-3.394066
65	1	0	-2.233486	5.608190	-3.562222
66	1	0	-0.086374	4.410495	-3.184745
67	1	0	-0.964359	3.638511	-4.511901
68	1	0	-1.770729	1.848115	-3.011592
69	1	0	-0.020726	1.926522	-2.922786
70	1	0	-0.821416	-1.875148	1.235557
71	1	0	-2.762965	-3.486771	1.156748
72	1	0	-1.213697	-4.260586	1.488559
73	1	0	-1.941954	-4.402870	-0.113966
74	1	0	3.580115	-4.773677	0.810537
75	1	0	3.626063	-3.025008	0.772362
76	1	0	3.409706	-3.956600	-0.745678
77	1	0	2.070884	-4.148483	2.682115
78	1	0	0.390754	-3.666590	2.419167
79	1	0	1.715366	-2.479015	2.258881
80	1	0	1.576016	-6.000979	1.080868
81	1	0	1.447525	-5.725795	-0.658262
82	1	0	0.039730	-5.475450	0.387574
83	1	0	-0.034724	-2.327585	-4.296897
84	1	0	0.770268	-1.189590	-3.191705
85	1	0	-0.938998	-1.592306	-2.959643
86	1	0	1.696837	-3.952997	-3.972423
87	1	0	2.041230	-4.734325	-2.421712
88	1	0	2.624953	-3.092737	-2.734232
89	1	0	-0.639518	-4.653361	-3.563915
90	1	0	-1.636352	-3.935053	-2.296491

91	1	0	-0.439632	-5.186246	-1.888212
92	1	0	2.843465	4.982105	-2.259373
93	1	0	3.829963	5.742423	-0.083419
94	1	0	3.854821	4.165837	1.867603
95	15	0	-0.658928	1.089101	-0.133045
96	15	0	0.703096	-2.502680	-0.528136
97	46	0	1.646531	0.200095	-0.533989
98	1	0	1.896031	2.714143	-2.473361
99	6	0	4.001749	-0.631930	-0.636393
100	1	0	3.787634	-1.688978	-0.766812
101	6	0	4.710208	-0.233220	0.634354
102	6	0	3.553766	-0.232631	-3.159247
103	1	0	4.490735	-0.190208	-3.736827
104	1	0	3.166223	-1.251429	-3.228028
105	1	0	2.845743	0.444422	-3.654314
106	1	0	2.903879	1.902554	1.662855
107	6	0	3.836906	0.193490	-1.734110
108	1	0	4.192942	1.215577	-1.635695
109	1	0	5.641957	-0.823038	0.687647
110	5	0	3.970315	-0.499713	2.060305
111	9	0	4.383144	0.472695	3.047003
112	9	0	2.481058	-0.381483	1.950799
113	9	0	4.231754	-1.834965	2.567830
114	1	0	5.000856	0.822240	0.581878

(CyPF-*t*-Bu)Pd(Ph)((*E*)-CH_3CH=$CHCH_2BF_3$), *si*, the chelated cyclic complex: optimaization (-13.9 kcal/mol (**32**)) from the chelated cyclic complex (-2225.97343686 (-330 kcal/mol))



E(RB+HF-LYP) = -2226.52108316 A.U.

Standard orientation:

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3	6	0	2.293480	1.552343	-0.357651
4	6	0	3.260568	2.171671	-1.232249
5	6	0	3.756207	1.185402	-2.151130
6	6	0	3.121719	-0.061639	-1.835586
7	6	0	5.056685	-0.561990	1.395174
8	6	0	5.052315	0.828257	1.776520
9	6	0	5.855443	1.550855	0.820864
10	6	0	6.348766	0.606830	-0.151818
11	6	0	5.852630	-0.700318	0.202794

12	6	0	1.641307	-1.997996	1.398137
13	6	0	1.625826	-1.084487	2.648718
14	6	0	2.219239	-1.794924	3.891181
15	6	0	1.524915	-3.145990	4.167834
16	6	0	1.563379	-4.047054	2.914970
17	6	0	0.926334	-3.341882	1.693056
18	6	0	0.795245	-2.429214	-1.508229
19	6	0	2.024691	-3.352884	-1.712370
20	6	0	1.669155	-4.485656	-2.709381
21	6	0	-0.020923	-2.960874	-3.860991
22	6	0	0.298718	-1.832283	-2.850689
23	6	0	1.497288	2.280594	0.699927
24	6	0	2.223666	3.552549	1.198213
25	6	0	-1.252298	3.427624	1.601306
26	6	0	-2.793177	3.271451	1.484703
27	6	0	-0.816423	2.747029	2.928025
28	6	0	-0.914809	4.940835	1.638973
29	6	0	-0.476882	3.427295	-1.569094
30	6	0	-0.223060	2.384238	-2.692676
31	6	0	-1.903693	4.000555	-1.768366
32	6	0	0.549350	4.582266	-1.685048
33	6	0	-2.069020	-1.833191	0.409719
34	6	0	-2.513667	-2.682203	-0.624124
35	6	0	-3.302176	-3.814079	-0.325113
36	6	0	-3.662459	-4.102469	1.005068
37	6	0	-3.242966	-3.241049	2.037621
38	6	0	-2.447664	-2.114186	1.741488
39	26	0	4.233503	0.627859	-0.182003
40	1	0	6.970949	0.841032	-1.004507
41	1	0	3.568830	3.205658	-1.194128
42	1	0	4.487934	1.346910	-2.929687
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45	1	0	4.552207	1.249599	2.637345
46	1	0	6.049618	2.614567	0.825976
47	1	0	6.049594	-1.620945	-0.328960

48	1	0	2.684235	-2.204929	1.119473
49	1	0	0.586726	-0.792135	2.861436
50	1	0	2.189711	-0.163826	2.452069
51	1	0	3.295874	-1.971091	3.737405
52	1	0	2.131462	-1.133002	4.764427
53	1	0	0.476680	-2.967879	4.453707
54	1	0	2.006421	-3.650636	5.017063
55	1	0	1.029661	-4.987997	3.107099
56	1	0	2.608737	-4.313515	2.688502
57	1	0	-0.134816	-3.163726	1.895422
58	1	0	0.973143	-4.010981	0.826379
59	1	0	-0.015710	-3.054900	-1.113580
60	1	0	2.879530	-2.797989	-2.115784
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62	1	0	0.880849	-5.119332	-2.274178
63	1	0	2.547817	-5.128384	-2.862661
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66	1	0	-0.885619	-3.538163	-3.499182
67	1	0	-0.318556	-2.516158	-4.820273
68	1	0	1.065559	-1.171585	-3.278480
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70	1	0	1.377674	1.615105	1.562021
71	1	0	3.268790	3.304993	1.425120
72	1	0	1.771225	3.935089	2.116015
73	1	0	2.222676	4.360426	0.462661
74	1	0	-3.252787	3.802508	2.332119
75	1	0	-3.108065	2.226701	1.515564
76	1	0	-3.196169	3.696804	0.563291
77	1	0	-1.401350	3.177555	3.752881
78	1	0	0.243291	2.896487	3.163689
79	1	0	-1.021523	1.668691	2.904416
80	1	0	-1.402424	5.382188	2.520969
81	1	0	-1.305972	5.461754	0.759254
82	1	0	0.155318	5.149895	1.714047
83	1	0	-0.264529	2.899973	-3.663355

84	1	0	-0.997726	1.609468	-2.691571
85	1	0	0.759285	1.908277	-2.608032
86	1	0	-1.962978	4.399672	-2.791846
87	1	0	-2.119526	4.829341	-1.084892
88	1	0	-2.687100	3.244717	-1.672076
89	1	0	0.372577	5.103490	-2.637454
90	1	0	1.580249	4.217301	-1.700632
91	1	0	0.444900	5.321847	-0.883180
92	1	0	-3.651906	-4.451905	-1.134956
93	1	0	-4.276854	-4.971151	1.231042
94	1	0	-3.536933	-3.437481	3.067262
95	15	0	0.912522	-1.082069	-0.137811
96	15	0	-0.383469	2.427714	0.130795
97	46	0	-1.212622	-0.012797	0.092190
98	1	0	-2.303779	-2.440870	-1.661567
99	6	0	-6.420194	0.250770	-0.199968
100	1	0	-2.150474	-1.450155	2.551600
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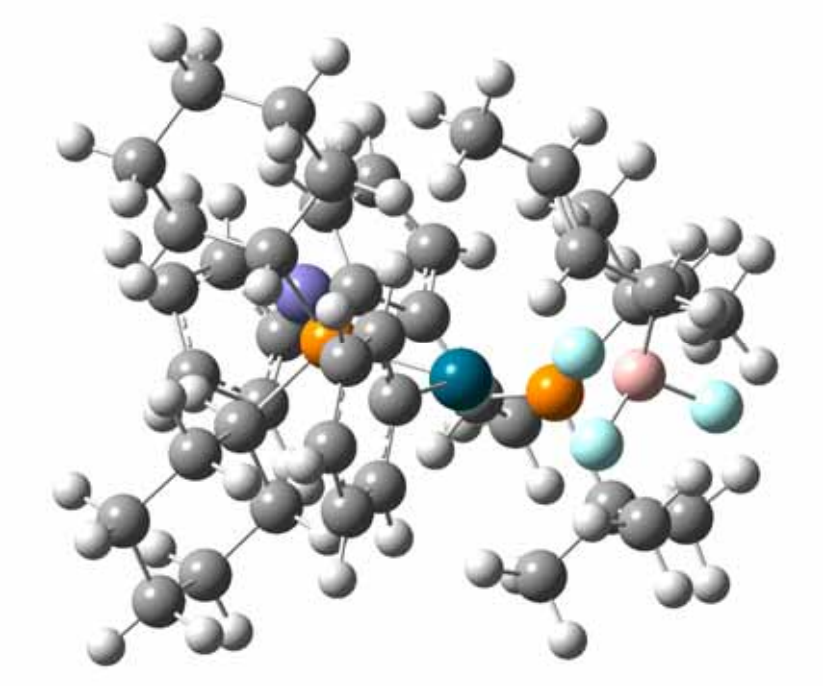
102	1	0	-6.416176	-1.301464	1.223941
103	6	0	-7.835747	0.268938	1.914576
104	1	0	-8.196820	1.241849	1.556582
105	1	0	-8.708612	-0.388568	2.048832
106	1	0	-7.392377	0.419136	2.911174
107	1	0	-6.827910	1.228513	-0.470802
108	6	0	-5.402258	-0.326325	-1.156767
109	1	0	-5.096293	-1.328389	-0.827980
110	1	0	-5.853989	-0.432985	-2.158304
111	5	0	-4.111686	0.593134	-1.341876
112	9	0	-4.397357	1.971081	-1.663121
113	9	0	-3.135468	0.088419	-2.302983
114	9	0	-3.289623	0.675900	-0.026743

(CyPF-*t*-Bu)Pd(Ph)((*E*)-$CH_3CH{=}CHCH_2BF_3$), *si*, the chelated cyclic complex: optimaization (-8.7 kcal/mol (**33**)) from the chelated cyclic complex (-2226.27434911 (-141 kcal/mol))



E(RB+HF-LYP) = -2226.51282224 A.U.

Standard orientation:

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9	6	0	6.002697	0.978630	-0.495823
10	6	0	6.149391	-0.149922	-1.382008

11	6	0	5.611830	-1.312249	-0.717822
12	6	0	1.681696	-1.808705	1.612127
13	6	0	2.065643	-0.708763	2.630172
14	6	0	2.835883	-1.291871	3.841295
15	6	0	2.053929	-2.435286	4.522524
16	6	0	1.677734	-3.528452	3.499118
17	6	0	0.882660	-2.941066	2.307760
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19	6	0	1.378399	-3.700227	-1.157714
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21	6	0	-0.982018	-3.500659	-2.989267
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28	6	0	-0.244284	5.163219	1.482654
29	6	0	-0.568094	3.423496	-1.602393
30	6	0	-0.615222	2.294771	-2.669793
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32	6	0	0.434783	4.516178	-2.046743
33	6	0	-2.221781	-1.371372	1.098208
34	6	0	-2.953808	-2.267855	0.297349
35	6	0	-3.806630	-3.219217	0.897339
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37	6	0	-3.225749	-2.365340	3.098532
38	6	0	-2.365055	-1.421735	2.502302
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79	1	0	0.108471	2.024445	2.999335
80	1	0	-0.473772	5.681486	2.425439
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82	1	0	0.804139	5.367010	1.240570

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97	46	0	-1.213800	0.254369	0.404351
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99	6	0	-5.610359	-0.493713	-1.423082
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104	1	0	-5.715936	-3.128080	-1.949311
105	1	0	-6.068032	-2.835469	-3.665481
106	1	0	-4.391252	-2.999924	-3.131816
107	1	0	-5.913376	-1.112182	-0.573998
108	6	0	-5.555063	0.989635	-1.159433
109	1	0	-5.223657	1.528144	-2.059998
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112	9	0	-4.920786	0.797042	1.333092
113	9	0	-4.668553	2.882569	0.263628
114	9	0	-3.146718	1.141940	-0.206235

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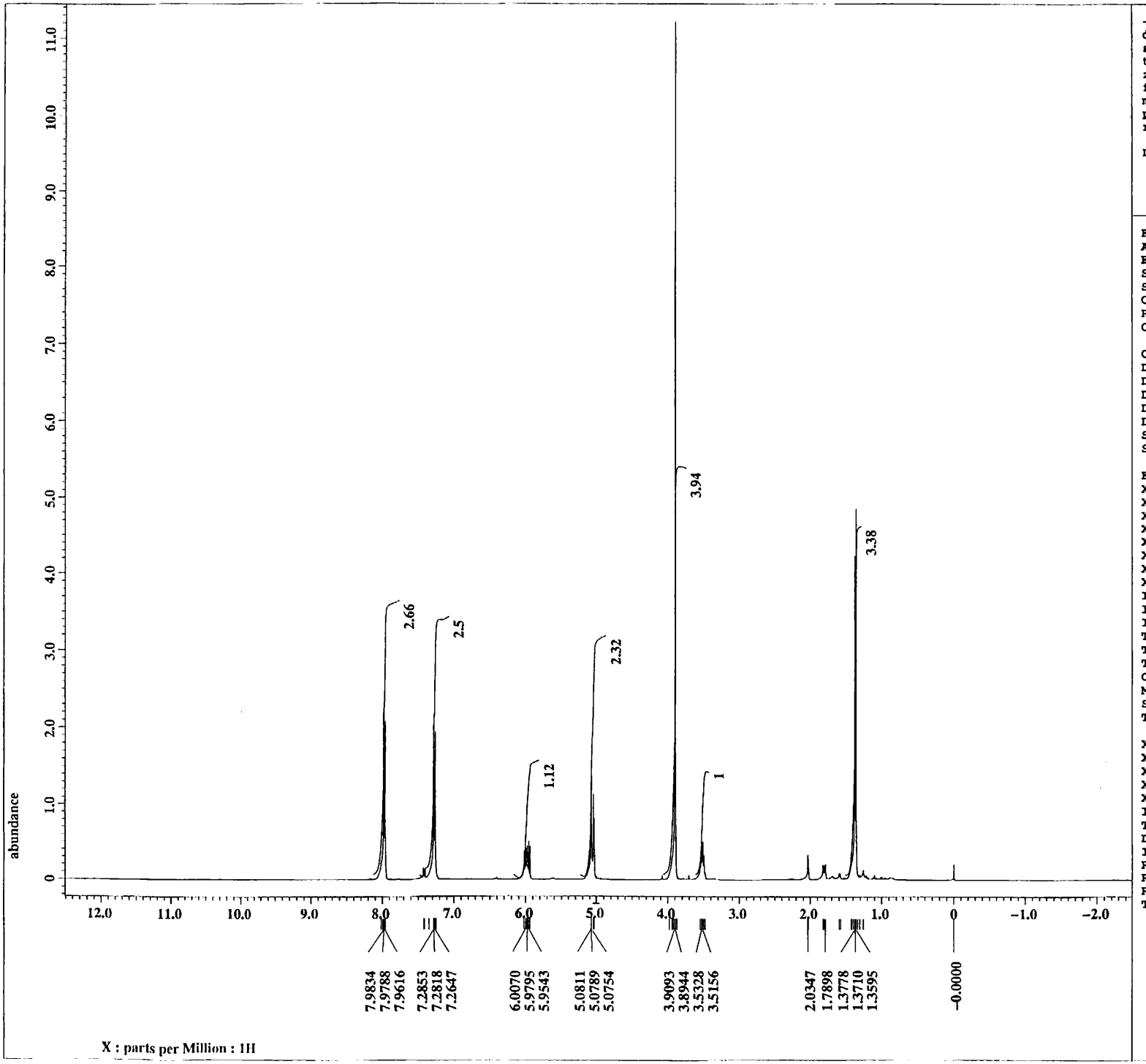
7) (a) Zhang, A.; RanjanBabu, T. V. *Org. Lett*. **2004**, *6*, 1515. (b) López, F.; van Zijl, A. W.; Minnaard, A. J.; Feringa, B. L. *Chem. Commun*. **2006**, 409.

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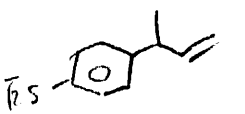
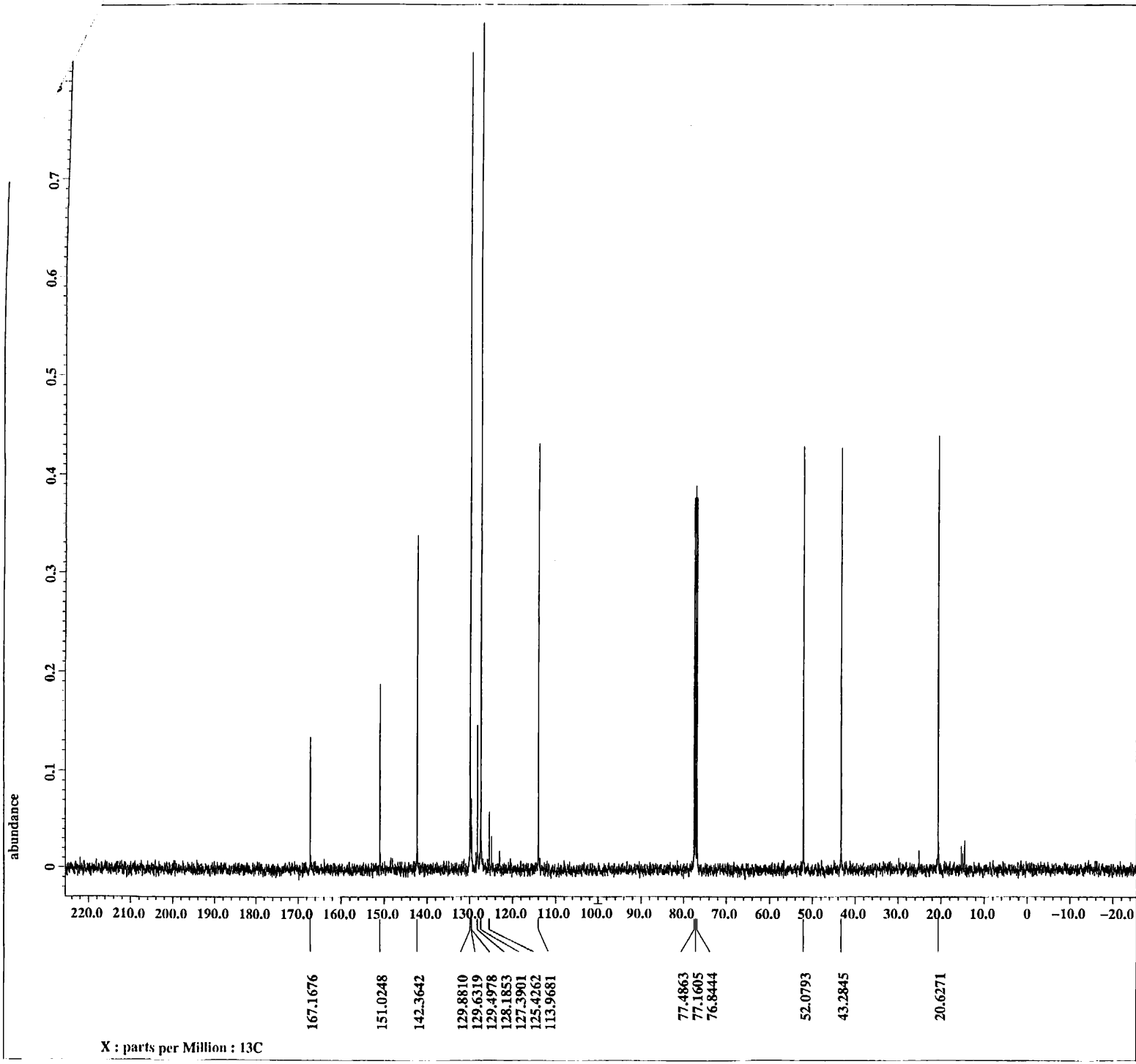
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.2[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 26
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 21.7[dC]

(4-MeO2CC6H4)CH(CH3)CH=CH2 (6a)

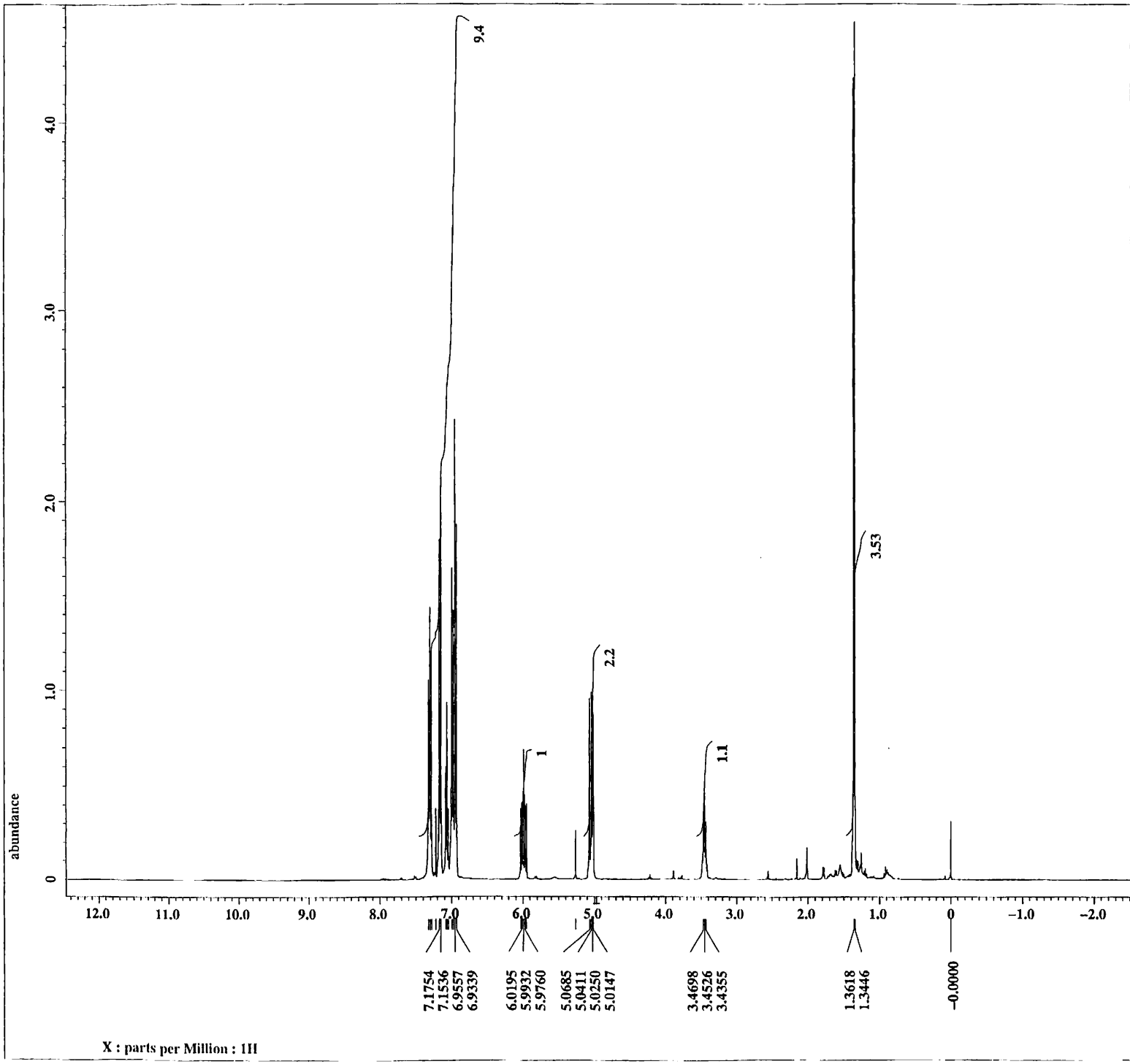





```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Es_C-1.jdf
```

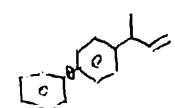
Filename	= Es_C-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#546124
Solvent	= CHLOROFORM-D
Creation_time	= 10-JUL-2007 15:17:46
Revision_time	= 10-JUL-2007 15:17:37
Current_time	= 10-JUL-2007 15:17:45
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 1.048576[s]
X_domain	= 13C
X_freq	= 99.54517646[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.95367432[Hz]
X_sweep	= 31.25[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 128
Total_scans	= 128
X_90_width	= 9.5[us]
X_acq_time	= 1.048576[s]
X_angle	= 30[deg]
X_atn	= 4.2[dB]
X_pulse	= 3.16666667[us]
Irr_atn_dec	= 21[dB]
Irr_atn_noe	= 21[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 52
Relaxation_delay	= 2[s]
Repetition_time	= 3.048576[s]
Temp_get	= 22[dC]

(4-MeO2CC6H4)CH(CH3)CH=CH2 (6a)

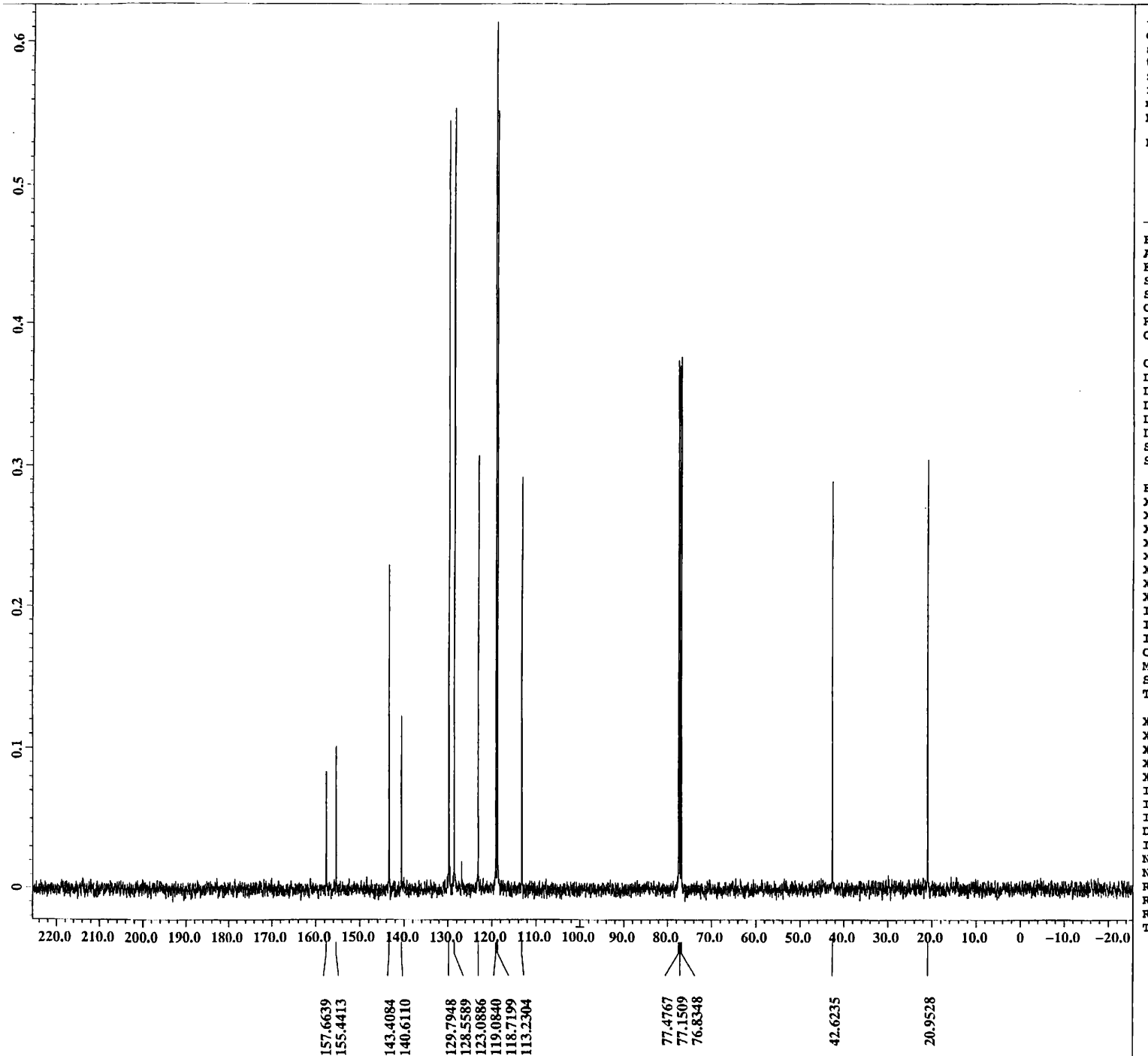



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Me_H-1.jdf
```

Filename	= Me_H-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#780632
Solvent	= CHLOROFORM-D
Creation_time	= 10-JUL-2007 21:44:11
Revision_time	= 10-JUL-2007 21:45:51
Current_time	= 10-JUL-2007 21:47:10
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.20725248[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.2[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 26
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 21.7[dC]



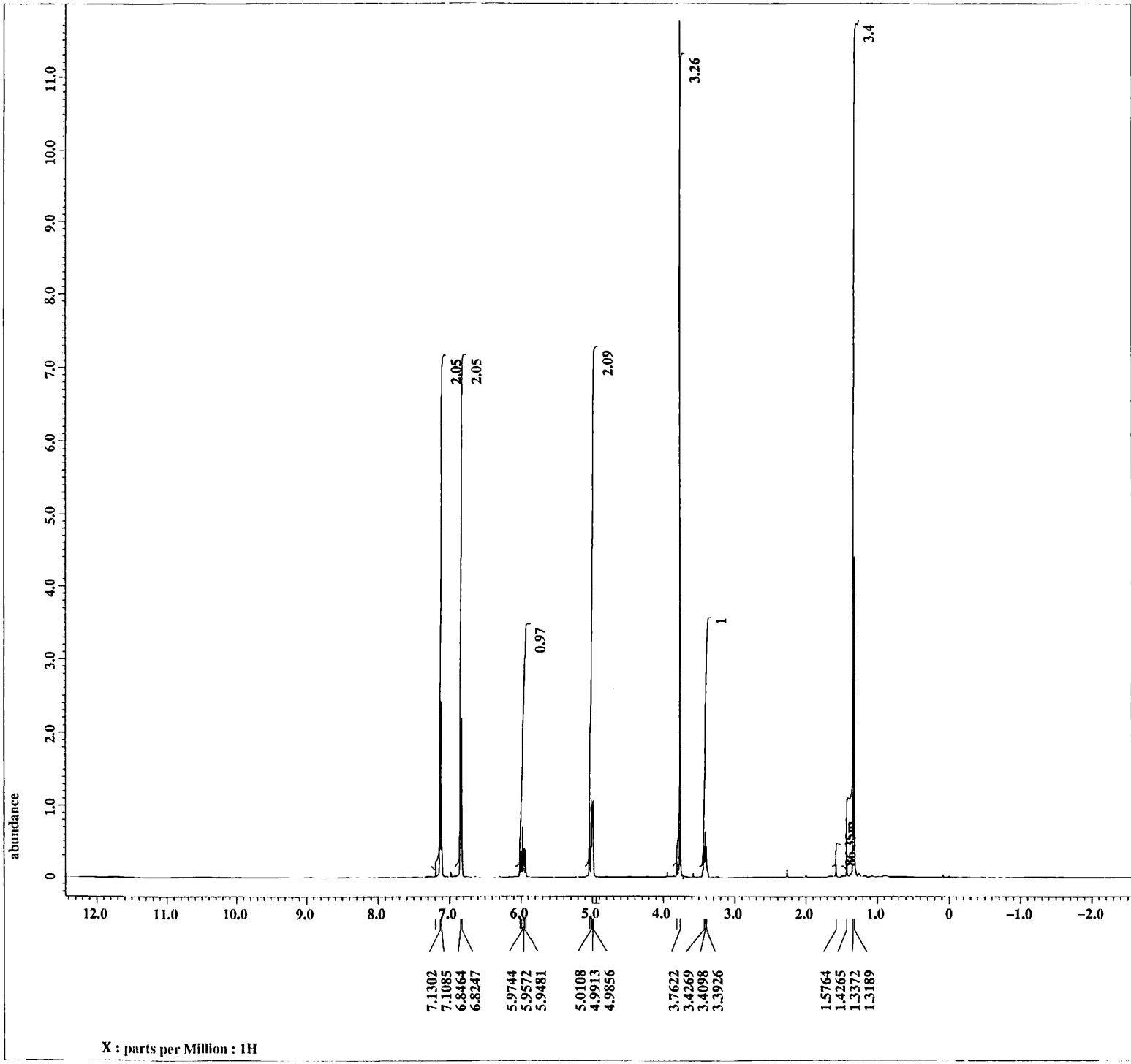
(4-PhOC6H4)CH(CH3)CH=CH2 (6b)




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Me_C-1.jdf
```

Filename	= Me_C-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#780677
Solvent	= CHLOROFORM-D
Creation_time	= 10-JUL-2007 21:51:13
Revision_time	= 10-JUL-2007 21:52:08
Current_time	= 10-JUL-2007 21:52:16
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 1.048576[s]
X_domain	= 13C
X_freq	= 99.54517646[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.95367432[Hz]
X_sweep	= 31.25[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 128
Total_scans	= 128
X_90_width	= 9.5[us]
X_acq_time	= 1.048576[s]
X_angle	= 30[deg]
X_atn	= 4.2[dB]
X_pulse	= 3.16666667[us]
Irr_atn_dec	= 21[dB]
Irr_atn_noe	= 21[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 50
Relaxation_delay	= 2[s]
Repetition_time	= 3.048576[s]
Temp_get	= 22.1[dC]

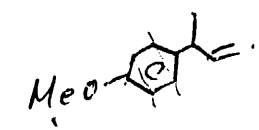
(4-PhOC6H4)CH(CH3)CH=CH2 (6b)

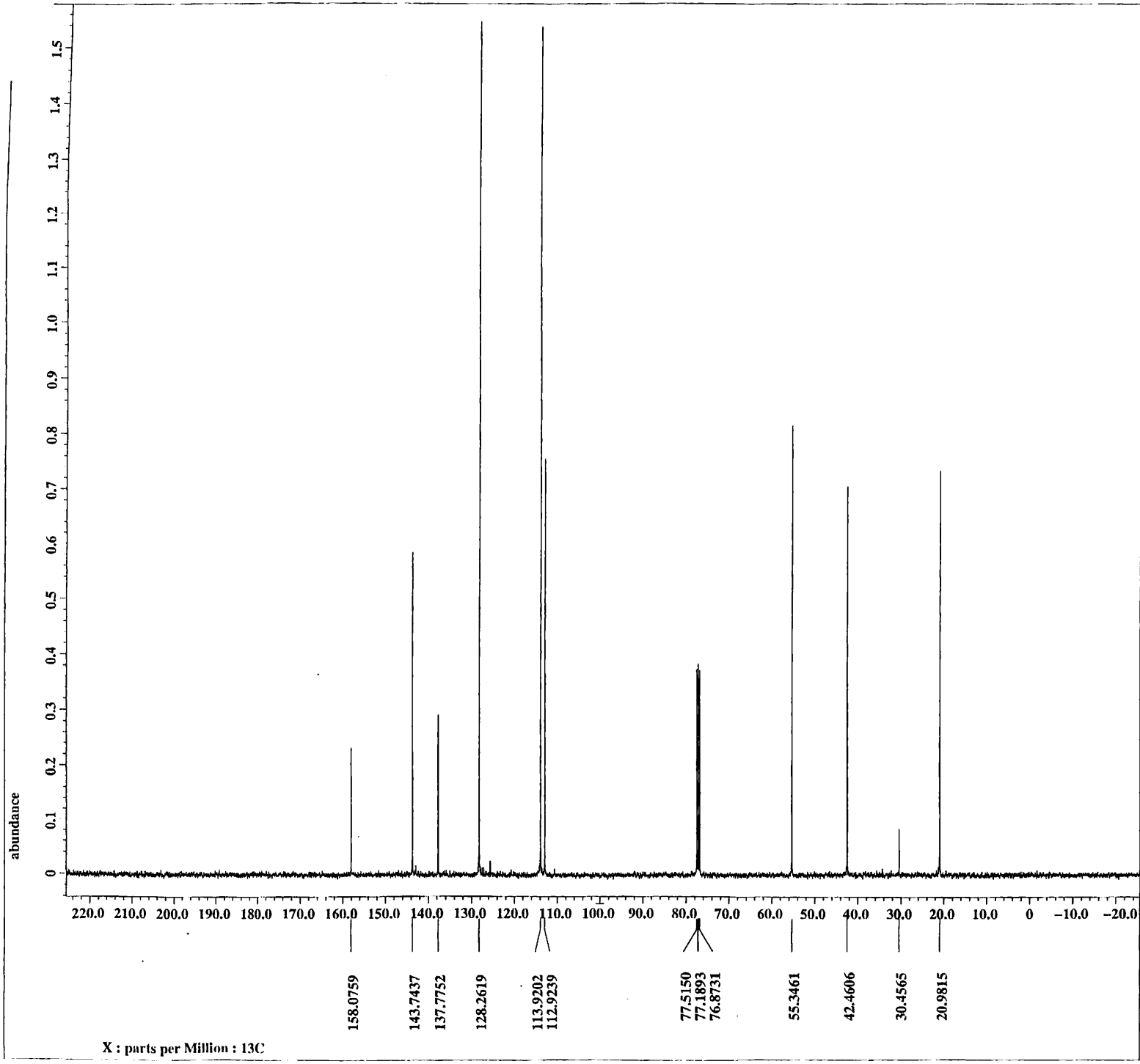



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: MeO_H2-1.jdf
```

Filename	= MeO_H2-5.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#777810
Solvent	= CHLOROFORM-D
Creation_time	= 12-JUL-2007 21:39:45
Revision_time	= 12-JUL-2007 21:42:23
Current_time	= 12-JUL-2007 21:42:31
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.20725248[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.2[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 22
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 22.2[dC]

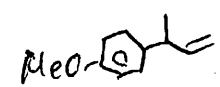
(4-MeOC6H4)CH(CH3)CH=CH2 (6c)



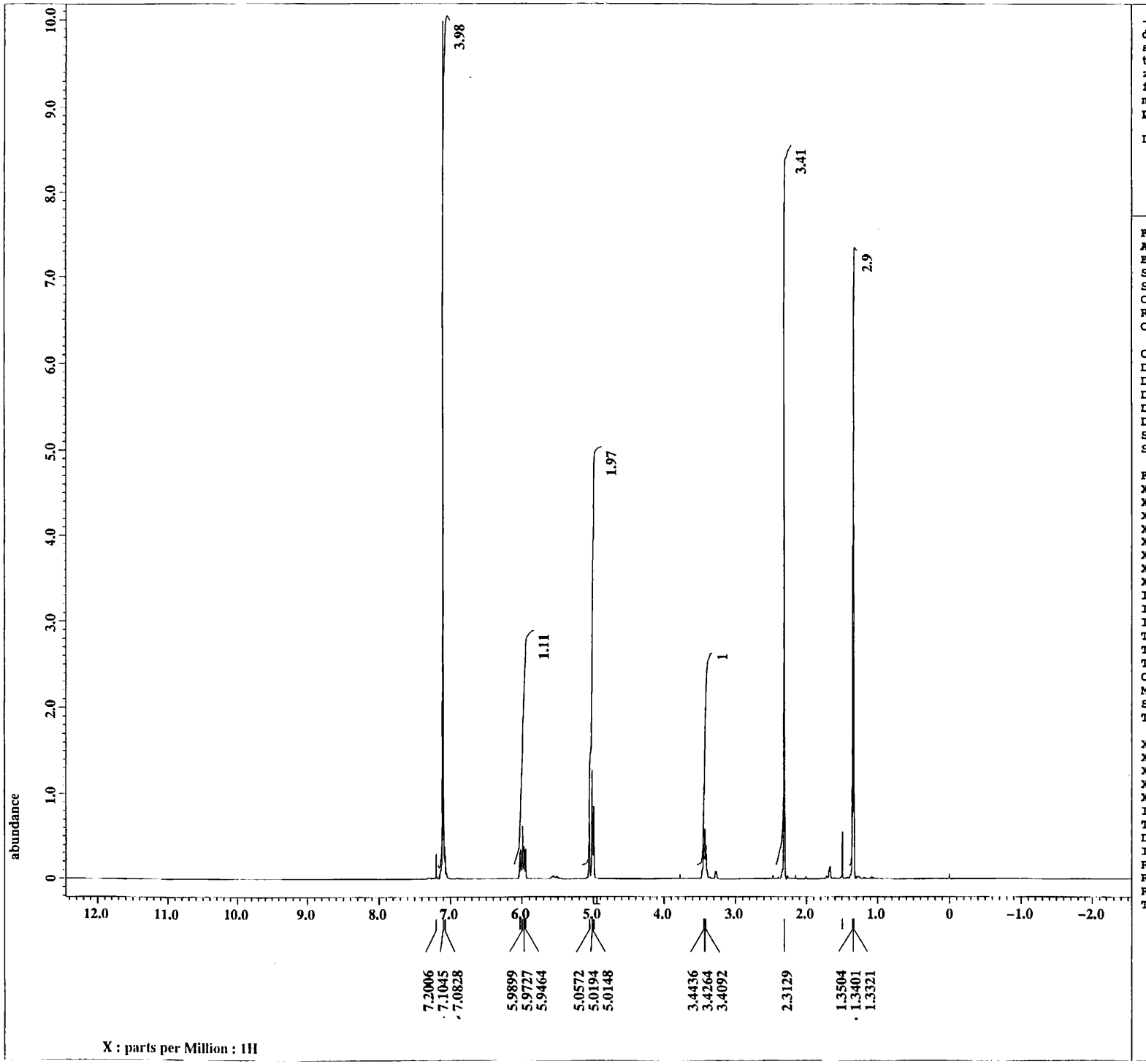



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: MeO_C2-1.jdf
```

Filename	= MeO_C2-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#778041
Solvent	= CHLOROFORM-D
Creation_time	= 12-JUL-2007 21:47:10
Revision_time	= 12-JUL-2007 21:48:08
Current_time	= 12-JUL-2007 21:48:23
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 1.048576[s]
X_domain	= 13C
X_freq	= 99.54517646[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.95367432[Hz]
X_sweep	= 31.25[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 128
Total_scans	= 128
X_90_width	= 9.5[us]
X_acq_time	= 1.048576[s]
X_angle	= 30[deg]
X_atn	= 4.2[dB]
X_pulse	= 3.16666667[us]
Irr_atn_dec	= 21[dB]
Irr_atn_noe	= 21[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 50
Relaxation_delay	= 2[s]
Repetition_time	= 3.048576[s]
Temp_get	= 22.3[dC]



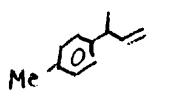
(4-MeOC6H4)CH(CH3)CH=CH2 (6c)

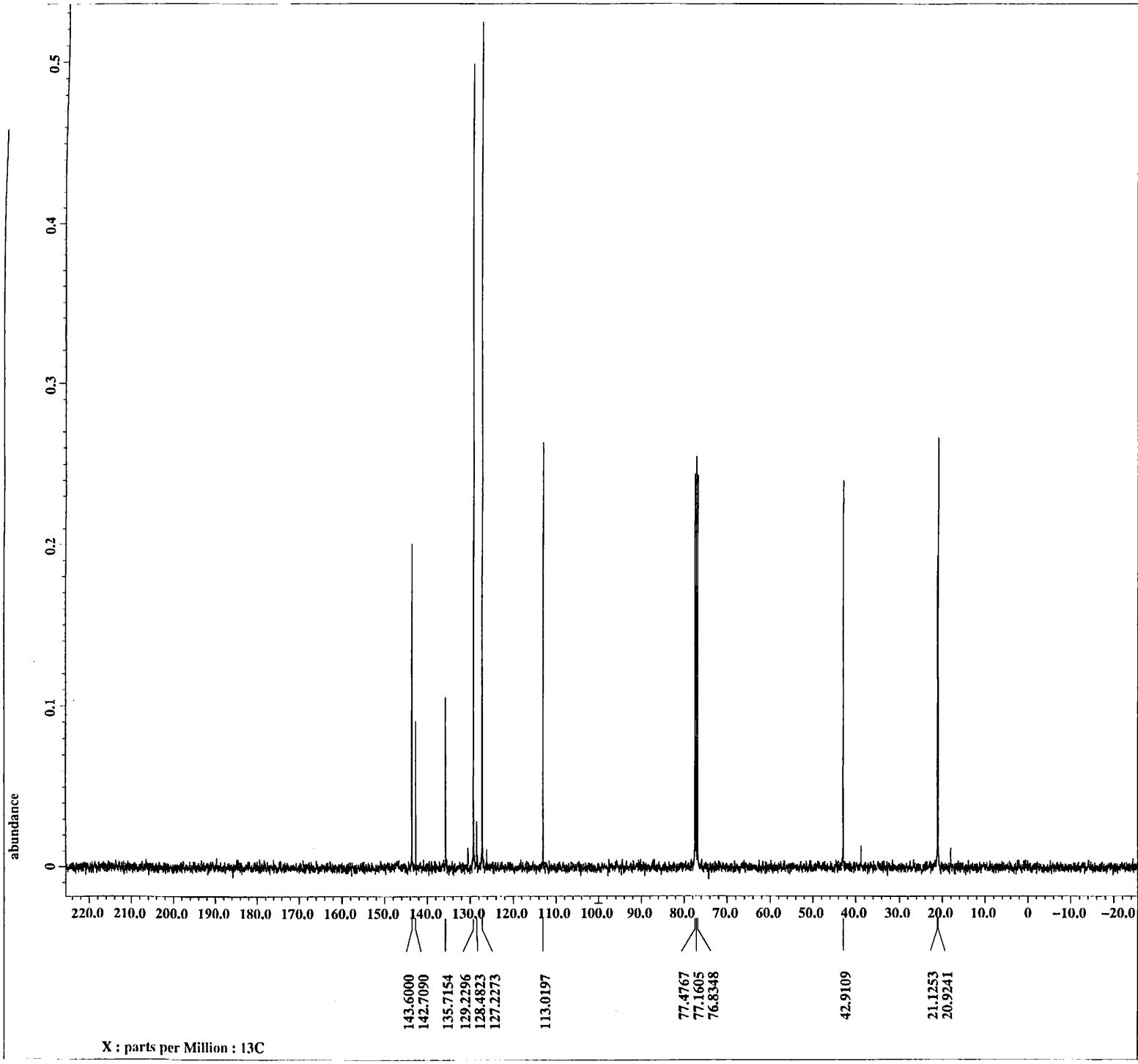



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Me_H3-1.jdf
```

Filename	= Me_H3-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#770785
Solvent	= CHLOROFORM-D
Creation_time	= 12-JUL-2007 21:27:48
Revision_time	= 12-JUL-2007 21:29:22
Current_time	= 12-JUL-2007 21:29:40
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.20725248[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.2[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 26
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 22[dC]

(4-MeC6H4)CH(CH3)CH=CH2 (6d)

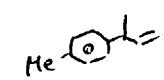


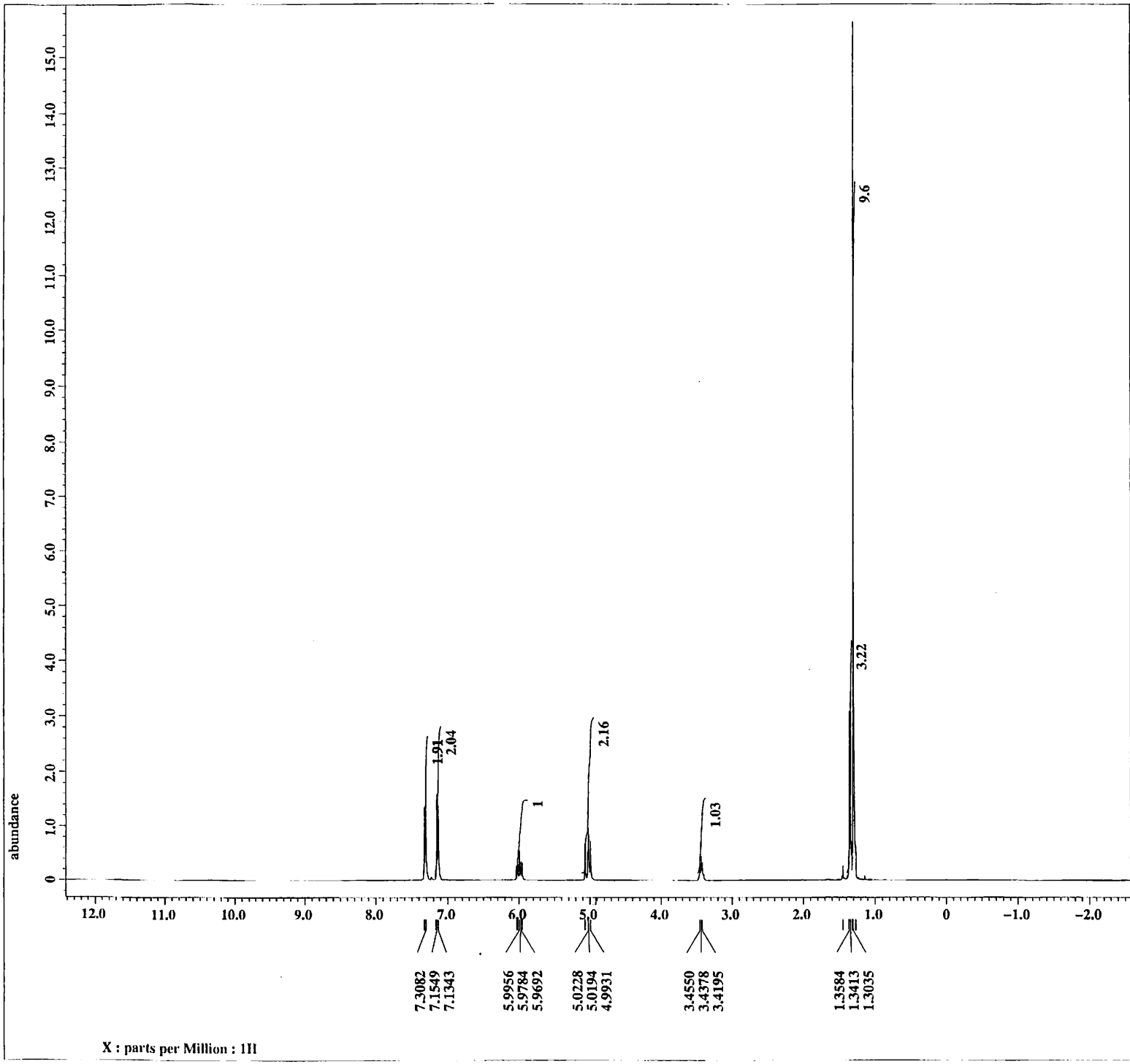



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Me_C3-1.jdf
```

```
Filename          = Me_C3-2.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#771135
Solvent           = CHLOROFORM-D
Creation_time     = 12-JUL-2007 21:35:01
Revision_time     = 12-JUL-2007 21:35:04
Current_time      = 12-JUL-2007 21:35:33

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 128
Total_scans       = 128

X_90_width        = 9.5[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 4.2[dB]
X_pulse           = 3.16666667[us]
Irr_atn_dec       = 21[dB]
Irr_atn_noe       = 21[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 46
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 22.7[dC]
```

(4-MeC6H4)CH(CH3)CH=CH2 (6d)

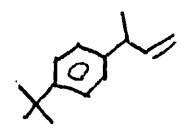


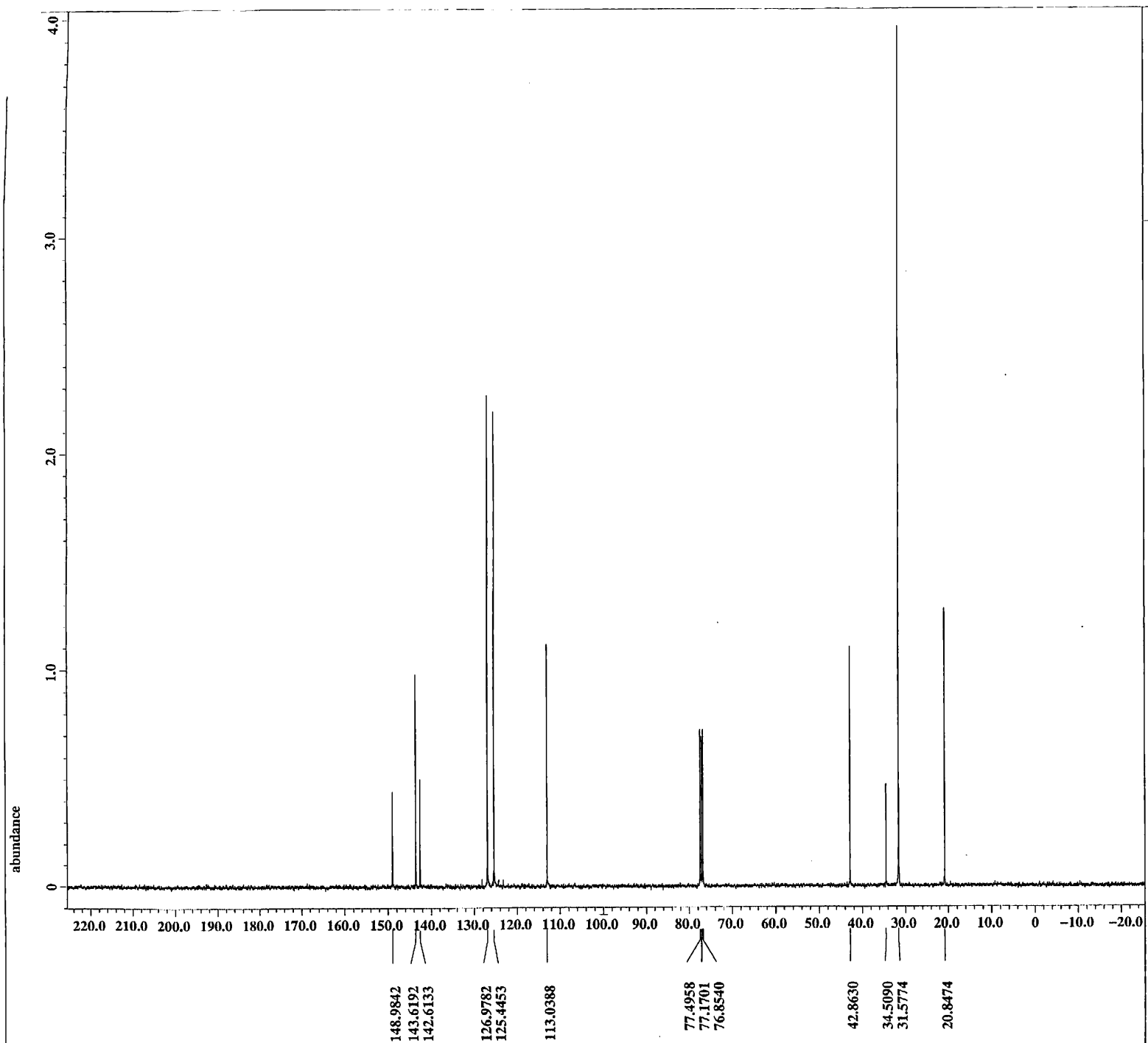



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: tBu_H2-1.jdf
```

Filename	= tBu_H2-5.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#786474
Solvent	= CHLOROFORM-D
Creation_time	= 12-JUL-2007 21:54:11
Revision_time	= 12-JUL-2007 21:58:07
Current_time	= 12-JUL-2007 21:58:16
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.20725248[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.2[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 20
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 21.8[dC]

(4-t-BuC6H4)CH(CH3)CH=CH2 (6e)

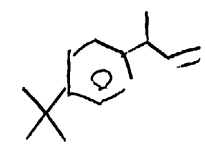


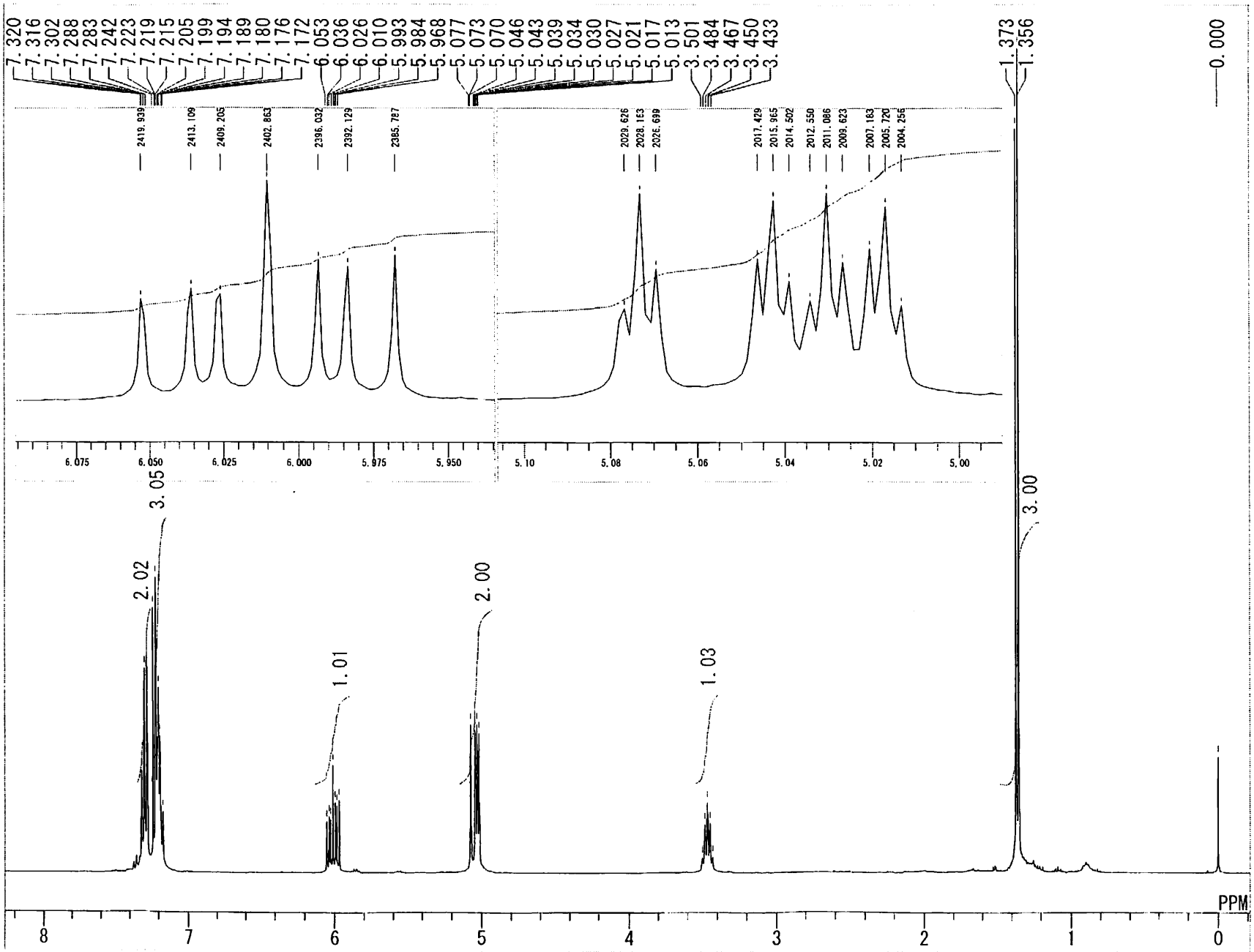



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: tBu_C2-1.jdf
```

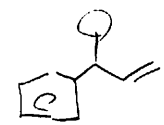
Filename	= tBu_C2-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#786519
Solvent	= CHLOROFORM-D
Creation_time	= 12-JUL-2007 22:01:26
Revision_time	= 12-JUL-2007 22:01:17
Current_time	= 12-JUL-2007 22:01:27
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 1.048576[s]
X_domain	= 13C
X_freq	= 99.54517646[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.95367432[Hz]
X_sweep	= 31.25[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Clipped	= TRUE
Mod_return	= 1
Scans	= 128
Total_scans	= 128
X_90_width	= 9.5[us]
X_acq_time	= 1.048576[s]
X_angle	= 30[deg]
X_atn	= 4.2[dB]
X_pulse	= 3.16666667[us]
Irr_atn_dec	= 21[dB]
Irr_atn_noe	= 21[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 56
Relaxation_delay	= 2[s]
Repetition_time	= 3.048576[s]
Temp_get	= 22.1[dC]

(4-t-BuC6H4)CH(CH3)CH=CH2 (6e)

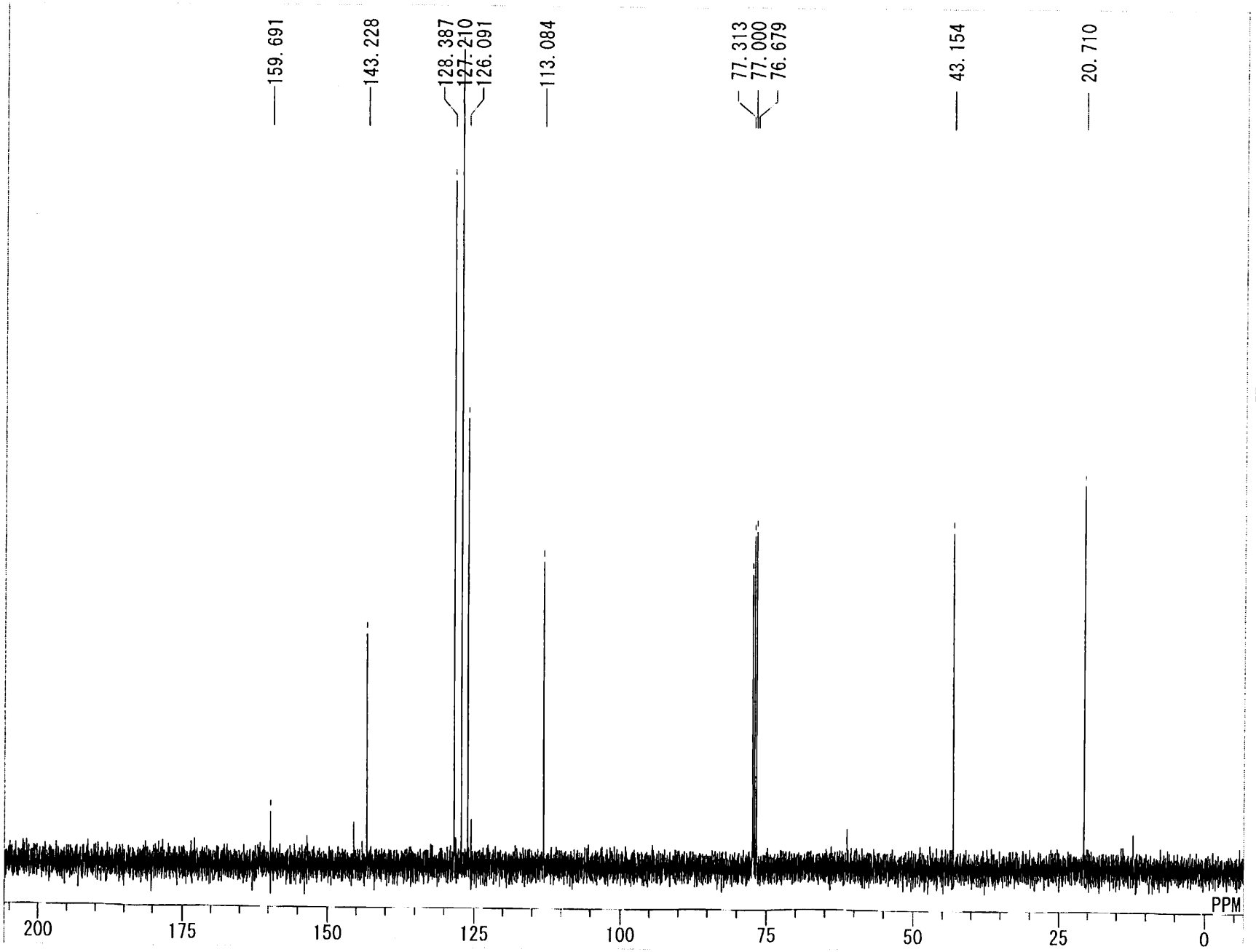




DFILE C:¥Documents and Setting
COMNT
DATIM Thu Jan 11 16:36:56 200
OBNUC 1H
EXMOD non
OBFRQ 399.65 MHz
OBSET 0.00 KHz
OBFIN 134300.00 Hz
POINT 16384
FREQU 7993.60 Hz
SCANS 16
ACQTM 2.0496 sec
PD 4.9504 sec
PW1 6.50 usec
IRNUC 1H
CTEMP 23.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15

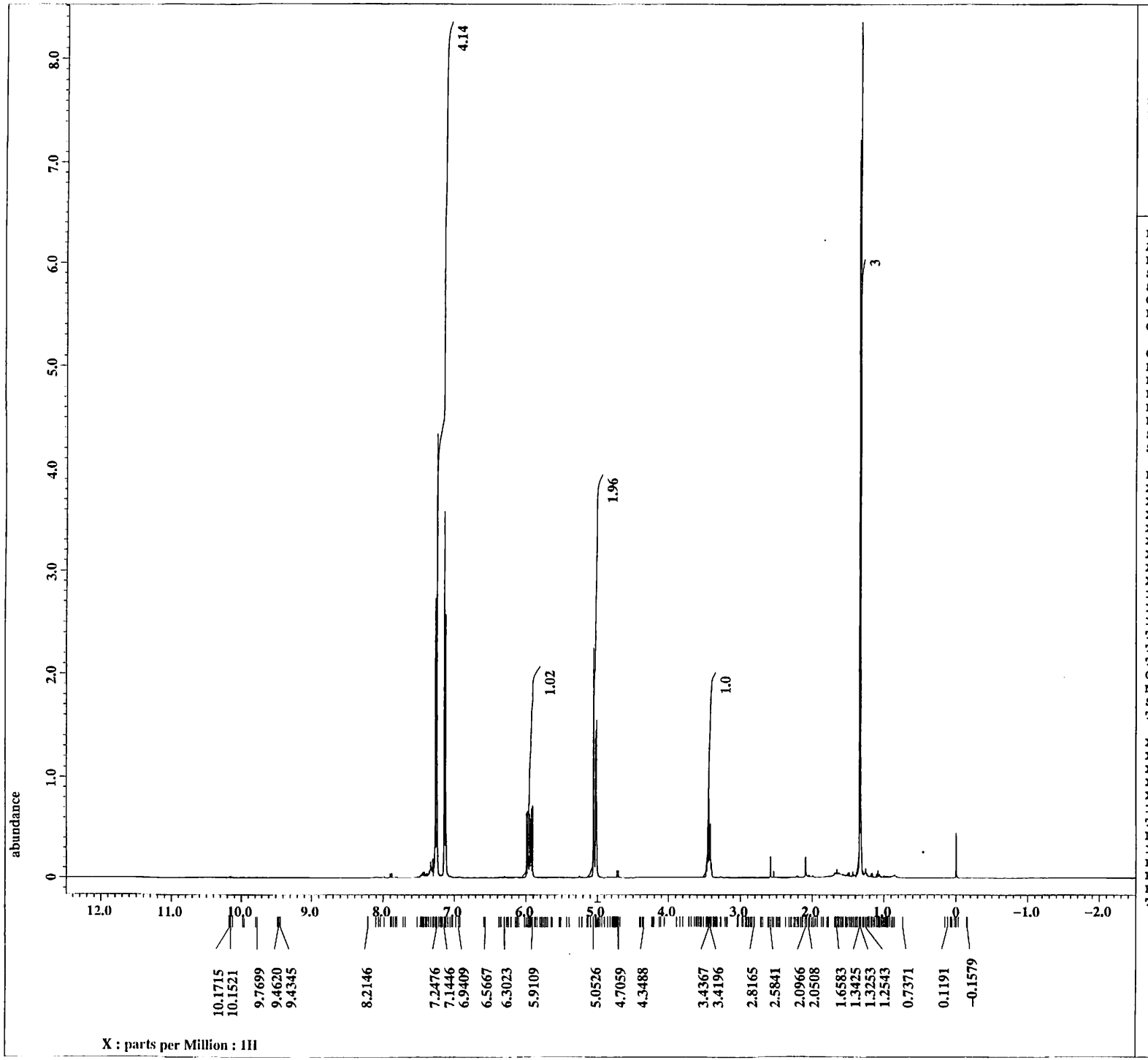


C6H4CH(CH3)CH=CH2 (6f)



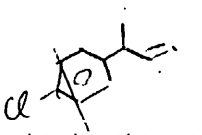
DFILE	C:¥Documents and Setting
COMNT	
DATIM	Thu Jan 11 16:42:55 2007
OBNUC	13C
EXMOD	bcm
OBFRQ	100.40 MHz
OBSET	0.00 KHz
OBFIN	135500.00 Hz
POINT	32768
FREQU	27100.27 Hz
SCANS	100
ACQTM	1.2091 sec
PD	1.7910 sec
PW1	4.50 usec
IRNUC	1H
CTEMP	23.9 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	30

C6H4CH(CH3)CH=CH2 (6f)

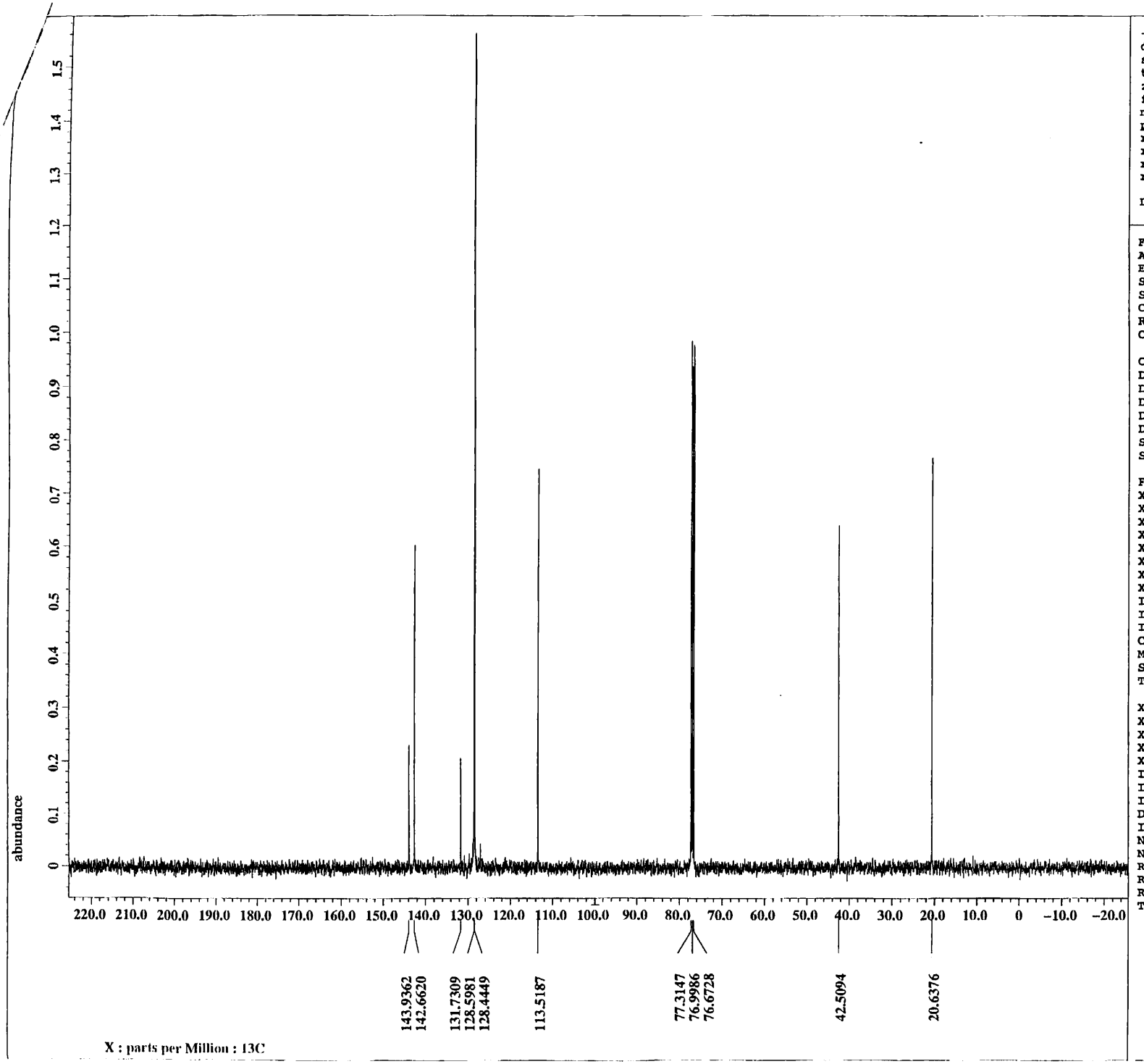



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Cl_H-1.jdf
```

Filename	= Cl_H-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#517478
Solvent	= CHLOROFORM-D
Creation_time	= 10-JUL-2007 14:25:22
Revision_time	= 10-JUL-2007 14:26:40
Current_time	= 10-JUL-2007 14:26:47
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.20725248[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.2[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 30
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 21.7[dC]



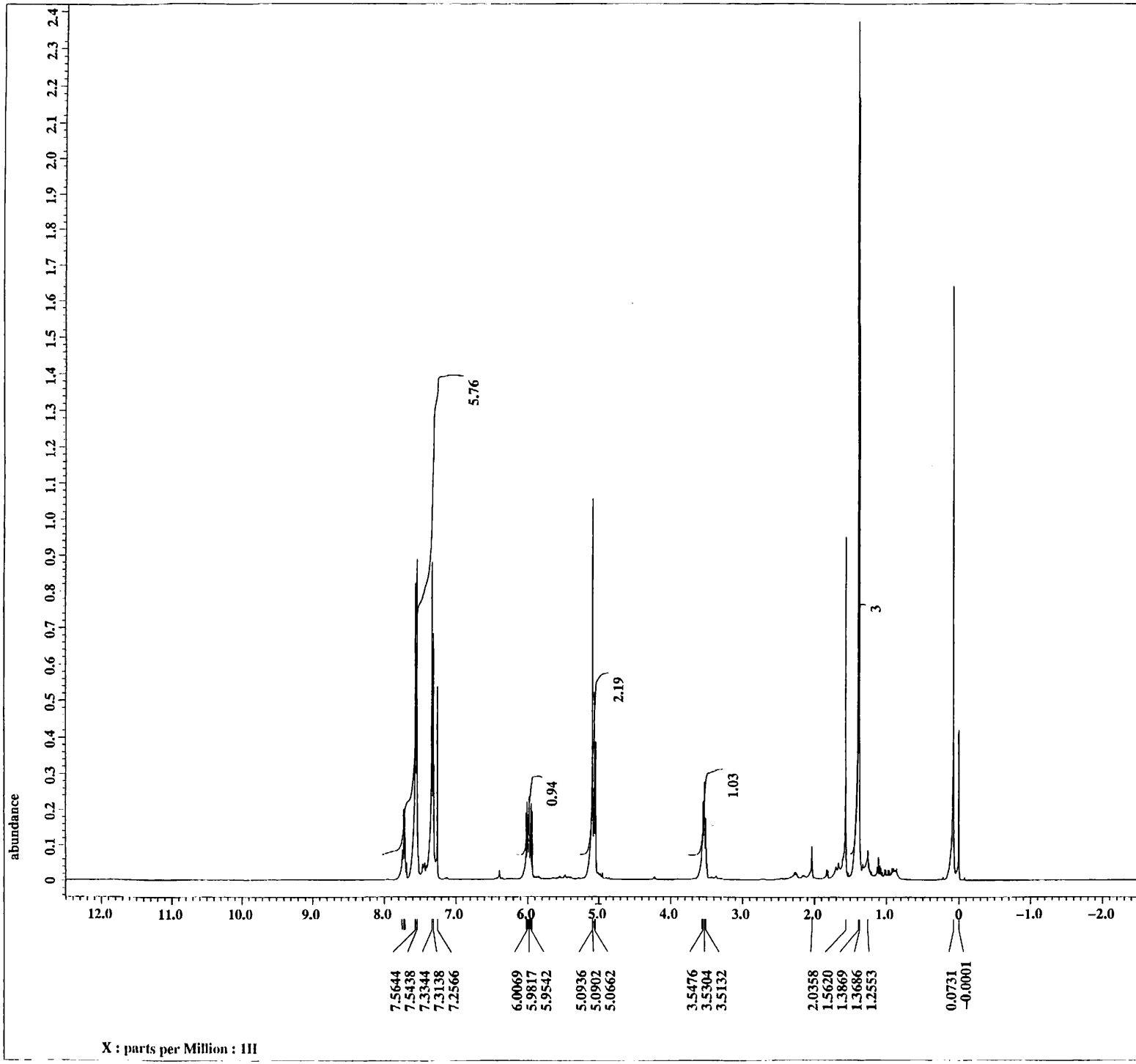
(4-ClC6H4)CH(CH3)CH=CH2 (6g)




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
reference : 77.119[ppm] : 77[ppm]
reference : 0.017[ppm] : 77[ppm]
reference : -0.004[ppm] : 77[ppm]
reference : 231.019[ppm] : 77[ppm]

Derived from: Cl_C-1.jdf
```

```
Filename          = Cl_C-6.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#519092
Solvent           = CHLOROFORM-D
Creation_time     = 10-JUL-2007 14:32:35
Revision_time     = 10-JUL-2007 14:34:47
Current_time      = 10-JUL-2007 14:34:58

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 128
Total_scans       = 128

X_90_width        = 9.5[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 4.2[dB]
X_pulse           = 3.16666667[us]
Irr_atn_dec       = 21[dB]
Irr_atn_noe       = 21[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 22.2[dC]
```

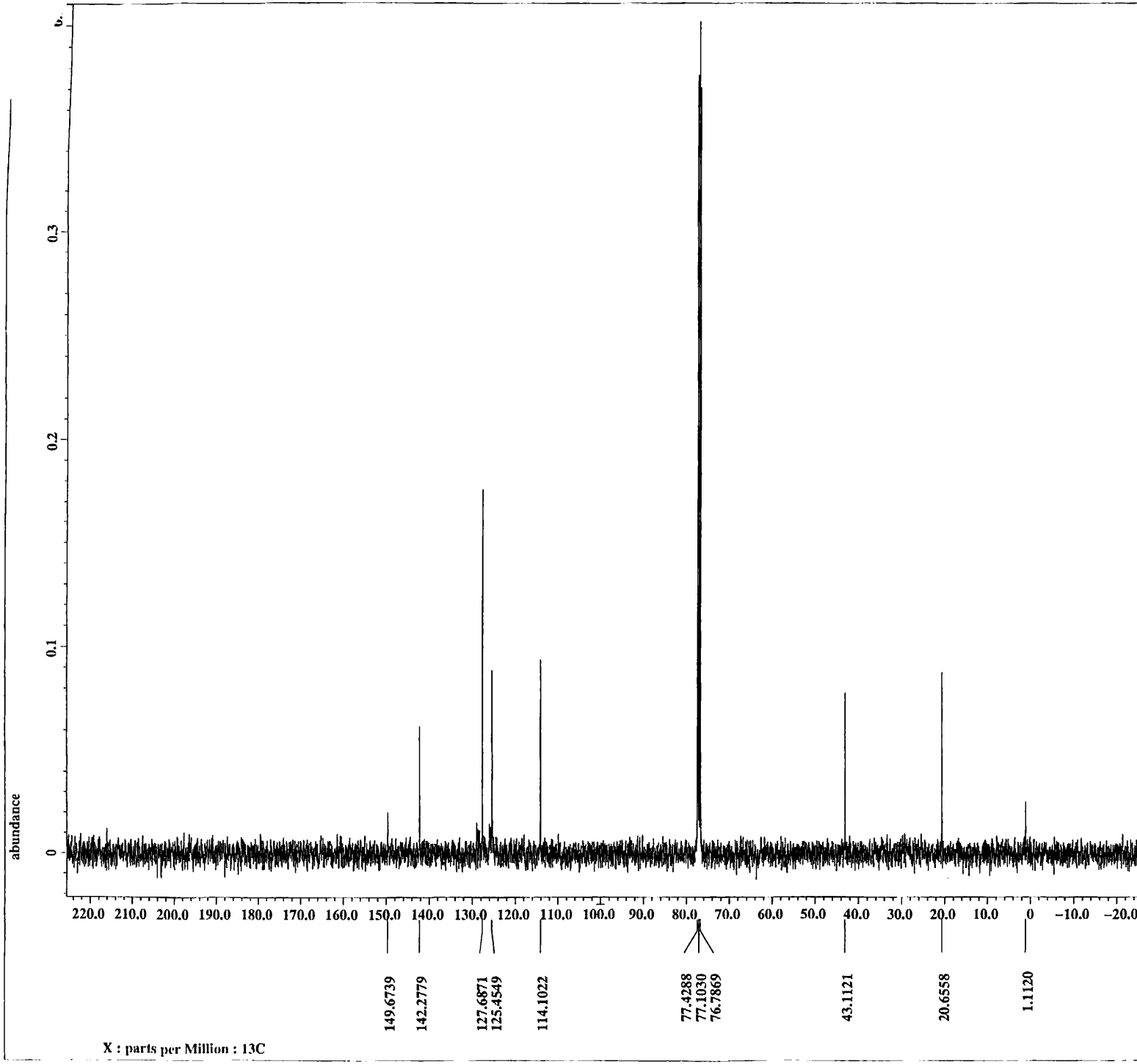
(4-ClC6H4)CH(CH3)CH=CH2 (6g)




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: CF3_H-1.jdf
```

Filename	= CF3_H-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#553184
Solvent	= CHLOROFORM-D
Creation_time	= 10-JUL-2007 15:25:06
Revision_time	= 10-JUL-2007 15:27:26
Current_time	= 10-JUL-2007 15:27:34
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.20725248[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.2[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 21.7[dC]

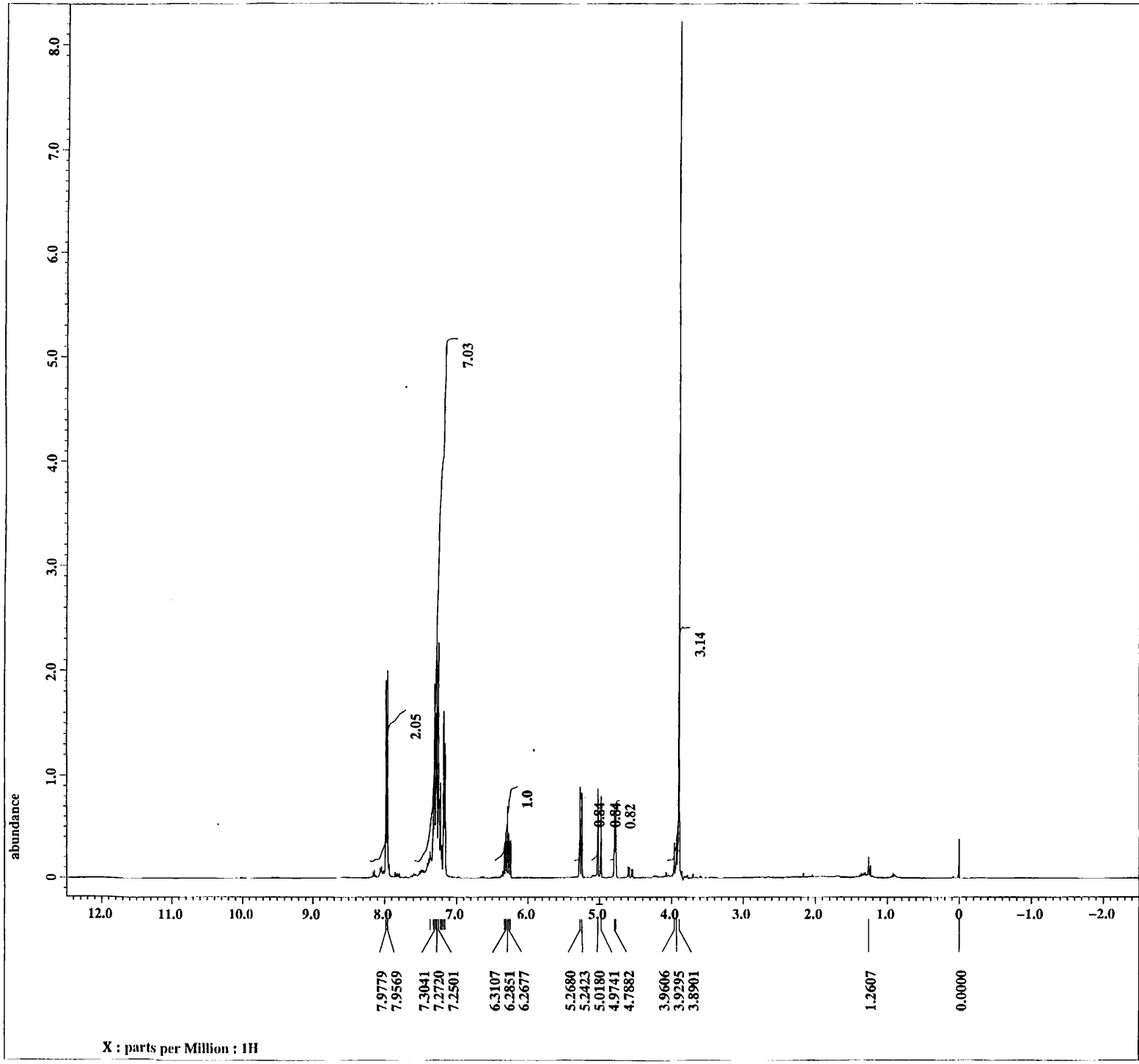
(4-CF3C6H4)CH(CH3)CH=CH2 (6h)




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: CF3_C-1.jdf
```

```
Filename          = CF3_C-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#553463
Solvent           = CHLOROFORM-D
Creation_time     = 10-JUL-2007 15:32:21
Revision_time     = 10-JUL-2007 15:32:23
Current_time      = 10-JUL-2007 15:32:39

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 128
Total_scans       = 128

X_90_width        = 9.5[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 4.2[dB]
X_pulse           = 3.16666667[us]
Irr_atn_dec       = 21[dB]
Irr_atn_noe       = 21[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 52
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 22[dC]
```

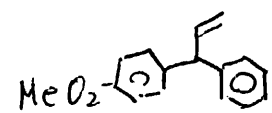
(4-CF3C6H4)CH(CH3)CH=CH2 (6h)

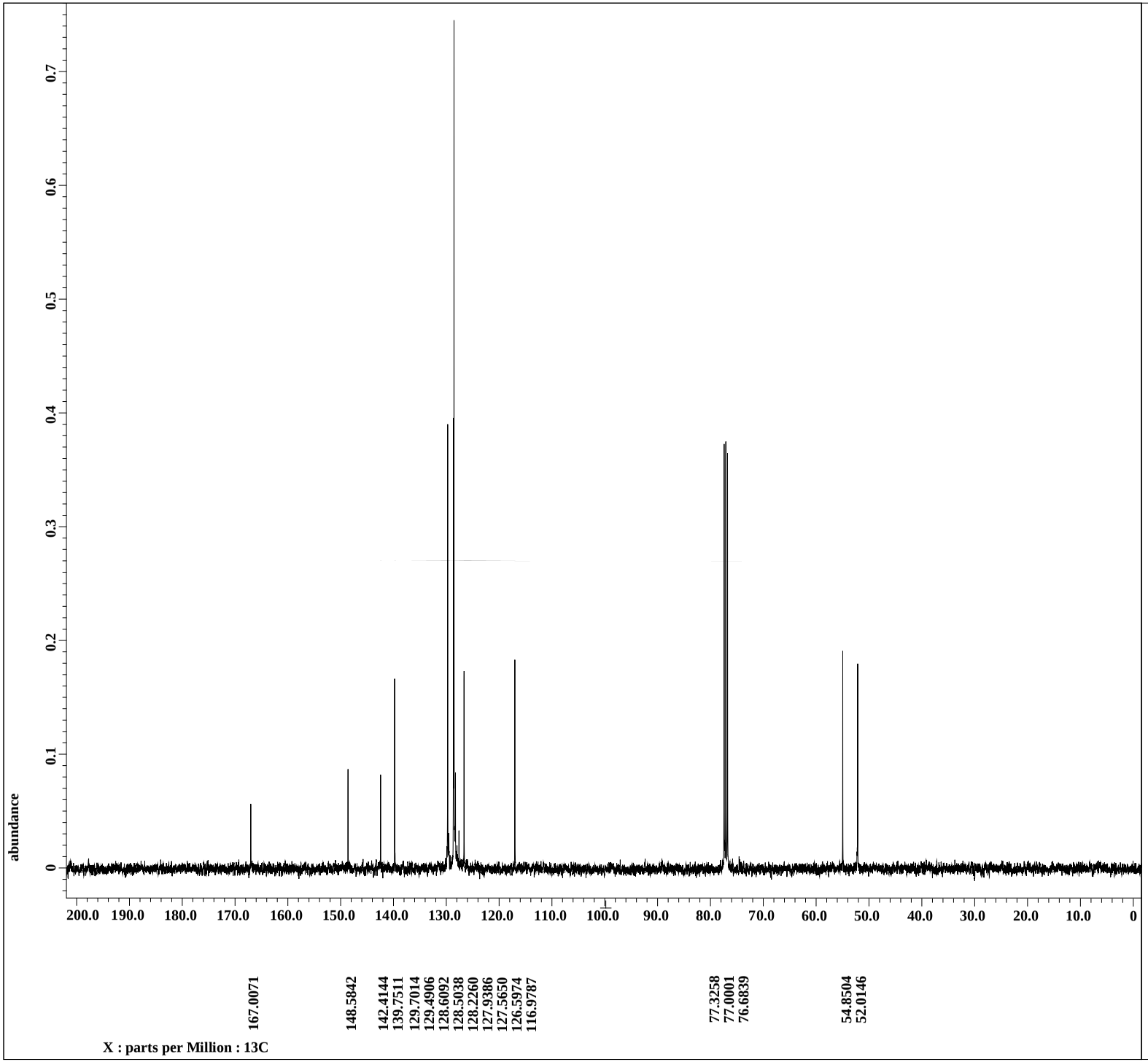



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: EsPh_H-1.jdf
```

Filename	= EsPh_H-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#803404
Solvent	= CHLOROFORM-D
Creation_time	= 10-JUL-2007 22:22:37
Revision_time	= 10-JUL-2007 22:26:55
Current_time	= 10-JUL-2007 22:27:01
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 16384
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.7590656[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.36244155[Hz]
X_sweep	= 5.93824228[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.2[us]
X_acq_time	= 2.7590656[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 34
Relaxation_delay	= 5[s]
Repetition_time	= 7.7590656[s]
Temp_get	= 21.5[dC]

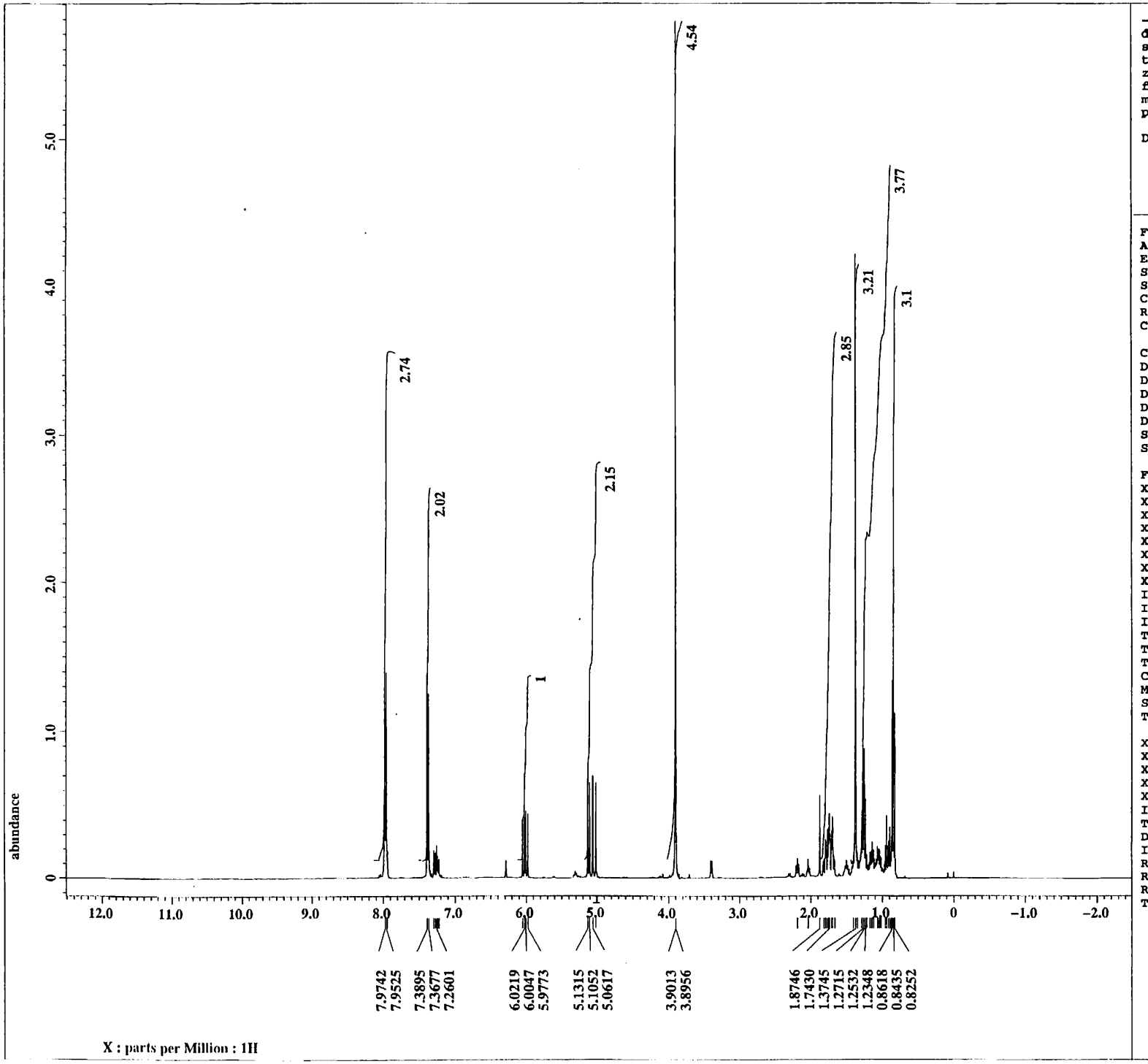
(4-MeO2CC6H4)CH(Ph)CH=CH2






```
Filename          = EsPh_C-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#803461
Solvent           = CHLOROFORM-D
Creation_time     = 10-JUL-2007 22:29:39
Revision_time     =  7-AUG-2008 11:16:59
Current_time      =  7-AUG-2008 11:32:34

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 1.048576[s]
X_domain          = 13C
X_freq            = 99.54517646[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95367432[Hz]
X_sweep           = 31.25[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 128
Total_scans       = 128

X_90_width        = 9.5[us]
X_acq_time        = 1.048576[s]
X_angle           = 30[deg]
X_atn             = 4.2[dB]
X_pulse           = 3.16666667[us]
Irr_atn_dec       = 21[dB]
Irr_atn_noe       = 21[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 50
Relaxation_delay  = 2[s]
Repetition_time   = 3.048576[s]
Temp_get          = 21.8[dC]
```

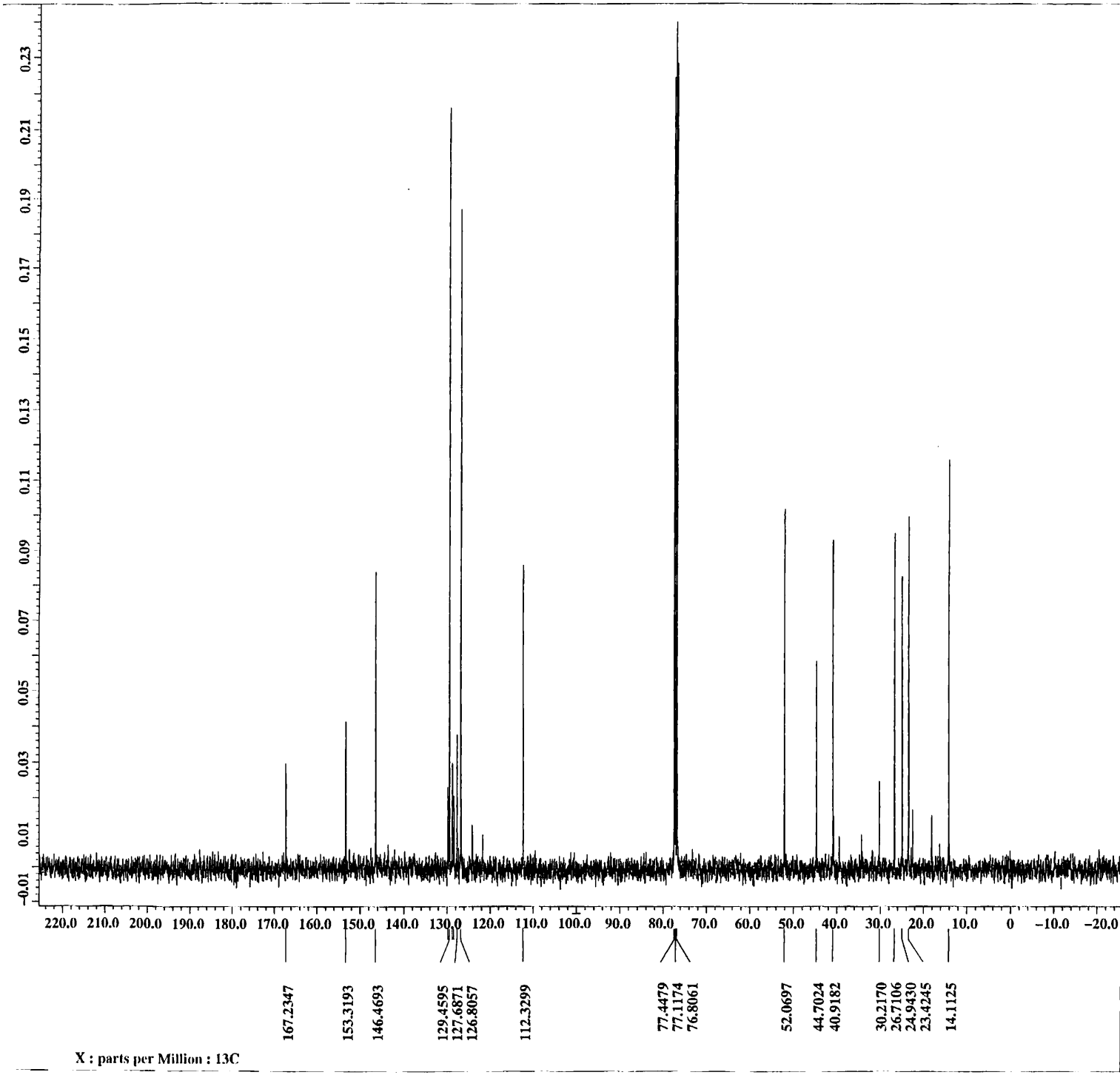
(4-MeO2CC6H4)CH(Ph)CH=CH2




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: BuMeEs_H2-1.jdf
```

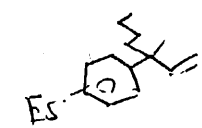
```
Filename          = BuMeEs_H2-4.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#761011
Solvent           = CHLOROFORM-D
Creation_time     = 12-JUL-2007 21:11:31
Revision_time     = 12-JUL-2007 21:14:54
Current_time      = 12-JUL-2007 21:15:12

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 2.20725248[s]
X_domain          = 1H
X_freq            = 395.88430144[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.45305193[Hz]
X_sweep           = 7.42280285[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 395.88430144[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 11.2[us]
X_acq_time        = 2.20725248[s]
X_angle           = 45[deg]
X_atn             = 1.5[dB]
X_pulse           = 5.6[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 24
Relaxation_delay  = 5[s]
Repetition_time   = 7.20725248[s]
Temp_get          = 22[dC]
```

(4-MeO2CC6H4)C(Me)(Bu)CH=CH2

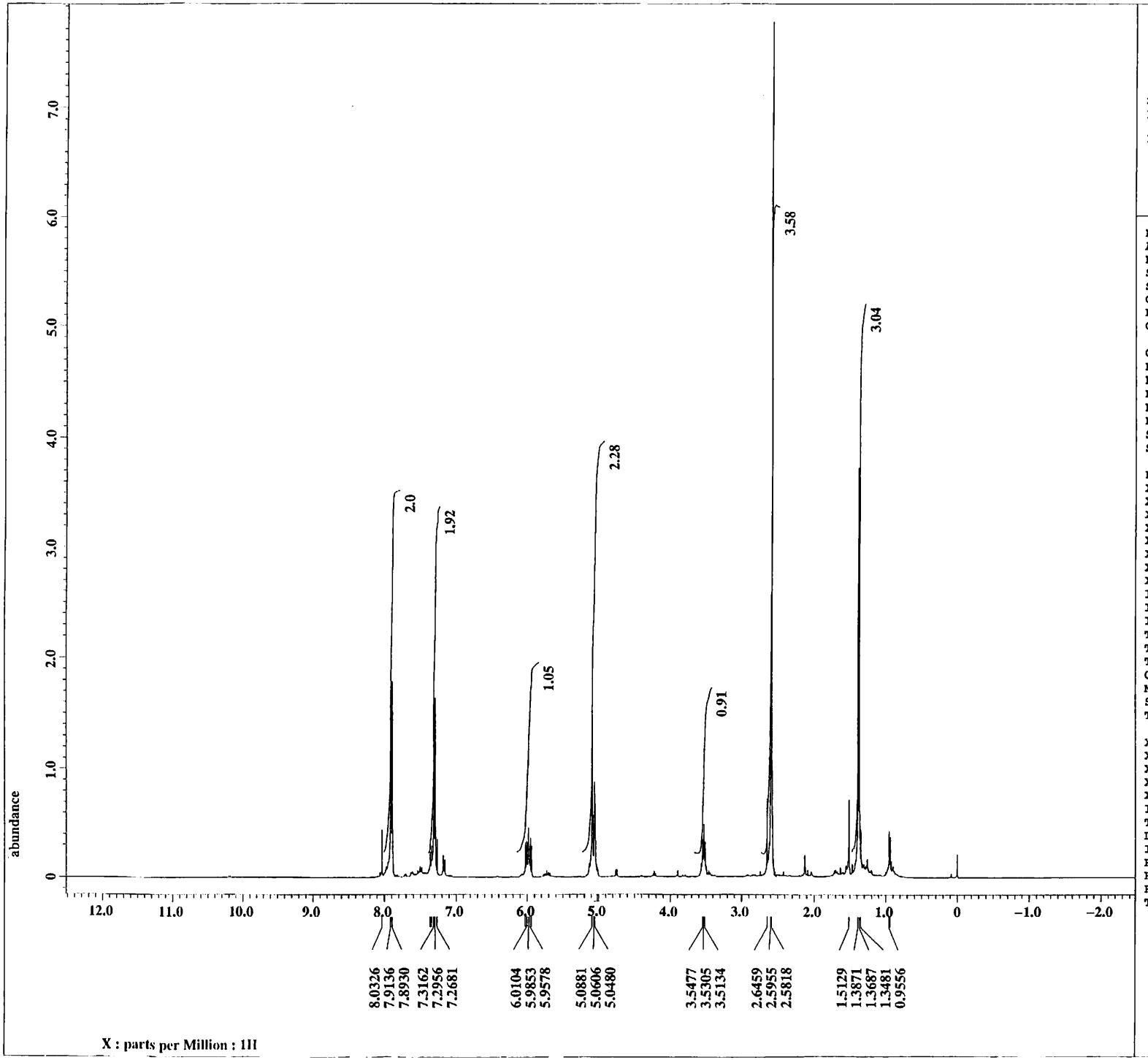



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: BuMeEs_C-1.jdf
```

Filename	= BuMeEs_C-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#506968
Solvent	= CHLOROFORM-D
Creation_time	= 10-JUL-2007 14:13:11
Revision_time	= 10-JUL-2007 14:15:50
Current_time	= 10-JUL-2007 14:15:52
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 1.048576[s]
X_domain	= 13C
X_freq	= 99.54517646[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.95367432[Hz]
X_sweep	= 31.25[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 128
Total_scans	= 128
X_90_width	= 9.5[us]
X_acq_time	= 1.048576[s]
X_angle	= 30[deg]
X_atn	= 4.2[dB]
X_pulse	= 3.16666667[us]
Irr_atn_dec	= 21[dB]
Irr_atn_noe	= 21[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 46
Relaxation_delay	= 2[s]
Repetition_time	= 3.048576[s]
Temp_get	= 22.2[dC]



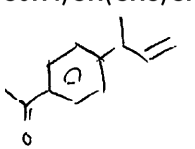
(4-MeO2CC6H4)C(Me)(Bu)CH=CH2

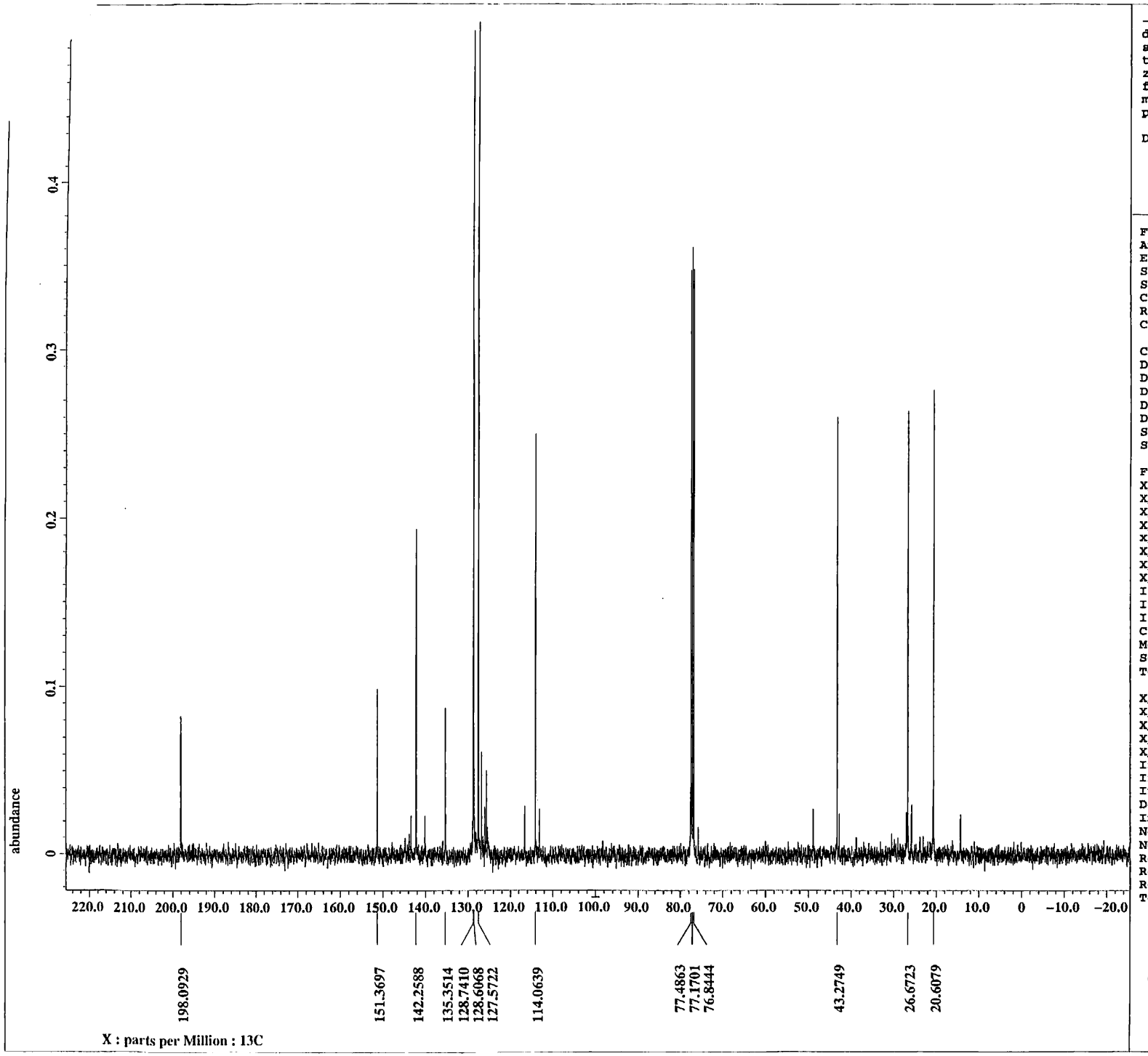



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Ac_H2-1.jdf
```

Filename	= Ac_H2-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#667746
Solvent	= CHLOROFORM-D
Creation_time	= 11-JUL-2007 18:39:53
Revision_time	= 11-JUL-2007 18:43:08
Current_time	= 11-JUL-2007 18:43:16
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.20725248[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 8
Total_scans	= 8
X_90_width	= 11.2[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 28
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 21.8[dC]

(4-CH3COC6H4)CH(CH3)CH=CH2

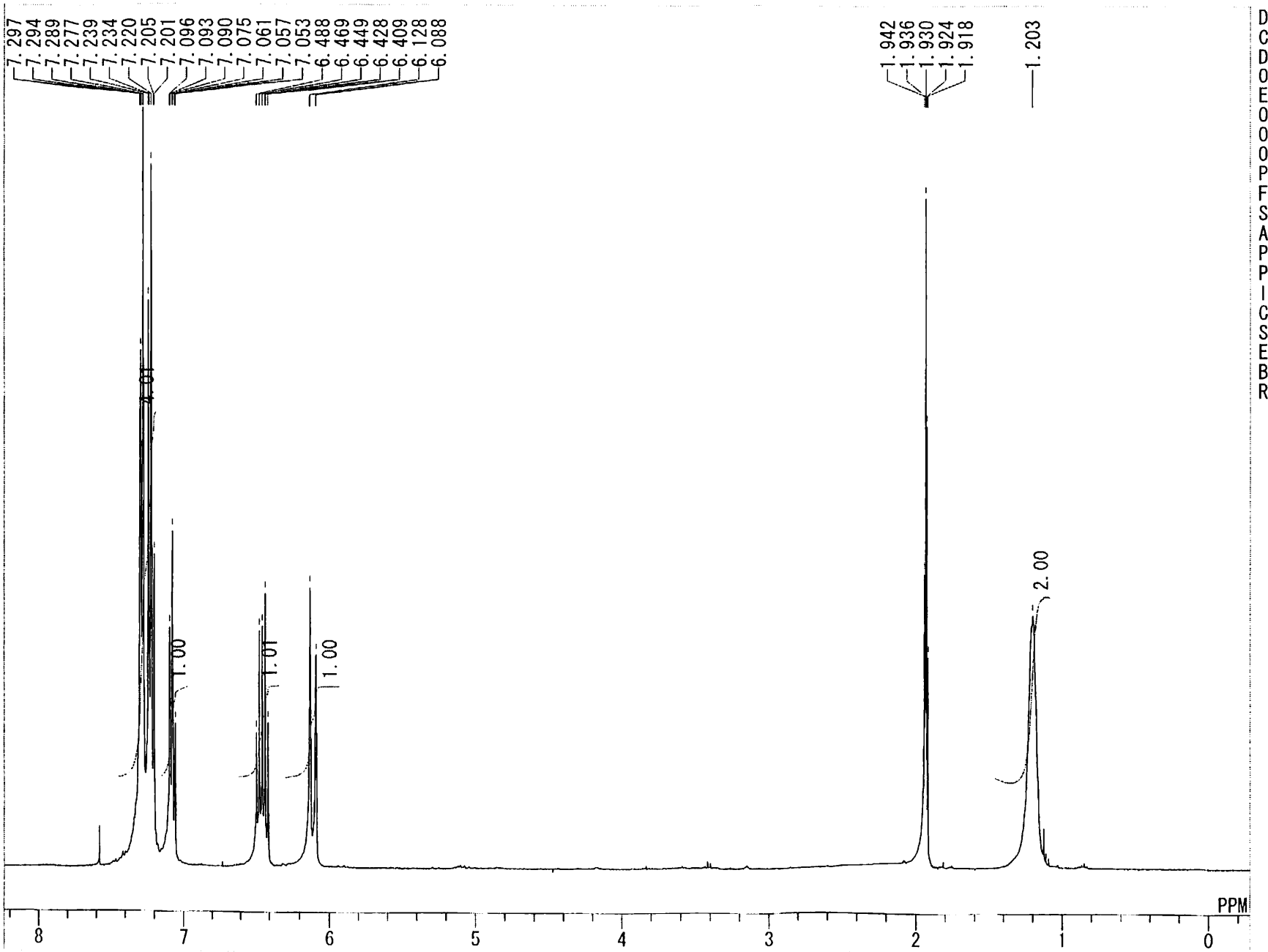




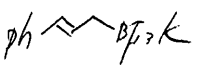

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Ac_C-1.jdf
```

Filename	= Ac_C-3.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#664529
Solvent	= CHLOROFORM-D
Creation_time	= 11-JUL-2007 18:37:02
Revision_time	= 11-JUL-2007 18:37:20
Current_time	= 11-JUL-2007 18:38:06
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 1.048576[s]
X_domain	= 13C
X_freq	= 99.54517646[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.95367432[Hz]
X_sweep	= 31.25[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 128
Total_scans	= 128
X_90_width	= 9.5[us]
X_acq_time	= 1.048576[s]
X_angle	= 30[deg]
X_atn	= 4.2[dB]
X_pulse	= 3.16666667[us]
Irr_atn_dec	= 21[dB]
Irr_atn_noe	= 21[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 50
Relaxation_delay	= 2[s]
Repetition_time	= 3.048576[s]
Temp_get	= 22.2[dC]

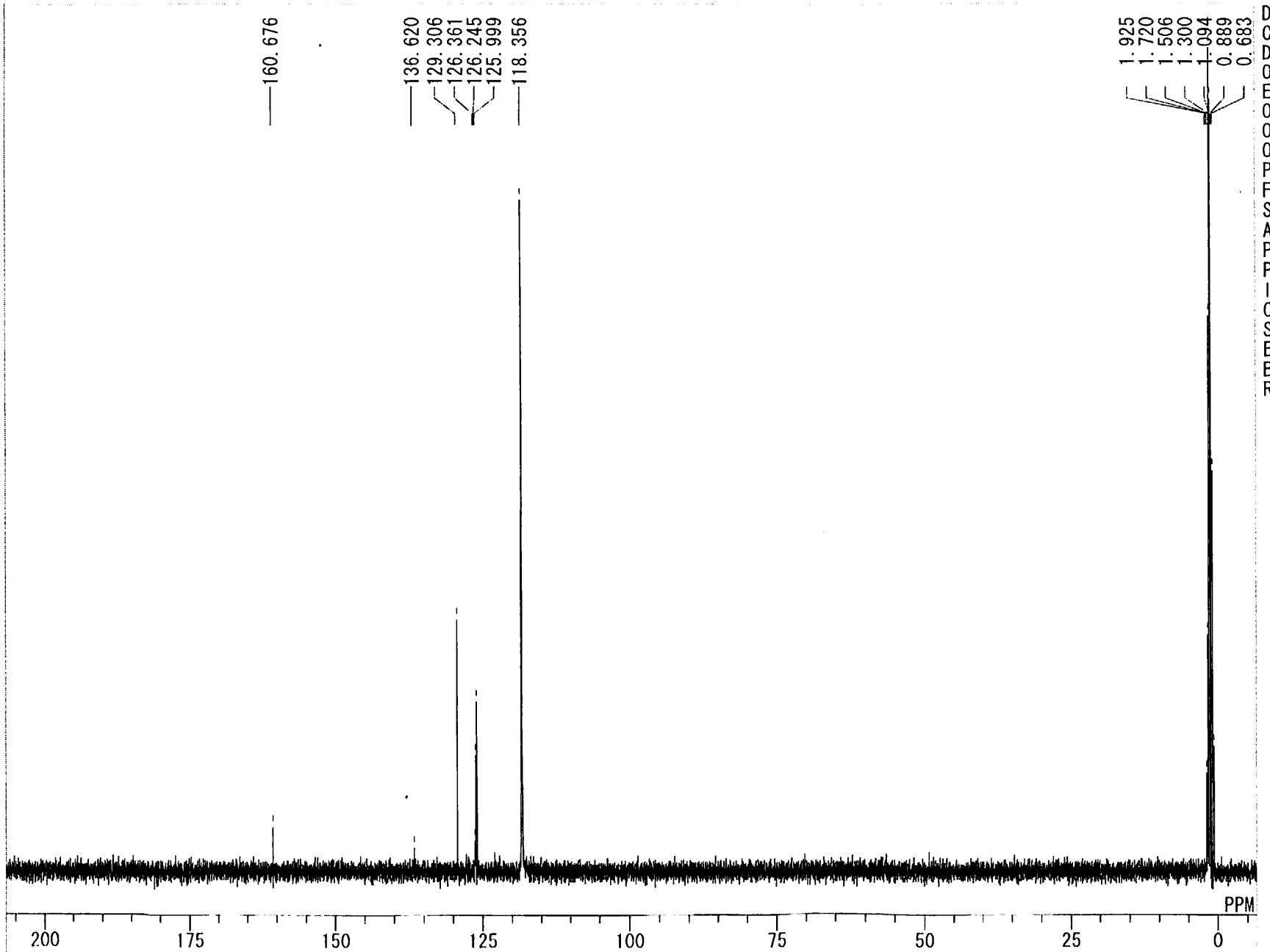
(4-CH3COC6H4)CH(CH3)CH=CH2



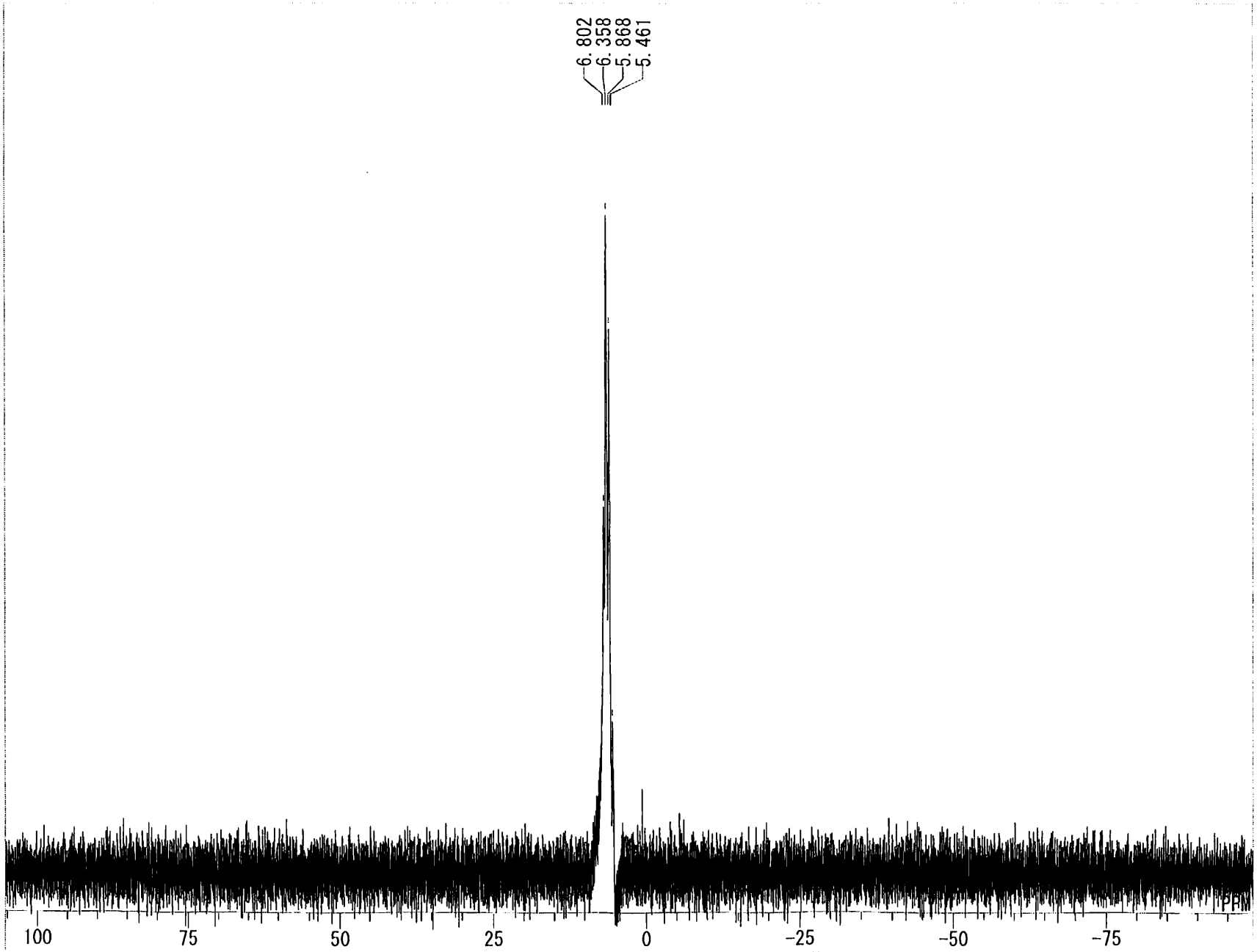
DFILE	C:¥Documents and Setting
COMNT	
DATIM	Thu Jan 11 16:59:02 200
OBNUC	1H
EXMOD	non
OBFRQ	399.65 MHz
OBSET	0.00 KHz
OBFIN	134300.00 Hz
POINT	16384
FREQU	7993.60 Hz
SCANS	16
ACQTM	2.0496 sec
PD	4.9500 sec
PW1	6.50 usec
IRNUC	1H
CTEMP	23.6 c
SLVNT	CD3CN
EXREF	1.93 ppm
BF	0.12 Hz
RGAIN	16



(*E*)-PhCH=CHCH$_2$BF$_3$K (**2c**)

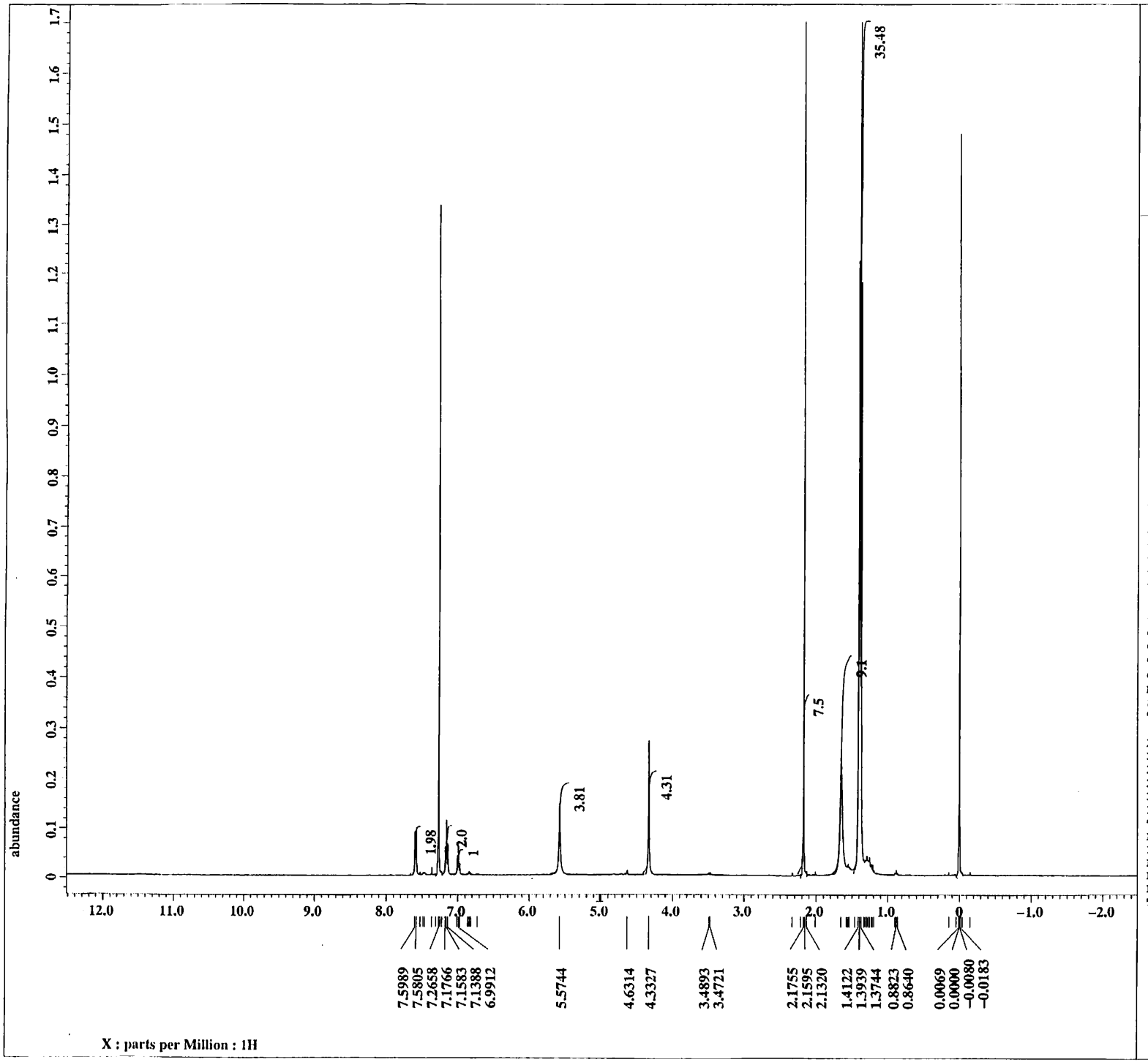


(*E*)-PhCH=CHCH$_2$BF$_3$K (**2c**)



DFILE	C:¥Documents and Setting
COMNT	
DATIM	Thu Jan 11 17:16:31 200
OBNUC	11B
EXMOD	bcm
OBFRQ	128.15 MHz
OBSET	0.00 KHz
OBFIN	116720.00 Hz
POINT	32768
FREQU	27100.27 Hz
SCANS	100
ACQTM	1.2091 sec
PD	1.7910 sec
PW1	4.50 usec
IRNUC	1H
CTEMP	24.3 c
SLVNT	CD3CN
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	21

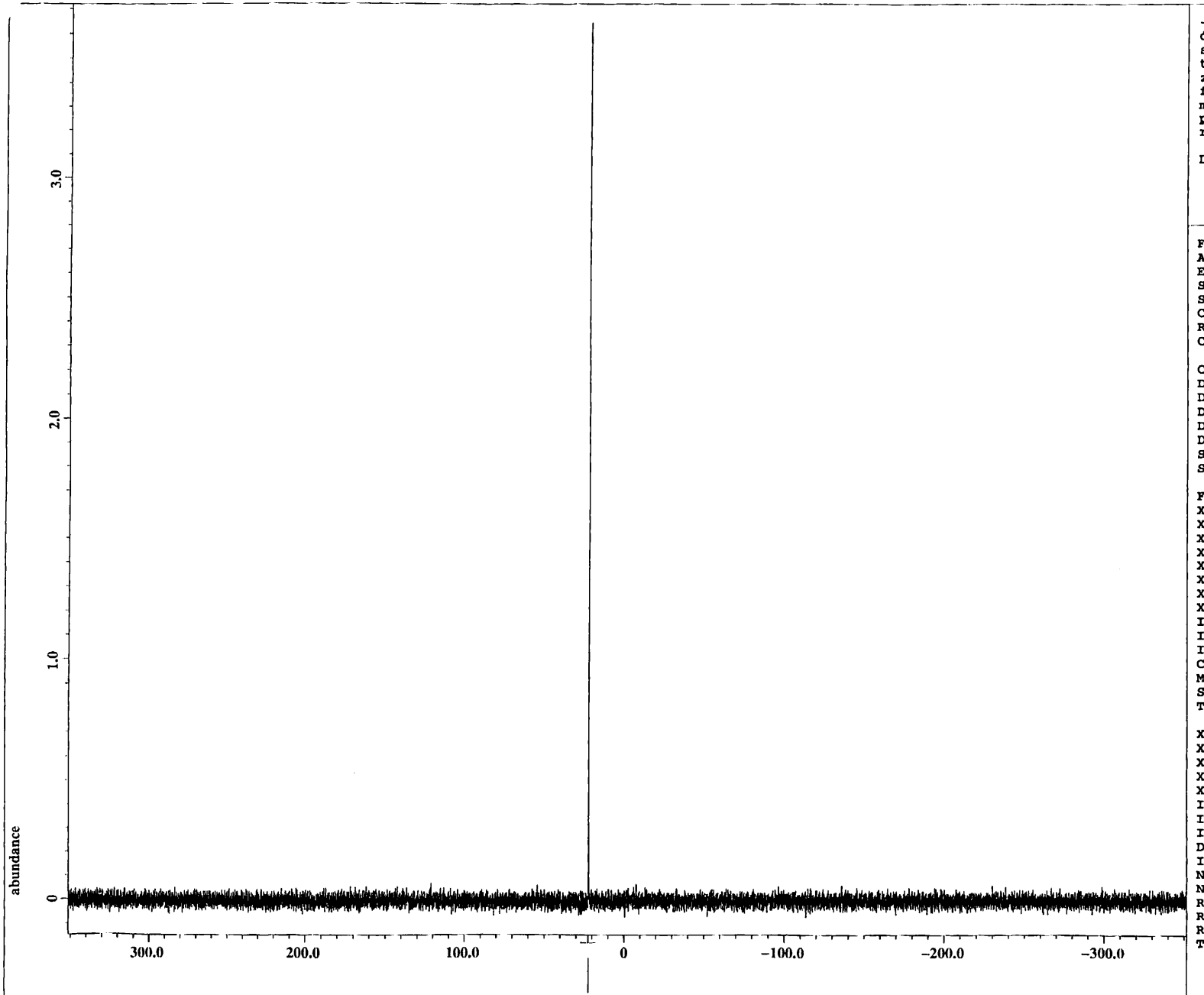
(*E*)-PhCH=CHCH$_2$BF$_3$K (**2c**)




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: DtBPF_PhBr_H-1.jdf
```

Filename	= DtBPF_PhBr_H-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#614693
Solvent	= CHLOROFORM-D
Creation_time	= 13-JUL-2007 17:07:38
Revision_time	= 13-JUL-2007 17:12:07
Current_time	= 13-JUL-2007 17:12:17
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.20725248[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.2[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 38
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 22[dC]

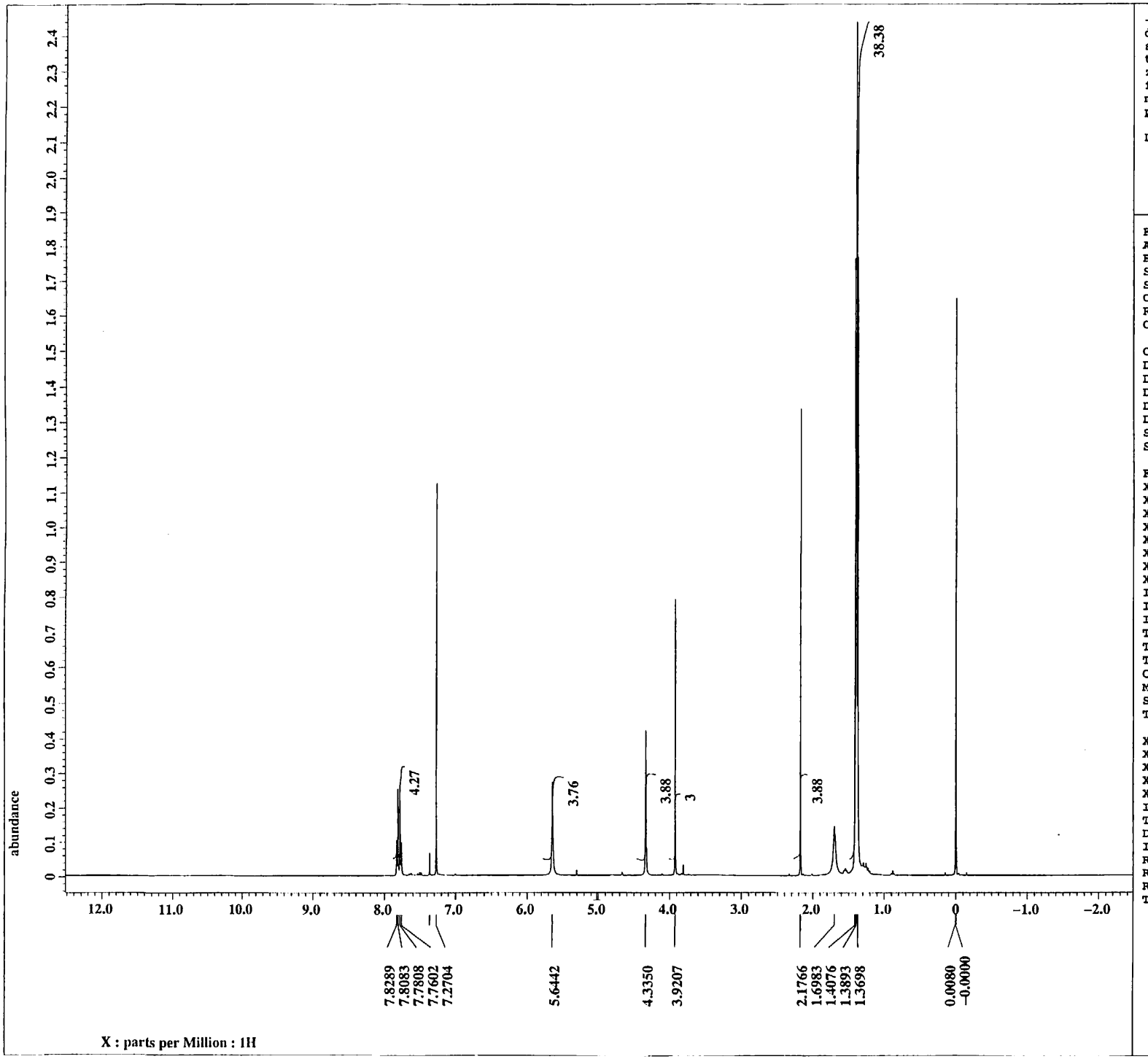
(D-*t*-BPF)Pd(Br)(C_6H_5)




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
reference : 0.171[ppm] : 0[ppm]

Derived from: DtBPF_PhBr_P-1.jdf
```

```
Filename          = DtBPF_PhBr_P-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#615781
Solvent           = CHLOROFORM-D
Creation_time     = 13-JUL-2007 17:27:05
Revision_time     = 13-JUL-2007 17:32:57
Current_time      = 13-JUL-2007 17:33:01

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 31P
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.2982153[T] (400[MHz
X_acq_duration    = 0.2326528[s]
X_domain          = 31P
X_freq            = 160.25679653[MHz]
X_offset          = 0[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 4.29825044[Hz]
X_sweep           = 140.84507042[kHz]
Irr_domain        = 1H
Irr_freq          = 395.88430144[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 100
Total_scans       = 100

X_90_width        = 9.5[us]
X_acq_time        = 0.2326528[s]
X_angle           = 30[deg]
X_atn             = 6.2[dB]
X_pulse           = 3.16666667[us]
Irr_atn_dec       = 21[dB]
Irr_atn_noe       = 21[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 56
Relaxation_delay  = 2[s]
Repetition_time   = 2.2326528[s]
Temp_get          = 22.1[dC]
```

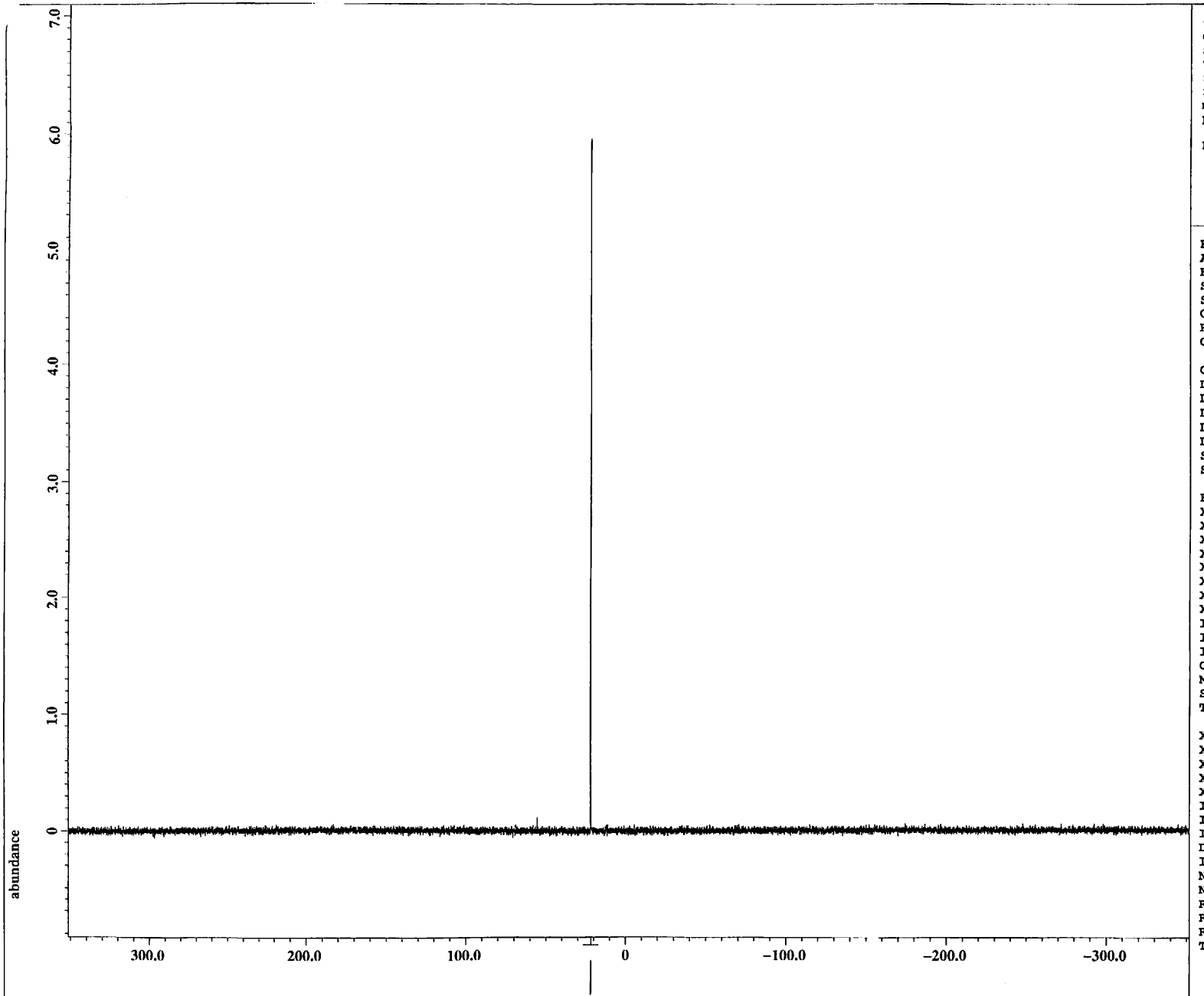
(D-*t*-BPF)Pd(Br)(C_6H_5)




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: DtBPF_EsPh_H-1.jdf
```

Filename	= DtBPF_EsPh_H-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= S#632533
Solvent	= CHLOROFORM-D
Creation_time	= 13-JUL-2007 17:37:31
Revision_time	= 13-JUL-2007 17:40:24
Current_time	= 13-JUL-2007 17:40:37
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 2.20725248[s]
X_domain	= 1H
X_freq	= 395.88430144[MHz]
X_offset	= 5[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.45305193[Hz]
X_sweep	= 7.42280285[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 395.88430144[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 16
Total_scans	= 16
X_90_width	= 11.2[us]
X_acq_time	= 2.20725248[s]
X_angle	= 45[deg]
X_atn	= 1.5[dB]
X_pulse	= 5.6[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 36
Relaxation_delay	= 5[s]
Repetition_time	= 7.20725248[s]
Temp_get	= 21.6[dC]

(D-*t*-BPF)Pd(Br)(4-$MeO_2CC_6H_4$)




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: DtBPF_EsPh_P-1.jdf
```

Filename	= DtBPF_EsPh_P-5.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= S#634273
Solvent	= CHLOROFORM-D
Creation_time	= 13-JUL-2007 17:42:45
Revision_time	= 13-JUL-2007 17:43:48
Current_time	= 13-JUL-2007 17:43:51
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 31P
Dim_units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_strength	= 9.2982153[T] (400[MHz
X_acq_duration	= 0.2326528[s]
X_domain	= 31P
X_freq	= 160.25679653[MHz]
X_offset	= 0[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 4.29825044[Hz]
X_sweep	= 140.84507042[kHz]
Irr_domain	= 1H
Irr_freq	= 395.88430144[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 128
Total_scans	= 128
X_90_width	= 9.5[us]
X_acq_time	= 0.2326528[s]
X_angle	= 30[deg]
X_atn	= 6.2[dB]
X_pulse	= 3.16666667[us]
Irr_atn_dec	= 21[dB]
Irr_atn_noe	= 21[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 56
Relaxation_delay	= 2[s]
Repetition_time	= 2.2326528[s]
Temp_get	= 22[dC]

(D-*t*-BPF)Pd(Br)(4-MeO$_2$CC$_6$H$_4$)