# Supporting Information

## Manganese(III) acetate-mediated radical reaction of [60]fullerene with phosphonate esters affording unprecedented separable singly-bonded [60]fullerene dimers

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**Synthesis of 2a in chlorobenzene:** A mixture of $C_{60}$ (36.0 mg, 0.05 mmol), **1a** (9.2 μL, 0.10 mmol) and $Mn(OAc)_3{\cdot}2H_2O$ (26.8 mg, 0.10 mmol) was dissolved in chlorobenzene (10 mL) and stirred at 135 °C (oil bath temperature) under argon atmosphere for 50 min. The reaction mixture was poured onto a silica gel column and eluted with $CS_2$ to afford recovered $C_{60}$ (24.1 mg, 67%), then with $CS_2$/AcOEt (10:1) to give dimer **2a** (11.9 mg, 29%). The meso and racemic mixture of dimer **2a** was further separated on a silica gel column wrapped by aluminum foil. Elution with cold $CS_2$/AcOEt (100:5) afforded the minor isomer and then major isomer. $^1$H NMR (400 MHz, $CDCl_3$) δ 4.10 (d, $J$ = 11.2 Hz, OC$H_3$, major), 4.11 (d, $J$ = 11.2 Hz, OC$H_3$, minor), 4.17 (d, $J$ = 11.2 Hz, OC$H_3$, major), 4.23 (d, $J$ = 11.2 Hz, OC$H_3$, minor); $^{13}$C NMR (75.5 MHz, $CS_2$–$CDCl_3$) δ 55.03-55.33 (m, O$CH_3$, major and minor), 61.68 (d, $J_{P\text{-}C}$ = 146.9 Hz, sp$^3$-C of $C_{60}$), 67.82-68.03 (m, sp$^3$-C of $C_{60}$), 137.42 (d, $J_{P\text{-}C}$ = 5.8 Hz), 137.49 (d, $J_{P\text{-}C}$ = 5.6 Hz), 138.07 (d, $J_{P\text{-}C}$ = 3.1 Hz), 138.21, 138.40 (d, $J_{P\text{-}C}$ = 2.1 Hz) 138.68, 139.05 (d, $J_{P\text{-}C}$ = 2.6 Hz), 139.15 (d, $J_{P\text{-}C}$ = 2.7 Hz), 140.90, 140.92, 141.53, 141.82, 142.23, 142.38, 142.44, 142.48, 142.59, 142.71, 142.74, 142.89, 142.96, 143.06, 143.13, 143.16, 143.31, 143.38, 143.45, 143.48, 143.58, 143.67, 143.72, 143.76, 143.88, 143.99, 144.09, 144.13, 144.19, 144.25, 144.33, 144.45, 144.48, 144.54, 144.58, 144.91, 145.02, 145.11, 145.17, 145.43, 145.46, 145.51, 145.64, 145.70, 145.76, 146.83, 146.96, 147.07, 147.09, 147.11, 147.33, 147.49, 147.51, 147.70 (d, $J_{P\text{-}C}$ = 7.4 Hz), 147.88, 148.07 (d, $J_{P\text{-}C}$ = 7.7 Hz), 148.62, 148.66, 148.83, 148.87, 148.93, 148.95, 149.14 (d, $J_{P\text{-}C}$ = 4.3 Hz), 149.33, 149.55, 149.99 (d, $J_{P\text{-}C}$ = 2.7 Hz), 150.29, 150.73, 154.29, 154.38, 154.47, 155.52 (d, $J_{P\text{-}C}$ = 3.1 Hz), 156.00 (d, $J_{P\text{-}C}$ = 3.6 Hz); $^{31}$P NMR (162 MHz, $CDCl_3$) δ 16.49 (major), 16.51 (minor); FT-IR $\nu$/cm$^{-1}$ (KBr) 2947, 2847, 1511, 1458, 1428, 1268, 1187, 1048, 1024, 905, 842, 762, 670, 630, 558, 526; UV−vis $\lambda_{max}$/nm (log ε) ($CHCl_3$) 257 (5.28), 325 (4.82), 446 (4.21); HRMS (-ESI): calcd. for $C_{62}H_6PO_3$ $[M/2]^-$ 829.0055, found 829.0068. **2a** (major isomer): $^1$H NMR (400 MHz, $CDCl_3$) δ 4.10 (d, 6H, $J$ = 11.2 Hz, OC$H_3$), 4.17 (d, 6H, $J$ = 11.2 Hz, OC$H_3$). **2a** (minor isomer): $^1$H NMR (400 MHz, $CDCl_3$) δ 4.11 (d, 6H, $J$ = 11.2 Hz, OC$H_3$), 4.23 (d, 6H, $J$ = 11.2 Hz, OC$H_3$).

**Synthesis of 2b in chlorobenzene:** A mixture of $C_{60}$ (36.0 mg, 0.05 mmol), **1b** (12.9 μL, 0.10 mmol) and $Mn(OAc)_3{\cdot}2H_2O$ (26.8 mg, 0.10 mmol) was dissolved in chlorobenzene (10 mL) and stirred at 135 °C (oil bath temperature) under argon atmosphere for 50 min. The reaction mixture was poured onto a silica gel column and eluted with $CS_2$ to afford recovered $C_{60}$ (24.6 mg, 68%), then with $CS_2$/AcOEt (20:1) to give dimer **2b** (12.0 mg, 28%). The meso and racemic mixture of dimer **2b** was further separated on a silica gel column wrapped by aluminum foil. Elution with cold $CS_2$/AcOEt (100:4) afforded the minor isomer and then major isomer. Spectral data of **2b**: $^1$H NMR (300 MHz, $CS_2$-$CDCl_3$) δ 1.37 (t, $J$ = 7.0 Hz, C$H_3$, major), 1.38 (t, $J$ = 6.9 Hz, C$H_3$, minor), 1.52 (t, $J$ = 6.9 Hz, C$H_3$, major and minor), 4.40-4.50 (m, C$H_2$, major and minor), 4.54-4.64 (m, C$H_2$, major and minor); $^{13}$C NMR (75.5 MHz, $CS_2$–$CDCl_3$ with $Cr(acac)_3$ as relaxation reagent) δ 16.43 (d, $J_{P\text{-}C}$ = 6.2 Hz, OCH$_2$$C$H$_3$, major), 16.46 (d, $J_{P\text{-}C}$ = 6.1 Hz, OCH$_2$$C$H$_3$, minor), 16.59 (d, $J_{P\text{-}C}$ = 6.1 Hz, OCH$_2$$C$H$_3$, major and minor), 62.22 (d, $J_{P\text{-}C}$ = 144.9 Hz, sp$^3$-C of $C_{60}$, major), 62.30 (d, $J_{P\text{-}C}$ = 144.9 Hz, sp$^3$-C of $C_{60}$, minor), 64.55 (d, $J_{P\text{-}C}$ = 7.0 Hz, O$C$H$_2$CH$_3$, major and minor),

64.65 (d, $J_{P\text{-}C}$ = 6.8 Hz, O*C*H$_2$CH$_3$, major and minor), 67.61–67.85 (sp$^3$-C of $C_{60}$, major and minor), 137.17 (d, $J_{P\text{-}C}$ = 5.0 Hz), 137.20 (d, $J_{P\text{-}C}$ = 4.5 Hz), 137.95 (d, $J_{P\text{-}C}$ = 3.8 Hz), 138.14, 138.40 (d, $J_{P\text{-}C}$ = 3.0 Hz), 138.57, 138.94 (d, $J_{P\text{-}C}$ = 3.0 Hz), 139.03 (d, $J_{P\text{-}C}$ = 2.7 Hz), 140.66, 141.40, 141.64, 142.11, 142.15, 142.23, 142.27, 142.34, 142.37, 142.41, 142.50, 142.55, 142.57, 142.70, 142.77, 142.81, 142.90, 142.92, 142.98, 143.05, 143.17, 143.22, 143.26, 143.40 (d, $J_{P\text{-}C}$ = 1.8 Hz), 143.48, 143.78, 143.88, 143.92, 143.97, 144.07, 144.12, 144.19, 144.24, 144.29, 144.33, 144.38, 144.60, 144.64, 144.80, 144.88, 144.92, 145.03, 145.30, 145.35, 145.43, 145.47, 145.55, 145.61, 146.13, 146.65, 146.80, 146.83, 146.89, 146.93, 147.07, 147.31, 147.53, 147.85 (d, $J_{P\text{-}C}$ = 7.1 Hz), 148.18 (d, $J_{P\text{-}C}$ = 7.2 Hz), 148.43, 148.46, 148.66, 148.70, 148.85 (d, $J_{P\text{-}C}$ = 5.5 Hz), 148.88 (d, $J_{P\text{-}C}$ = 5.4 Hz), 149.30, 149.48, 149.97 (d, $J_{P\text{-}C}$ = 1.9 Hz), 150.67 (d, $J_{P\text{-}C}$ = 2.2 Hz), 154.99, 155.16, 155.51 (d, $J_{P\text{-}C}$ = 3.1 Hz), 155.94 (d, $J_{P\text{-}C}$ = 3.6 Hz); $^{31}$P NMR (162 MHz, $CDCl_3$) δ 13.39 (major), 13.50 (minor); FT-IR $\nu$/cm$^{-1}$ (KBr) 2974, 1510, 1428, 1388, 1365, 1265, 1188, 1159, 1093, 1043, 1016, 968, 843, 821, 760, 733, 669, 643, 630, 567, 526; UV−vis $\lambda_{max}$/nm (log ε) ($CHCl_3$) 260 (5.25), 326 (4.78), 446 (4.18); HRMS (-ESI): calcd. for $C_{64}H_{10}PO_3$ $[M/2]^-$ 857.0368, found 857.0324. **2b** (major isomer): $^1$H NMR (400 MHz, $CDCl_3$) δ 1.38 (t, 6H, $J$ = 7.0 Hz, C*H*$_3$), 1.52 (t, 6H, $J$ = 7.2 Hz, C*H*$_3$), 4.47 (dq, 4H, $J$ = 7.2 Hz, OC*H*$_2$), 4.54-4.65 (m, 4H, OC*H*$_2$). **2b** (minor isomer): $^1$H NMR (400 MHz, $CDCl_3$) δ 1.39 (t, 6H, $J$ = 7.0 Hz, C*H*$_3$), 1.53 (t, 6H, $J$ = 7.0 Hz, C*H*$_3$), 4.43-4.53 (m, 4H, OC*H*$_2$), 4.55-4.71 (m, 4H, OC*H*$_2$).

**Synthesis of 2c in chlorobenzene:** A mixture of $C_{60}$ (36.0 mg, 0.05 mmol), **1c** (15.0 mg, 0.10 mmol) and $Mn(OAc)_3{\cdot}2H_2O$ (53.6 mg, 0.20 mmol) was dissolved in chlorobenzene (10 mL) and stirred at 100 $^o$C (oil bath temperature) under argon atmosphere for 90 min. The reaction mixture was poured onto a silica gel column and eluted with $CS_2$ to afford recovered $C_{60}$ (23.3 mg, 65%), then with $CS_2$/AcOEt (10:1) to give dimer **2c** (14.6 mg, 34%). The meso and racemic mixture of dimer **2c** was further separated on a silica gel column wrapped by aluminum foil. Elution with cold $CS_2$/AcOEt (100:7) afforded the minor isomer and then major isomer. Spectral data of **2c**: $^1$H NMR (300 MHz, $CDCl_3$) δ 1.11 (s, C*H*$_3$, major), 1.13 (s, C*H*$_3$, minor), 1.31 (s, C*H*$_3$, major), 1.32 (s, C*H*$_3$, minor), 4.25-4.57 (m, C*H*$_2$, major and minor); $^{13}$C NMR (75 MHz, $CS_2$–ODCB-$d_4$) δ 21.62 (*C*H$_3$), 21.68 (*C*H$_3$), 21.92 (*C*H$_3$), 21.98 (*C*H$_3$), 32.96 (d, $J_{P\text{-}C}$ = 6.1 Hz, *C*CH$_3$), 61.61 (d, $J_{P\text{-}C}$ = 144.6 Hz, sp$^3$-C of $C_{60}$), 67.83-68.10 (m, sp$^3$-C of $C_{60}$), 77.36-78.33 (m, *C*H$_2$), 137.60 (d, $J_{P\text{-}C}$ = 5.6 Hz), 137.70 (d, $J_{P\text{-}C}$ = 5.2 Hz), 138.56, 138.75 (d, $J_{P\text{-}C}$ = 3.8 Hz), 138.81, 138.94 (d, $J_{P\text{-}C}$ = 3.8 Hz), 139.15 (d, $J_{P\text{-}C}$ = 3.3 Hz), 141.01, 141.06, 141.83, 141.93, 142.31, 142.35, 142.47, 142.51, 142.55, 142.71, 142.79, 142.86, 143.00, 143.05, 143.14, 143.19, 143.24, 143.27, 143.39, 143.46, 143.49, 143.59, 143.72, 143.86, 144.04, 144.26, 144.32, 144.39, 144.50, 144.57, 144.63, 144.70, 145.07, 145.10, 145.13, 145.25, 145.54, 145.57, 145.60, 145.63, 145.73, 145.88, 146.23, 146.97, 147.07, 147.16, 147.25, 147.39, 147.62, 148.34 (d, $J_{P\text{-}C}$ = 7.3 Hz), 148.54 (d, $J_{P\text{-}C}$ = 7.6 Hz), 148.77, 148.97, 149.15 (d, $J_{P\text{-}C}$ = 5.6 Hz), 149.38, 149.54, 149.69, 150.07 (d, $J_{P\text{-}C}$ = 3.1 Hz), 150.56 (d, $J_{P\text{-}C}$ = 2.2 Hz), 153.52, 153.62, 153.70, 153.80, 155.48 (d, $J_{P\text{-}C}$ = 3.7 Hz), 155.84 (d, $J_{P\text{-}C}$ = 4.1 Hz); $^{31}$P NMR (162 MHz, $CDCl_3$) δ 9.70 (minor), 9.79 (major); FT-IR $\nu$/cm$^{-1}$ (KBr)

2922, 1510, 1462, 1427, 1370, 1270, 1189, 1052, 998, 909, 839, 762, 670, 645, 557, 526; UV−vis $\lambda_{max}$/nm (log ε) ($CHCl_3$) 259 (5.32), 325 (4.93), 447 (4.23); HRMS (-ESI): calcd. for $C_{65}H_{10}PO_3$ $[M/2]^-$ 869.0368, found 869.0376. **2c** (major isomer): $^1$H NMR (400 MHz, $CDCl_3$) δ 1.11 (s, 6H, OC*H*$_3$), 1.31 (s, 6H, OC*H*$_3$) 4.28-4.39 (m, 4H, C*H*$_2$), 4.48 (dd, 2H, *J* = 10.8, 6.8 Hz, C*H*$_2$), 4.53 (dd, 2H, *J* = 10.8, 6.4 Hz, C*H*$_2$). **2c** (minor isomer): $^1$H NMR (400 MHz, $CDCl_3$) δ 1.13 (s, 6H, OC*H*$_3$), δ 1.32 (s, 6H, OC*H*$_3$) 4.35-4.55 (m, 8H, C*H*$_2$).

**Synthesis of 2a in toluene:** A mixture of $C_{60}$ (36.0 mg, 0.05 mmol), **1a** (9.2 μL, 0.10 mmol), and $Mn(OAc)_3{\cdot}2H_2O$ (26.8 mg, 0.10 mmol) was dissolved in toluene (30 mL) and refluxed under argon atmosphere for 3 h. The reaction mixture was poured onto a silica gel column, and eluted with $CS_2$ to afford recovered $C_{60}$ (29.4 mg, 82%), then with $CS_2$/AcOEt (10:1) to give dimer **2a** (6.1 mg, 15%).

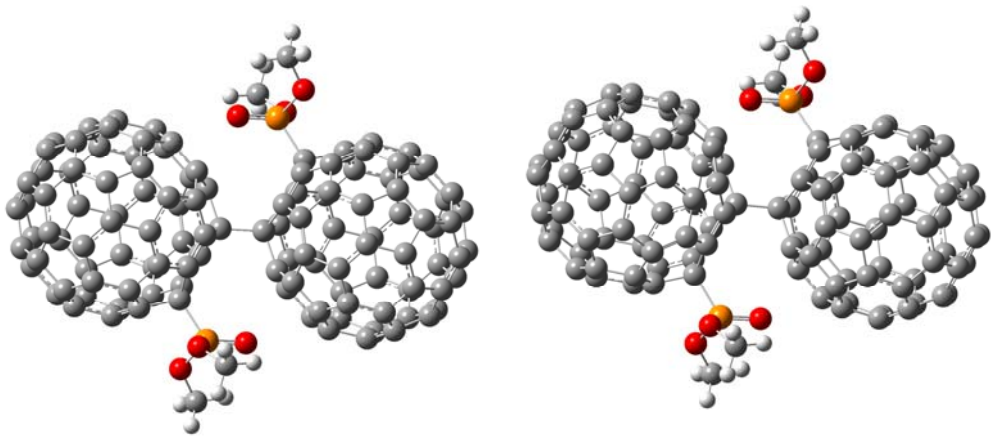
**Heating of 2a in chlorobenzene: 2a** (10.6 mg) was dissolved in chlorobenzene (3 mL) and refluxed under argon atmosphere for 12 h. The reaction mixture was poured onto a silica gel column, and eluted with $CS_2$ to afford $C_{60}$ (3.2 mg, 35%), then with $CS_2$/AcOEt (10:1) to give recovered dimer **2a** (6.1 mg, 58%).

**Crystal structure and refinement details for the minor isomer of 2a:** The single crystals of the minor isomer of **2a** was grown in $CS_2/CHCl_3$ at about –5 $^o$C. The single crystal was coated with silicone oil and mounted in the 100 K dinitrogen stream of a Bruker SMART APEX CCD diffractometer equipped with low-temperature apparatus and intensity data were collected using graphite-monochromated Mo Kα radiation. The data integration and reduction were processed with the SAINT software. An empirical absorption correction (SADABS) was applied. Structures were solved by the direct method using SHELXS-97 and refined on $F^2$ by a full-matrix least-squares technique using the SHELXL-97 program package. The independent moiety is the monomer unit of the dimer. The monomer unit has disorder as to the position of $C_{60}$ cage. The major part was refined anisotropically and the minor part was refined isotropically. Crystal structure refinement parameters are given in Table S1. CCDC contains the supplementary crystallographic data for this paper with a deposition number of CCDC 802193 for the minor isomer of **2a**. Copies of this information can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK. [Fax: +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk].

Table S1. Crystal data and structure refinement for the minor isomer of **2a**.

| | | |
|---|---|---|
| Empirical formula | $C_{64}H_8Cl_6O_3P$ | |
| Formula weight | 1068.37 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P-1 | |
| Unit cell dimensions | a = 9.9401(10) Å | α = 100.529(2)$^o$ |
| | b = 13.7583(15) Å | β = 96.973(2)$^o$ |
| | c = 14.9042(16) Å | γ = 102.216(2)$^o$ |

| | |
|---|---|
| Volume | 1931.2(4) $Å^3$ |
| Z | 2 |
| Density (calculated) | 1.837 $Mg/m^3$ |
| Absorption coefficient | 0.551 $mm^{-1}$ |
| F(000) | 1066 |
| Crystal size | 0.28 x 0.24 x 0.20 $mm^3$ |
| Theta range for data collection | 1.86 to 26.00°. |
| Index ranges | -12<=h<=11, -16<=k<=16, -18<=l<=12 |
| Reflections collected | 10469 |
| Independent reflections | 7352 [R(int) = 0.0180] |
| Completeness to theta = 26.00° | 96.8 % |
| Absorption correction | Empirical (SADABS) |
| Max. and min. transmission | 0.8979 and 0.8611 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7352 / 6 / 922 |
| Goodness-of-fit on $F^2$ | 1.090 |
| Final R indices [I>2sigma(I)] | R1 = 0.0690, wR2 = 0.1686 |
| R indices (all data) | R1 = 0.0848, wR2 = 0.1786 |
| Largest diff. peak and hole | 1.326 and -1.143 $e.Å^{-3}$ |



Optimized structures of meso and racemic isomers of **2a**

Table S2. Cartesian coordinates and energies of meso and racemic isomers of **2a** at the B3LYP/6-31G*//B3LYP/3-21G* level

*meso*-**2a**
-B3LYP/6-31G*//B3LYP/3-21G*-

| | | | |
|---|---|---|---|
| C | 1.869941 | 2.158766 | -0.904595 |
| C | 2.221766 | 1.487305 | -2.178141 |
| C | 2.008647 | 0.134476 | -2.320996 |
| C | 1.442763 | -0.660218 | -1.205391 |
| C | 0.796849 | 0.001086 | 0.002668 |
| C | 1.333871 | 1.441918 | 0.137906 |
| C | 2.879944 | 3.166628 | -0.649763 |
| C | 3.849958 | 3.129267 | -1.736875 |
| C | 3.437783 | 2.099334 | -2.685540 |
| C | 4.399885 | 1.319509 | -3.326801 |
| C | 3.006859 | -0.684425 | -2.986775 |
| C | 2.065784 | -1.878965 | -1.183592 |
| C | 2.189094 | -2.759345 | 0.040578 |
| C | 1.992319 | -1.883919 | 1.303697 |
| C | 1.393590 | -0.648632 | 1.275998 |
| C | 1.842282 | 0.392286 | 2.171601 |
| C | 1.785626 | 1.675701 | 1.479856 |
| C | 2.739752 | 2.659993 | 1.748308 |
| C | 3.301684 | 3.426855 | 0.654158 |
| C | 5.198570 | 3.342487 | -1.478915 |
| C | 5.644989 | 3.593159 | -0.111550 |
| C | 4.719278 | 3.630806 | 0.925687 |
| C | 5.031019 | 2.994054 | 2.204060 |
| C | 3.805620 | 2.389670 | 2.708787 |
| C | 3.854546 | 1.170099 | 3.374537 |
| C | 2.843451 | 0.150885 | 3.110576 |
| C | 3.487635 | -1.144001 | 3.132791 |
| C | 3.087585 | -2.119459 | 2.219912 |
| C | 3.053852 | -1.950982 | -2.281233 |
| C | 6.416730 | -2.810649 | 0.767949 |
| C | 5.974735 | -3.030756 | -0.537077 |
| C | 6.547101 | -2.271087 | -1.643568 |
| C | 7.520827 | -1.312179 | -1.394635 |
| C | 7.970386 | -1.065596 | -0.026141 |
| C | 7.091617 | -1.129247 | 2.281732 |
| C | 5.864557 | -1.729880 | 2.786809 |
| C | 5.449916 | -2.764257 | 1.844938 |
| C | 4.092548 | -2.946087 | 1.564088 |

| | | | |
|---|---|---|---|
| C | 3.662047 | -3.205372 | 0.223126 |
| C | 4.569214 | -3.246358 | -0.807565 |
| C | 5.486638 | -2.007773 | -2.611918 |
| C | 5.450210 | -0.787569 | -3.287031 |
| C | 6.467488 | 0.223830 | -3.016510 |
| C | 7.475877 | -0.031243 | -2.094608 |
| C | 7.889410 | 1.006298 | -1.154022 |
| C | 8.194013 | 0.367537 | 0.120475 |
| C | 7.871348 | 1.005262 | 1.316032 |
| C | 7.305916 | 0.238716 | 2.421323 |
| C | 4.906840 | -0.939221 | 3.411574 |
| C | 5.132487 | 0.493797 | 3.563172 |
| C | 6.304512 | 1.069787 | 3.079816 |
| C | 6.251288 | 2.349585 | 2.381844 |
| C | 7.220428 | 2.309166 | 1.292046 |
| C | 6.923142 | 2.916228 | 0.074149 |
| C | 7.268566 | 2.250997 | -1.176570 |
| C | 6.204439 | 2.516349 | -2.140472 |
| C | 5.815765 | 1.531713 | -3.040795 |
| C | 4.258697 | -2.597515 | -2.105042 |
| C | 4.178103 | -0.109486 | -3.481123 |
| C | 7.432404 | -1.796834 | 1.026771 |
| P | 1.156299 | -4.275247 | -0.077512 |
| O | -0.295232 | -4.184012 | -0.398068 |
| O | 2.014176 | -5.045274 | -1.193560 |
| O | 1.497991 | -4.931804 | 1.342793 |
| C | 0.515569 | -5.776993 | 2.065974 |
| H | 0.622298 | -5.539228 | 3.124028 |
| H | -0.493879 | -5.549636 | 1.716588 |
| C | 1.366994 | -5.972406 | -2.154316 |
| H | 0.302089 | -5.741612 | -2.227281 |
| H | 1.863643 | -5.821961 | -3.112477 |
| C | -0.796849 | -0.001086 | -0.002668 |
| C | -1.393590 | 0.648632 | -1.275998 |
| C | -1.442763 | 0.660218 | 1.205391 |
| C | -1.333871 | -1.441918 | -0.137906 |
| C | -1.992319 | 1.883919 | -1.303697 |
| C | -1.842282 | -0.392286 | -2.171601 |
| C | -2.065784 | 1.878965 | 1.183592 |
| C | -2.008647 | -0.134476 | 2.320996 |
| C | -1.785626 | -1.675701 | -1.479856 |
| C | -1.869941 | -2.158766 | 0.904595 |
| C | -2.189094 | 2.759345 | -0.040578 |
| C | -3.087585 | 2.119459 | -2.219912 |

| | | | |
|---|---|---|---|
| C | -2.843451 | -0.150885 | -3.110576 |
| C | -3.053852 | 1.950982 | 2.281233 |
| C | -3.006859 | 0.684425 | 2.986775 |
| C | -2.739752 | -2.659993 | -1.748308 |
| C | -2.879944 | -3.166628 | 0.649763 |
| C | -3.662047 | 3.205372 | -0.223126 |
| C | -4.092548 | 2.946087 | -1.564088 |
| C | -3.487635 | 1.144001 | -3.132791 |
| C | -3.854546 | -1.170099 | -3.374537 |
| C | -4.258697 | 2.597515 | 2.105042 |
| C | -4.178103 | 0.109486 | 3.481123 |
| C | -3.437783 | -2.099334 | 2.685540 |
| C | -3.301684 | -3.426855 | -0.654158 |
| C | -3.805620 | -2.389670 | -2.708787 |
| C | -3.849958 | -3.129267 | 1.736875 |
| C | -4.569214 | 3.246358 | 0.807565 |
| C | -5.449916 | 2.764257 | -1.844938 |
| C | -4.906840 | 0.939221 | -3.411574 |
| C | -5.132487 | -0.493797 | -3.563172 |
| C | -5.486638 | 2.007773 | 2.611918 |
| C | -4.399885 | -1.319509 | 3.326801 |
| C | -5.450210 | 0.787569 | 3.287031 |
| C | -4.719278 | -3.630806 | -0.925687 |
| C | -5.031019 | -2.994054 | -2.204060 |
| C | -5.198570 | -3.342487 | 1.478915 |
| C | -5.974735 | 3.030756 | 0.537077 |
| C | -6.416730 | 2.810649 | -0.767949 |
| C | -5.864557 | 1.729880 | -2.786809 |
| C | -6.304512 | -1.069787 | -3.079816 |
| C | -6.547101 | 2.271087 | 1.643568 |
| C | -5.815765 | -1.531713 | 3.040795 |
| C | -6.467488 | -0.223830 | 3.016510 |
| C | -5.644989 | -3.593159 | 0.111550 |
| C | -6.251288 | -2.349585 | -2.381844 |
| C | -6.204439 | -2.516349 | 2.140472 |
| C | -7.432404 | 1.796834 | -1.026771 |
| C | -7.091617 | 1.129247 | -2.281732 |
| C | -7.305916 | -0.238716 | -2.421323 |
| C | -7.520827 | 1.312179 | 1.394635 |
| C | -7.475877 | 0.031243 | 2.094608 |
| C | -6.923142 | -2.916228 | -0.074149 |
| C | -7.220428 | -2.309166 | -1.292046 |
| C | -7.268566 | -2.250997 | 1.176570 |
| C | -7.970386 | 1.065596 | 0.026141 |

| | | | |
|---|---|---|---|
| C | -7.871348 | -1.005262 | -1.316032 |
| C | -7.889410 | -1.006298 | 1.154022 |
| C | -8.194013 | -0.367537 | -0.120475 |
| C | -2.221766 | -1.487305 | 2.178141 |
| P | -1.156299 | 4.275247 | 0.077512 |
| O | 0.295232 | 4.184012 | 0.398068 |
| O | -2.014176 | 5.045274 | 1.193560 |
| O | -1.497991 | 4.931804 | -1.342793 |
| C | -1.366994 | 5.972406 | 2.154316 |
| H | -0.302089 | 5.741612 | 2.227281 |
| H | -1.863643 | 5.821961 | 3.112477 |
| C | -0.515569 | 5.776993 | -2.065974 |
| H | 0.493879 | 5.549636 | -1.716588 |
| H | -0.622298 | 5.539228 | -3.124028 |
| H | -1.513176 | 6.999489 | 1.811664 |
| H | -0.752315 | 6.829007 | -1.890795 |
| H | 0.752315 | -6.829007 | 1.890795 |
| H | 1.513176 | -6.999489 | -1.811664 |

-B3LYP/6-31G*// B3LYP/3-21G*-
E(RB+HF-LYP) = -5866.11319277 a.u.

*racemic*-**2a**
-B3LYP/6-31G*//B3LYP/3-21G*-

| | | | |
|---|---|---|---|
| C | 1.837220 | -2.072598 | 1.088526 |
| C | 2.146498 | -1.293149 | 2.311742 |
| C | 1.931403 | 0.067180 | 2.333119 |
| C | 1.408469 | 0.763465 | 1.137451 |
| C | 0.797459 | 0.001067 | -0.023899 |
| C | 1.340163 | -1.443696 | -0.028061 |
| C | 2.857243 | -3.092838 | 0.952923 |
| C | 3.789560 | -2.960887 | 2.066978 |
| C | 3.344254 | -1.855951 | 2.910712 |
| C | 4.282967 | -1.020680 | 3.516631 |
| C | 2.902001 | 0.943798 | 2.963469 |
| C | 2.018216 | 1.984651 | 1.036055 |
| C | 2.186145 | 2.753512 | -0.257337 |
| C | 2.038098 | 1.771207 | -1.443637 |
| C | 1.428596 | 0.546093 | -1.334127 |
| C | 1.914824 | -0.563894 | -2.122745 |
| C | 1.838000 | -1.784146 | -1.329878 |
| C | 2.801790 | -2.784276 | -1.482604 |
| C | 3.324357 | -3.456812 | -0.310356 |
| C | 5.146669 | -3.188074 | 1.872955 |
| C | 5.640017 | -3.548674 | 0.546871 |

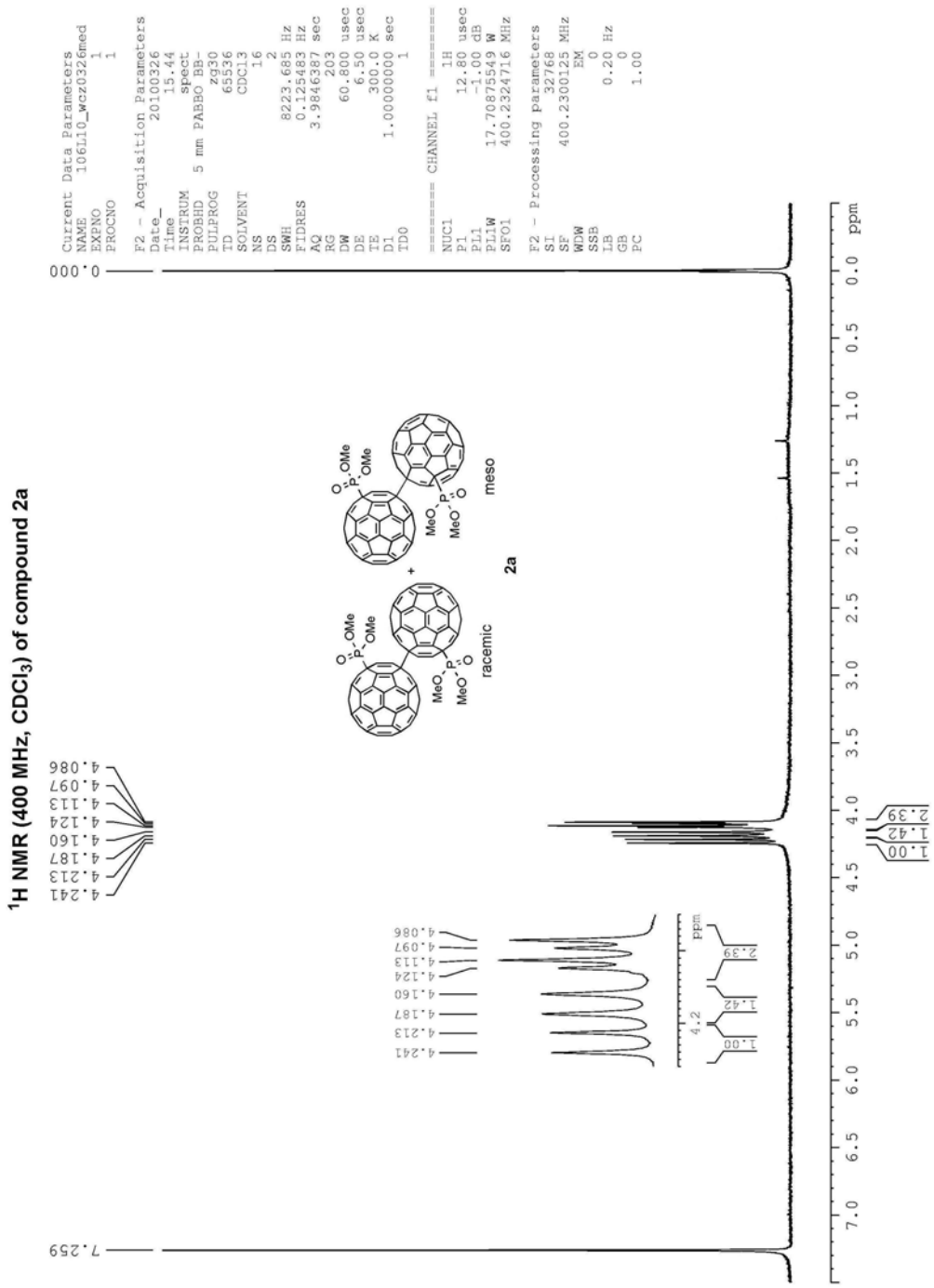
| | | | |
|---|---|---|---|
| C | 4.751055 | -3.677647 | -0.514718 |
| C | 5.106740 | -3.148719 | -1.830463 |
| C | 3.899381 | -2.591506 | -2.424777 |
| C | 3.969588 | -1.431081 | -3.186722 |
| C | 2.948233 | -0.398063 | -3.043971 |
| C | 3.592995 | 0.892066 | -3.154141 |
| C | 3.161401 | 1.938298 | -2.339993 |
| C | 2.970010 | 2.149657 | 2.157991 |
| C | 6.436075 | 2.761410 | -0.836320 |
| C | 5.949890 | 3.088867 | 0.429704 |
| C | 6.483308 | 2.425991 | 1.614617 |
| C | 7.465858 | 1.452701 | 1.479992 |
| C | 7.961689 | 1.094220 | 0.153386 |
| C | 7.164518 | 0.962251 | -2.180433 |
| C | 5.955483 | 1.514053 | -2.776555 |
| C | 5.507416 | 2.622143 | -1.939258 |
| C | 4.141678 | 2.820685 | -1.720266 |
| C | 3.664257 | 3.188490 | -0.420386 |
| C | 4.534352 | 3.320833 | 0.633528 |
| C | 5.390414 | 2.240233 | 2.565150 |
| C | 5.332461 | 1.079743 | 3.336999 |
| C | 6.359542 | 0.053480 | 3.187218 |
| C | 7.398507 | 0.234754 | 2.282075 |
| C | 7.844755 | -0.876494 | 1.446538 |
| C | 8.193002 | -0.344956 | 0.134415 |
| C | 7.912081 | -1.081396 | -1.014125 |
| C | 7.384567 | -0.411762 | -2.198001 |
| C | 5.021122 | 0.670483 | -3.366798 |
| C | 5.252638 | -0.769075 | -3.389420 |
| C | 6.407811 | -1.298620 | -2.819610 |
| C | 6.331663 | -2.516260 | -2.019379 |
| C | 7.262216 | -2.381011 | -0.904041 |
| C | 6.922852 | -2.884864 | 0.349356 |
| C | 7.224632 | -2.117004 | 1.551696 |
| C | 6.128381 | -2.306106 | 2.498018 |
| C | 5.708048 | -1.250537 | 3.298329 |
| C | 4.180141 | 2.782607 | 1.970400 |
| C | 4.055547 | 0.415840 | 3.543930 |
| C | 7.460882 | 1.733711 | -0.974764 |
| P | 1.147475 | 4.263817 | -0.372476 |
| O | -0.338485 | 4.167620 | -0.396270 |
| O | 1.745917 | 5.043035 | 0.892970 |
| O | 1.782912 | 4.915774 | -1.691612 |
| C | 0.955335 | 5.687616 | -2.651608 |

| | | | |
|---|---|---|---|
| H | 1.282438 | 5.396809 | -3.649721 |
| H | -0.100031 | 5.448994 | -2.503264 |
| C | 0.912421 | 5.976557 | 1.690671 |
| H | 1.206099 | 5.840220 | 2.731054 |
| H | -0.144144 | 5.737662 | 1.550574 |
| C | -0.797465 | -0.001038 | -0.023898 |
| C | -1.340180 | 1.443721 | -0.028060 |
| C | -1.408469 | -0.763440 | 1.137452 |
| C | -1.428599 | -0.546069 | -1.334125 |
| C | -1.837243 | 2.072619 | 1.088527 |
| C | -1.838022 | 1.784166 | -1.329876 |
| C | -1.931408 | -0.067160 | 2.333121 |
| C | -2.018205 | -1.984631 | 1.036058 |
| C | -1.914837 | 0.563913 | -2.122743 |
| C | -2.038090 | -1.771189 | -1.443634 |
| C | -2.146515 | 1.293167 | 2.311743 |
| C | -2.857276 | 3.092849 | 0.952924 |
| C | -2.801821 | 2.784287 | -1.482602 |
| C | -2.901998 | -0.943787 | 2.963472 |
| C | -2.969996 | -2.149646 | 2.157994 |
| C | -2.948245 | 0.398072 | -3.043968 |
| C | -3.161392 | -1.938291 | -2.339989 |
| C | -3.344275 | 1.855959 | 2.910714 |
| C | -3.789591 | 2.960890 | 2.066980 |
| C | -3.324394 | 3.456819 | -0.310355 |
| C | -3.899412 | 2.591507 | -2.424775 |
| C | -4.055548 | -0.415838 | 3.543933 |
| C | -4.180121 | -2.782607 | 1.970404 |
| C | -3.664235 | -3.188488 | -0.420381 |
| C | -3.592995 | -0.892063 | -3.154138 |
| C | -3.969608 | 1.431081 | -3.186720 |
| C | -4.141659 | -2.820687 | -1.720261 |
| C | -4.282981 | 1.020679 | 3.516634 |
| C | -5.146702 | 3.188065 | 1.872958 |
| C | -4.751094 | 3.677640 | -0.514715 |
| C | -5.106775 | 3.148710 | -1.830460 |
| C | -5.332456 | -1.079753 | 3.337003 |
| C | -4.534328 | -3.320838 | 0.633533 |
| C | -5.390399 | -2.240244 | 2.565155 |
| C | -5.021124 | -0.670493 | -3.366794 |
| C | -5.252652 | 0.769063 | -3.389416 |
| C | -5.507400 | -2.622157 | -1.939253 |
| C | -5.708064 | 1.250523 | 3.298332 |
| C | -6.128407 | 2.306089 | 2.498021 |

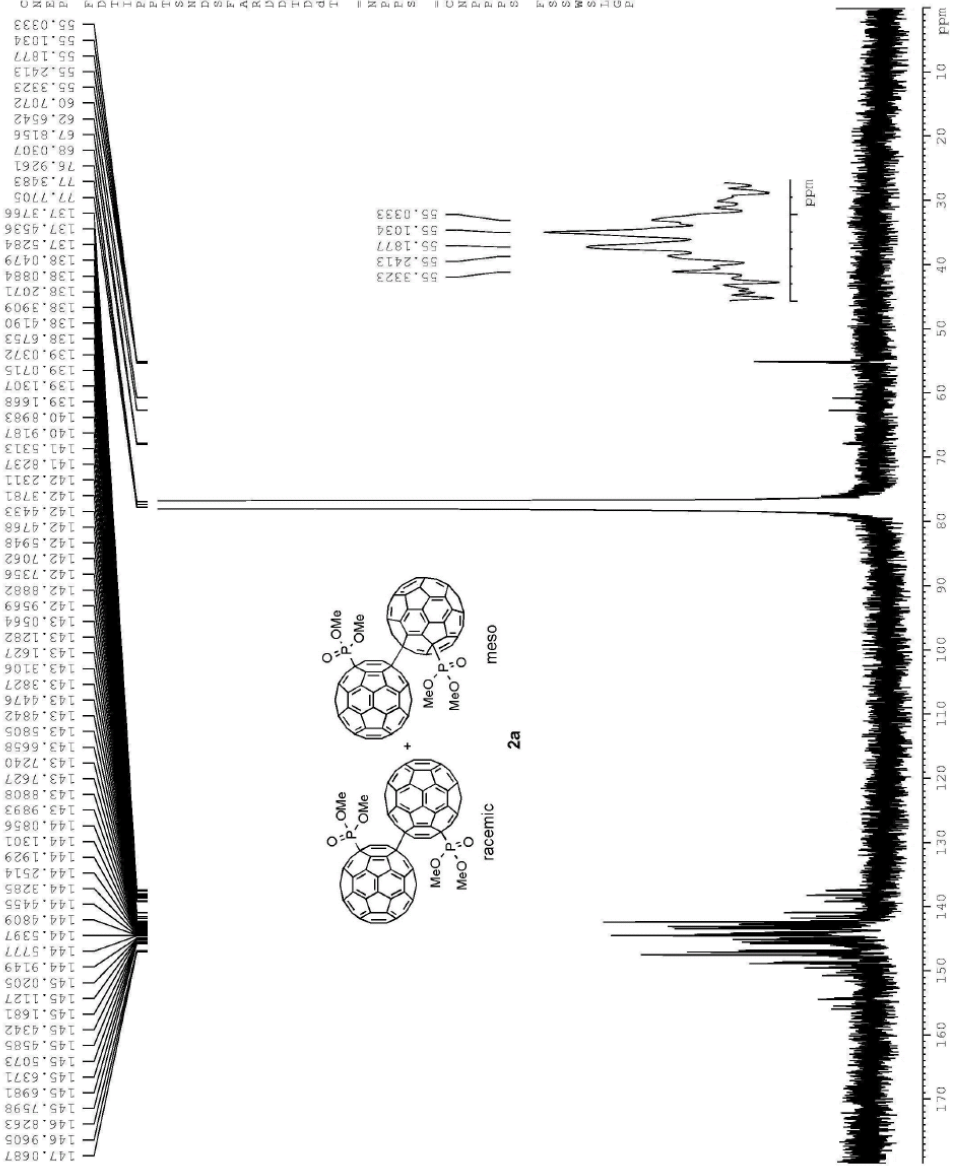
| | | | |
|---|---|---|---|
| C | -5.640055 | 3.548660 | 0.546873 |
| C | -6.331692 | 2.516239 | -2.019375 |
| C | -6.359547 | -0.053500 | 3.187222 |
| C | -5.949868 | -3.088884 | 0.429710 |
| C | -6.483292 | -2.426012 | 1.614622 |
| C | -5.955477 | -1.514071 | -2.776550 |
| C | -6.407830 | 1.298598 | -2.819606 |
| C | -6.436057 | -2.761431 | -0.836315 |
| C | -7.224656 | 2.116977 | 1.551700 |
| C | -6.922883 | 2.884838 | 0.349360 |
| C | -7.262244 | 2.380982 | -0.904037 |
| C | -7.398510 | -0.234783 | 2.282080 |
| C | -7.465851 | -1.452731 | 1.479998 |
| C | -7.164517 | -0.962279 | -2.180428 |
| C | -7.384578 | 0.411731 | -2.197996 |
| C | -7.460873 | -1.733742 | -0.974758 |
| C | -7.844768 | 0.876461 | 1.446542 |
| C | -7.912097 | 1.081361 | -1.014120 |
| C | -7.961686 | -1.094255 | 0.153391 |
| C | -8.193012 | 0.344919 | 0.134420 |
| C | -2.186127 | -2.753495 | -0.257334 |
| P | -1.147436 | -4.263786 | -0.372471 |
| O | 0.338523 | -4.167568 | -0.396262 |
| O | -1.782862 | -4.915751 | -1.691609 |
| O | -1.745870 | -5.043013 | 0.892974 |
| C | -0.955271 | -5.687582 | -2.651602 |
| H | 0.100091 | -5.448947 | -2.503255 |
| H | -1.282376 | -5.396779 | -3.649716 |
| C | -0.912363 | -5.976523 | 1.690676 |
| H | -1.206044 | -5.840190 | 2.731059 |
| H | 0.144199 | -5.737614 | 1.550581 |
| H | 1.132315 | 6.753811 | -2.493339 |
| H | 1.118114 | 7.001095 | 1.372076 |
| H | -1.132238 | -6.753780 | -2.493334 |
| H | -1.118042 | -7.001064 | 1.372082 |

-B3LYP/6-31G*// B3LYP/3-21G*-

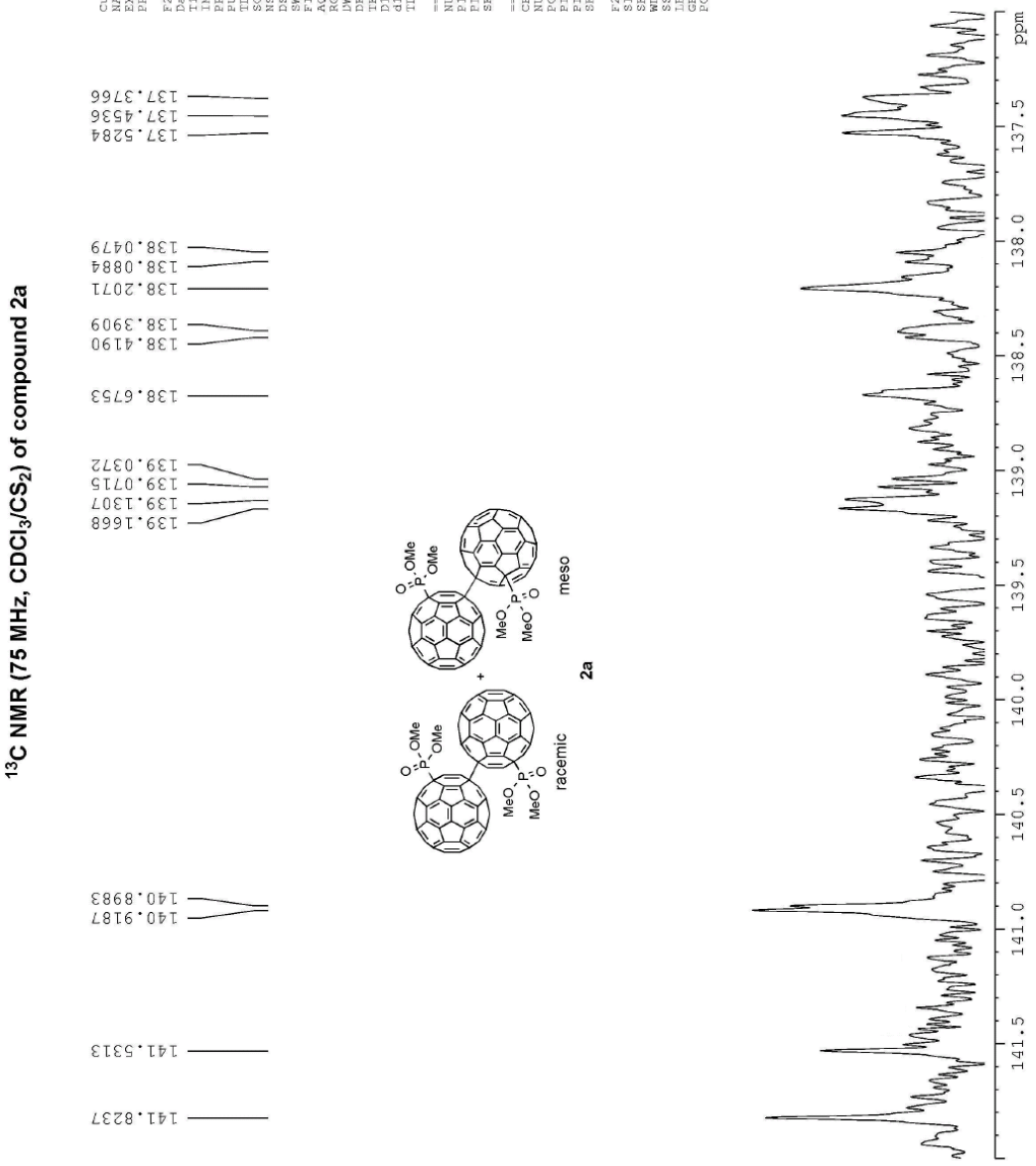
E(RB+HF-LYP) = -5866.11415505 hartree

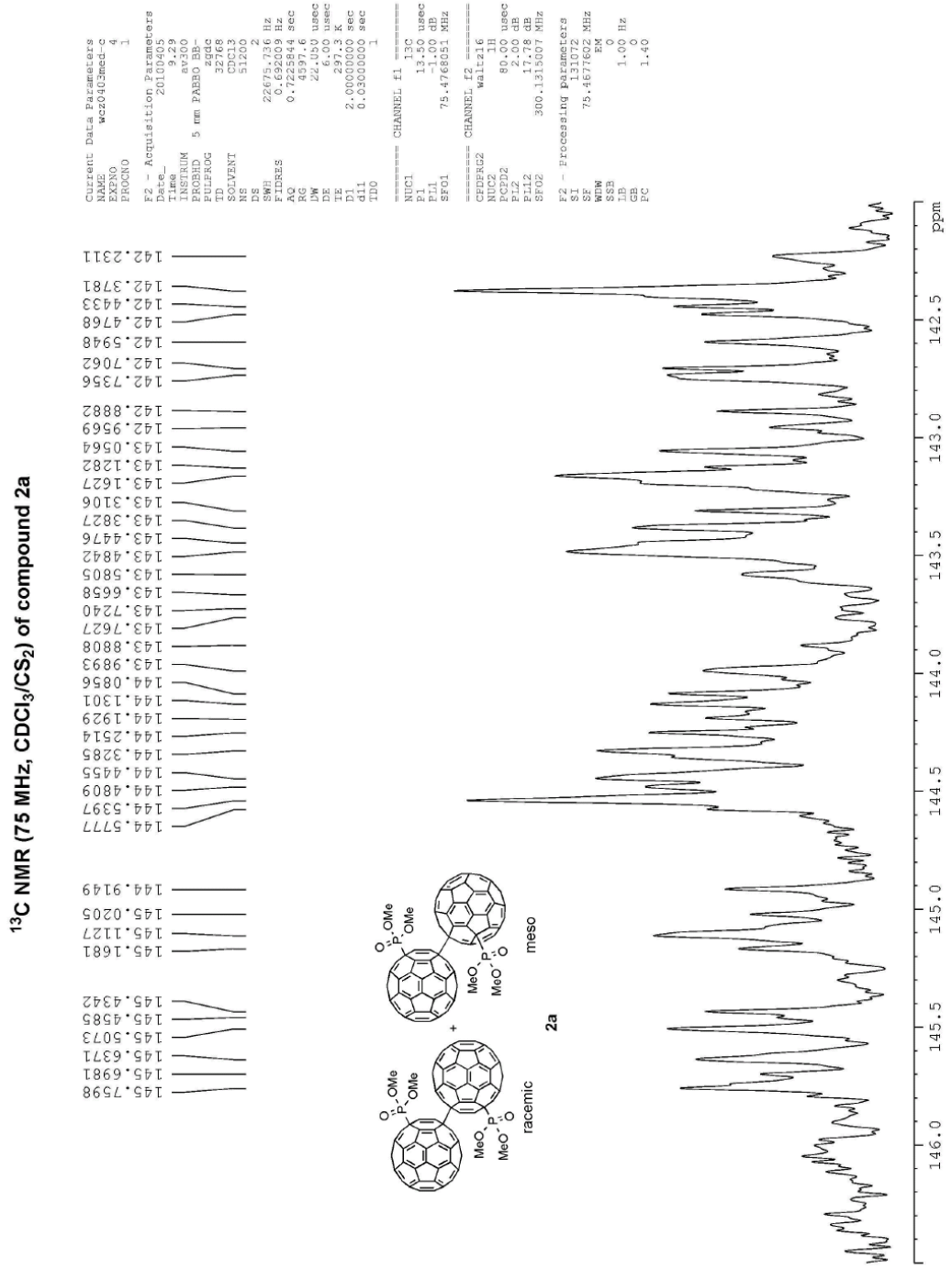

$^1$H NMR (400 MHz, $CDCl_3$) of compound 2a
Current Data Parameters
NAME 106L10_wcz0326med
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100326
Time 15.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 -1.00 dB
PL1W 17.70875549 W
SFO1 400.2324716 MHz
F2 - Processing parameters
SI 32768
SF 400.2300125 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
meso
racemic
2a
ppm

**$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2a**

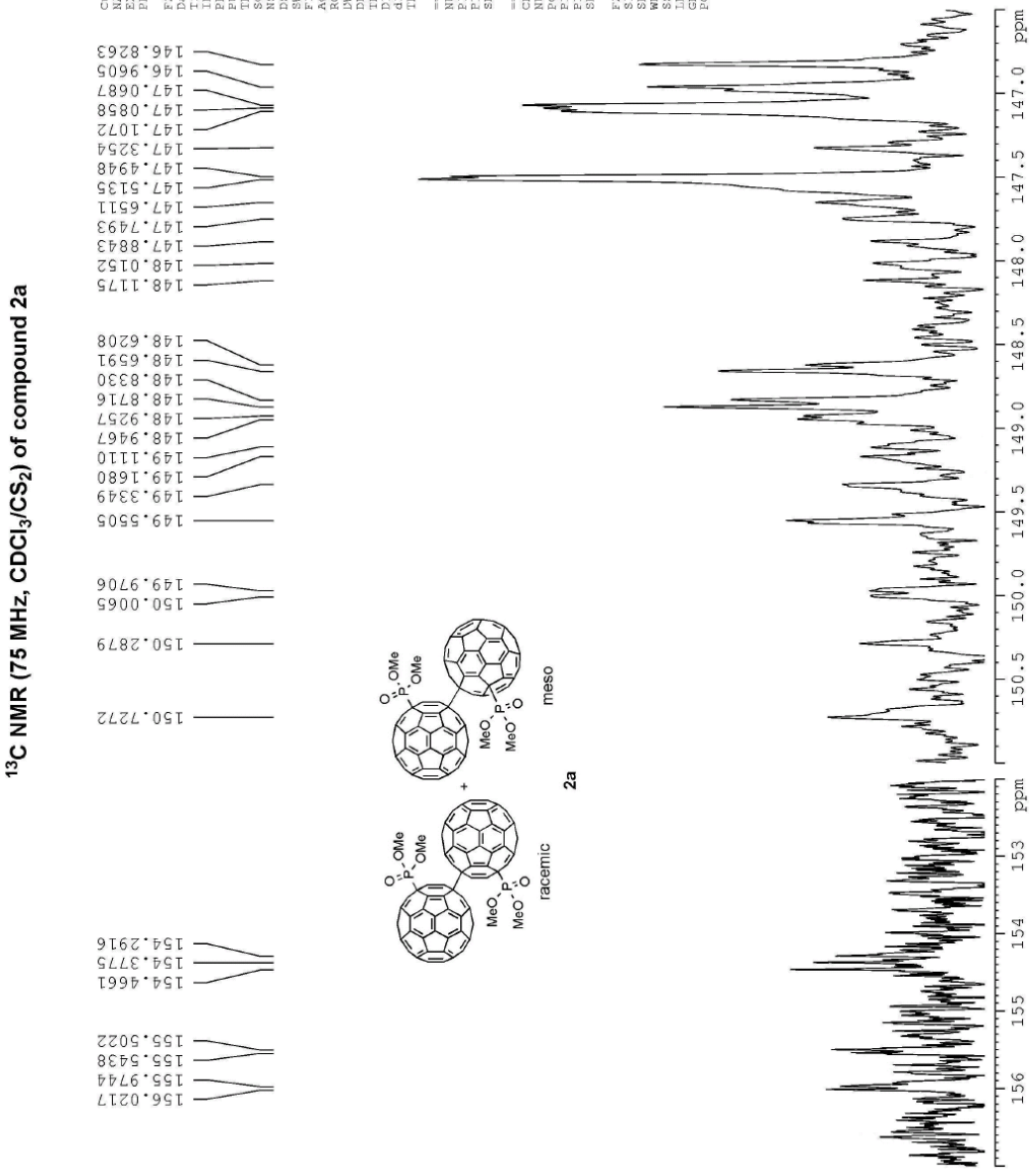


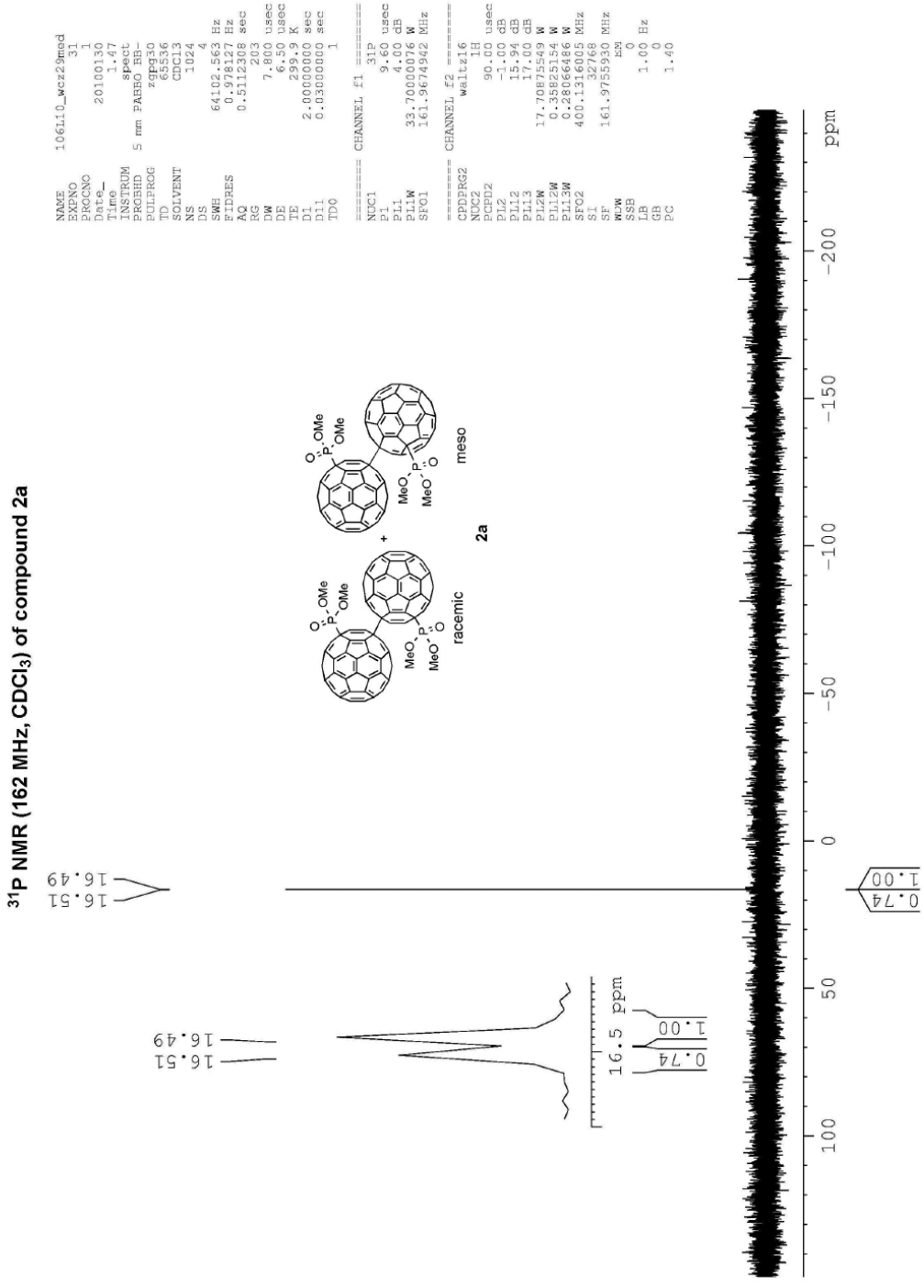
**$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2a**

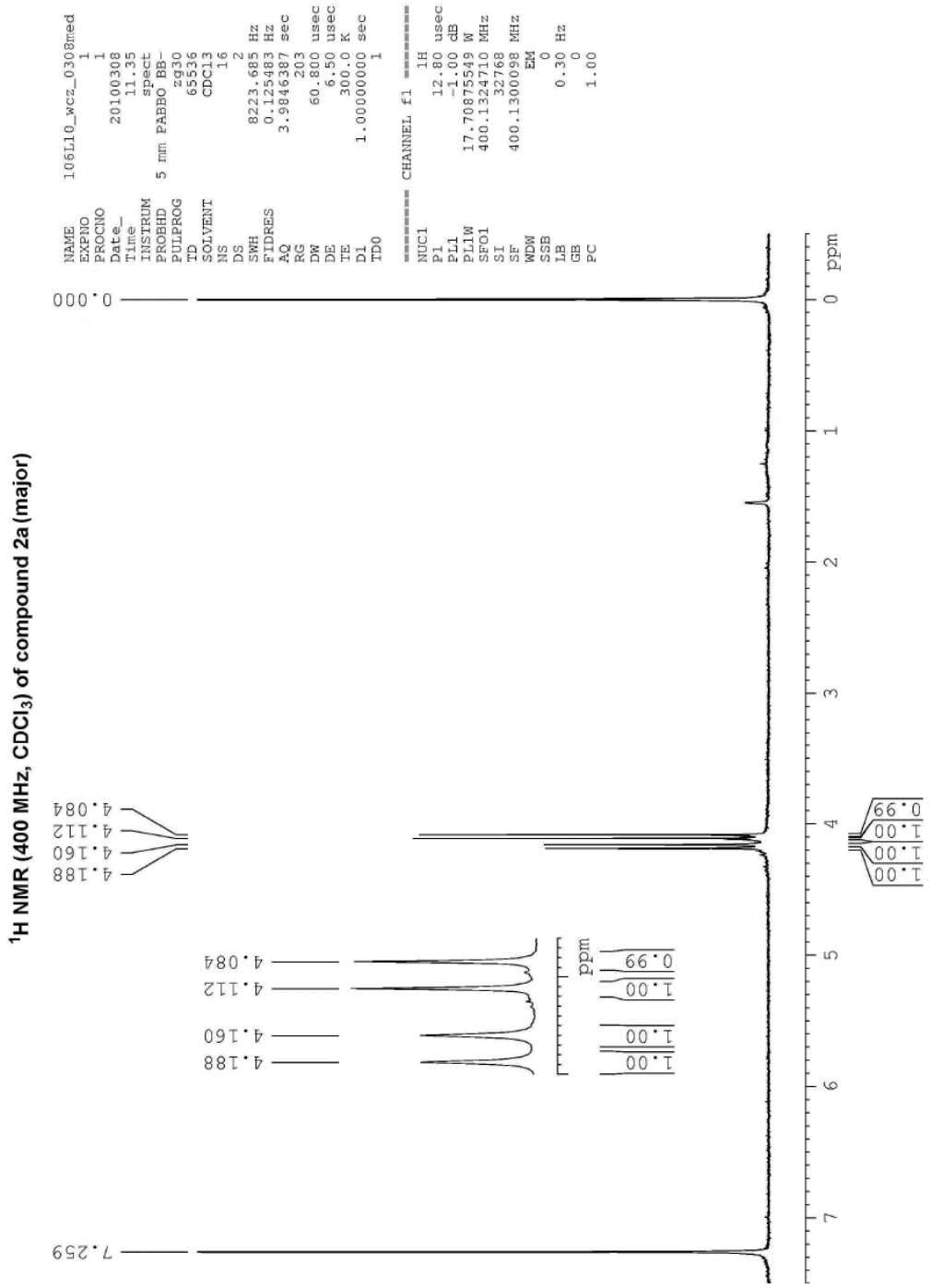



$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2a
Current Data Parameters
NAME wz20403med-c
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100405
Time 9.29
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 51200
DS 2
SWH 22675.736 Hz
FIDRES 0.692049 Hz
AQ 0.7225344 sec
RG 4591.6
DW 22.050 usec
DE 6.00 usec
TE 297.3 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.50 usec
PL1 1.00 dB
SFO1 75.4768051 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.78 dB
SFO2 300.1315007 MHz
F2 - Processing parameters
SI 131072
SF 75.4677622 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
142.2311
142.3781
142.4433
142.4768
142.5948
142.7062
142.7356
142.8882
142.9569
143.0564
143.1282
143.1627
143.3106
143.3827
143.4476
143.4842
143.5805
143.6658
143.7240
143.7627
143.8808
143.9893
144.0856
144.1301
144.1929
144.2514
144.3285
144.4455
144.4809
144.5397
144.5777
144.9149
145.0205
145.1127
145.1681
145.4342
145.4585
145.5073
145.6371
145.6981
145.7598
meso
racemic
2a
146.0
145.5
145.0
144.5
144.0
143.5
143.0
142.5
ppm

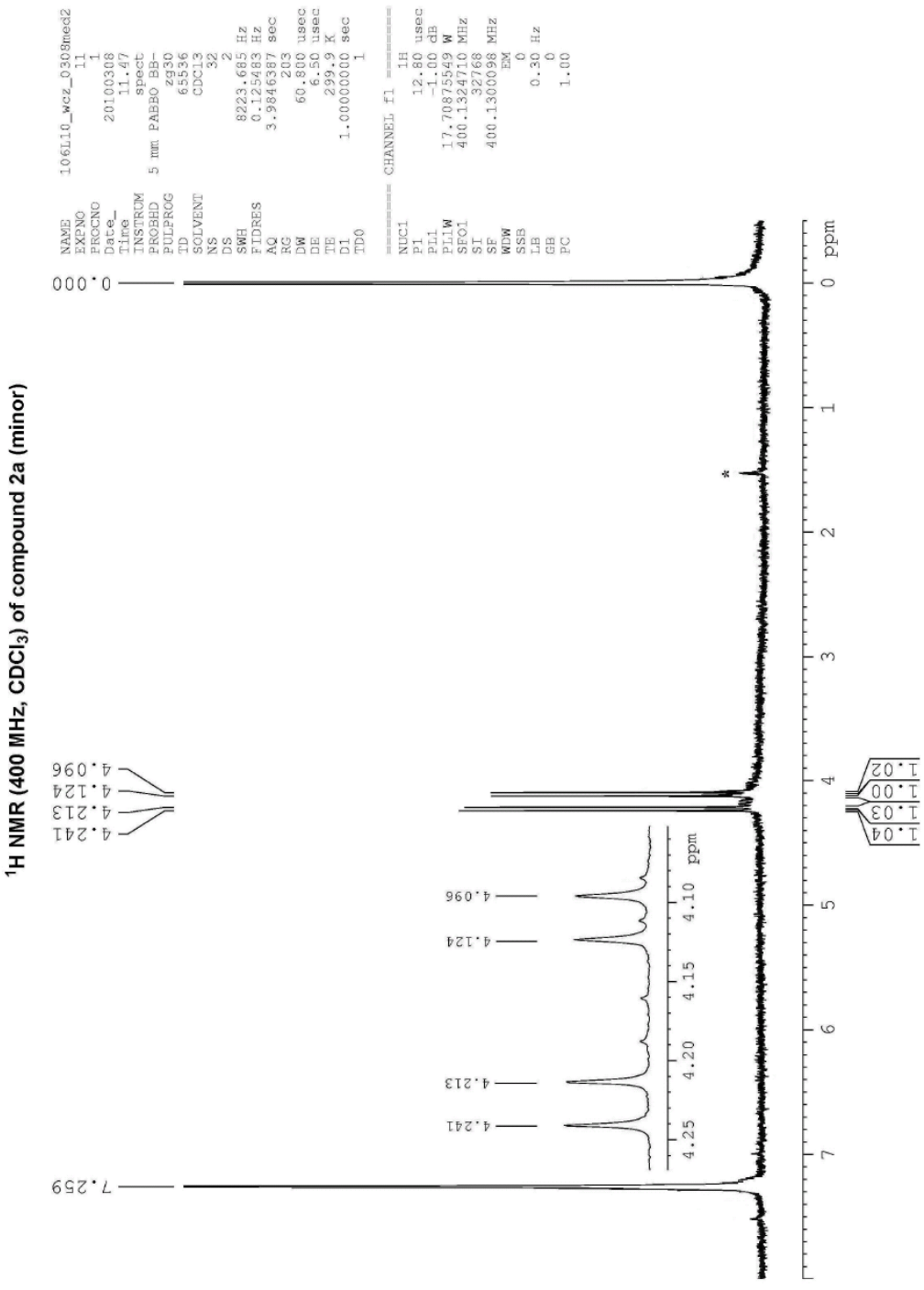
**$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2a**

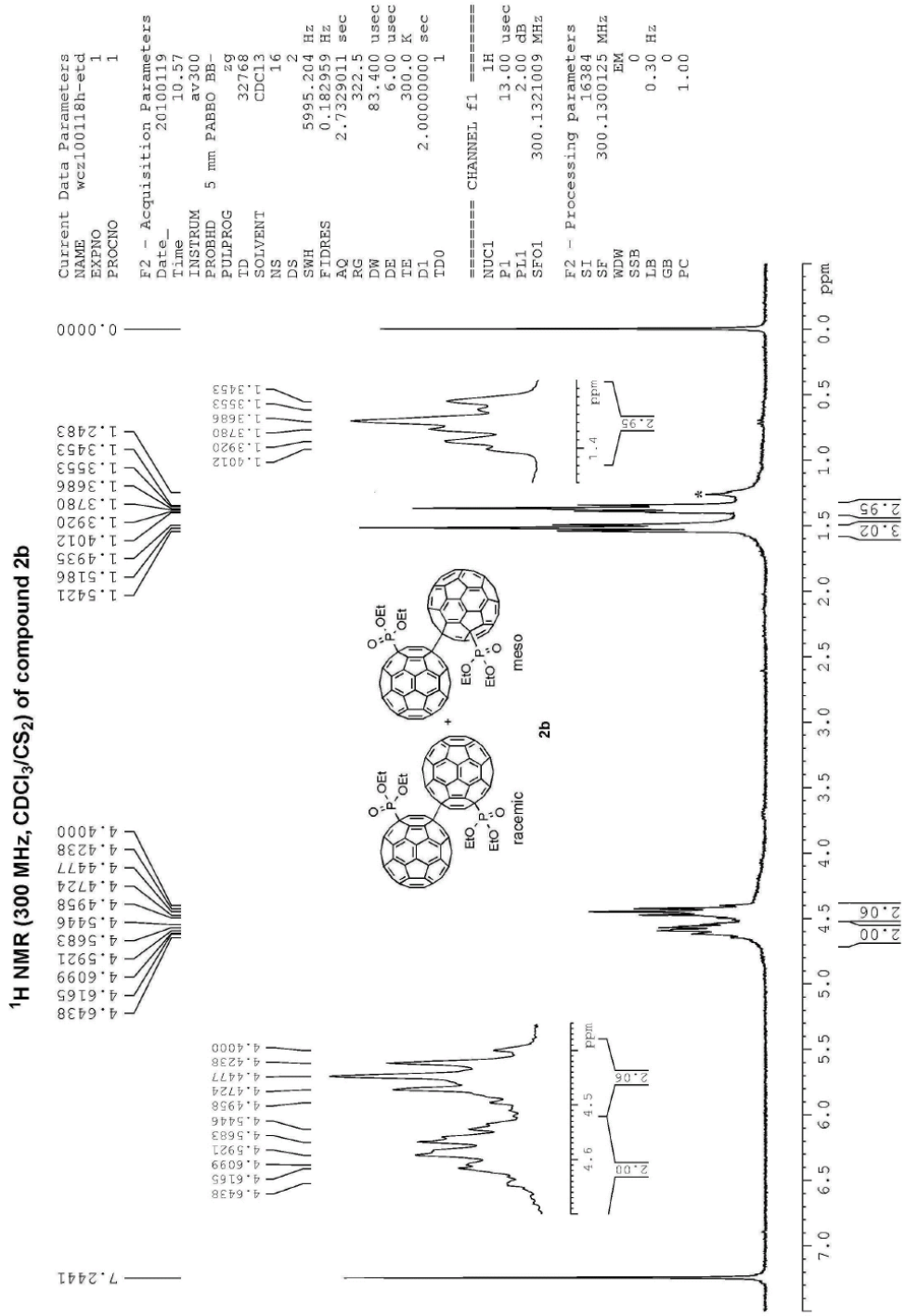



31P NMR (162 MHz, CDCl3) of compound 2a
16.51
16.49
16.51
16.49
16.5 ppm
0.74
1.00
0.74
1.00
ppm
racemic
meso
2a

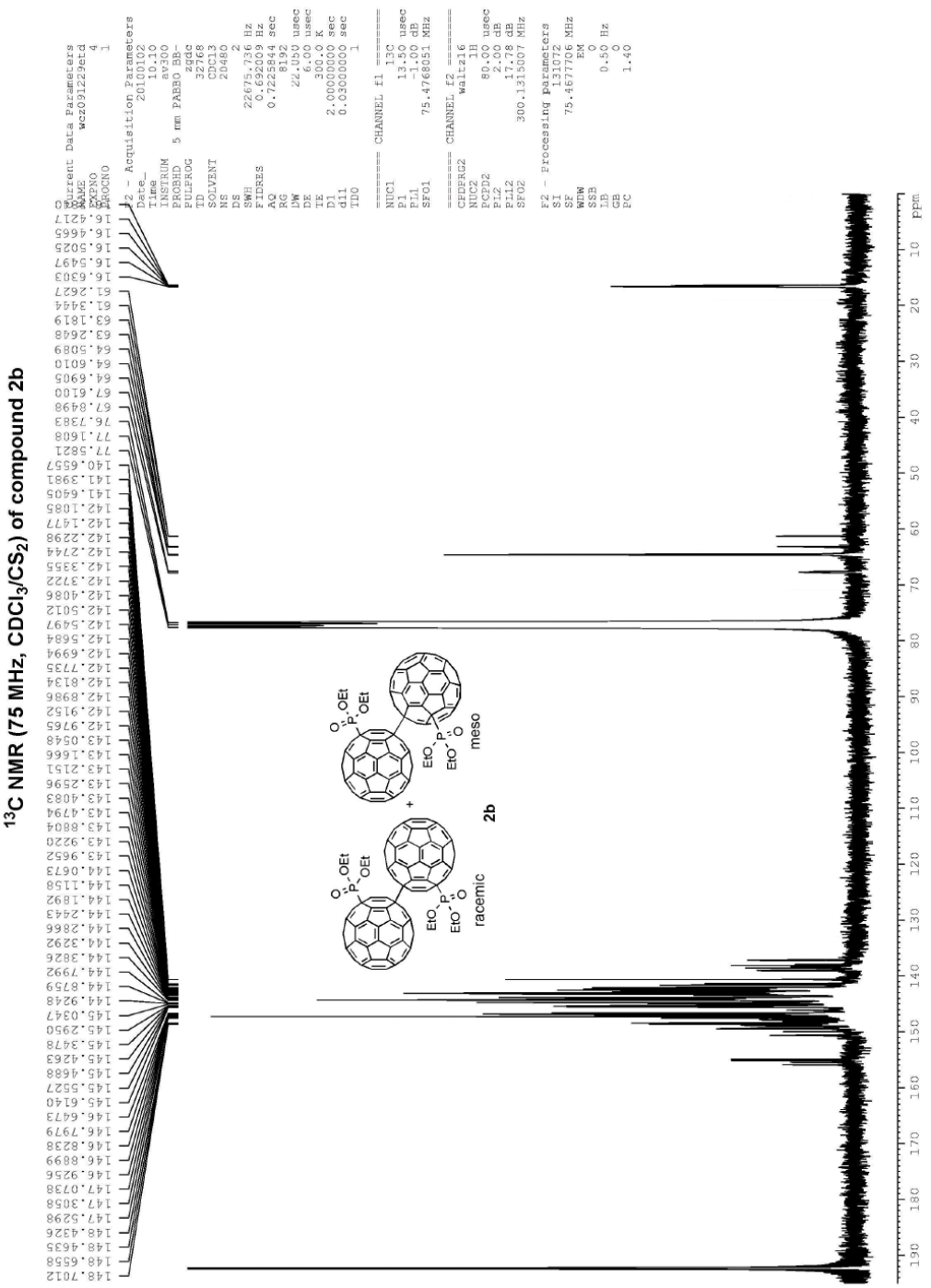



**$^1$H NMR (400 MHz, $CDCl_3$) of compound 2a (major)**

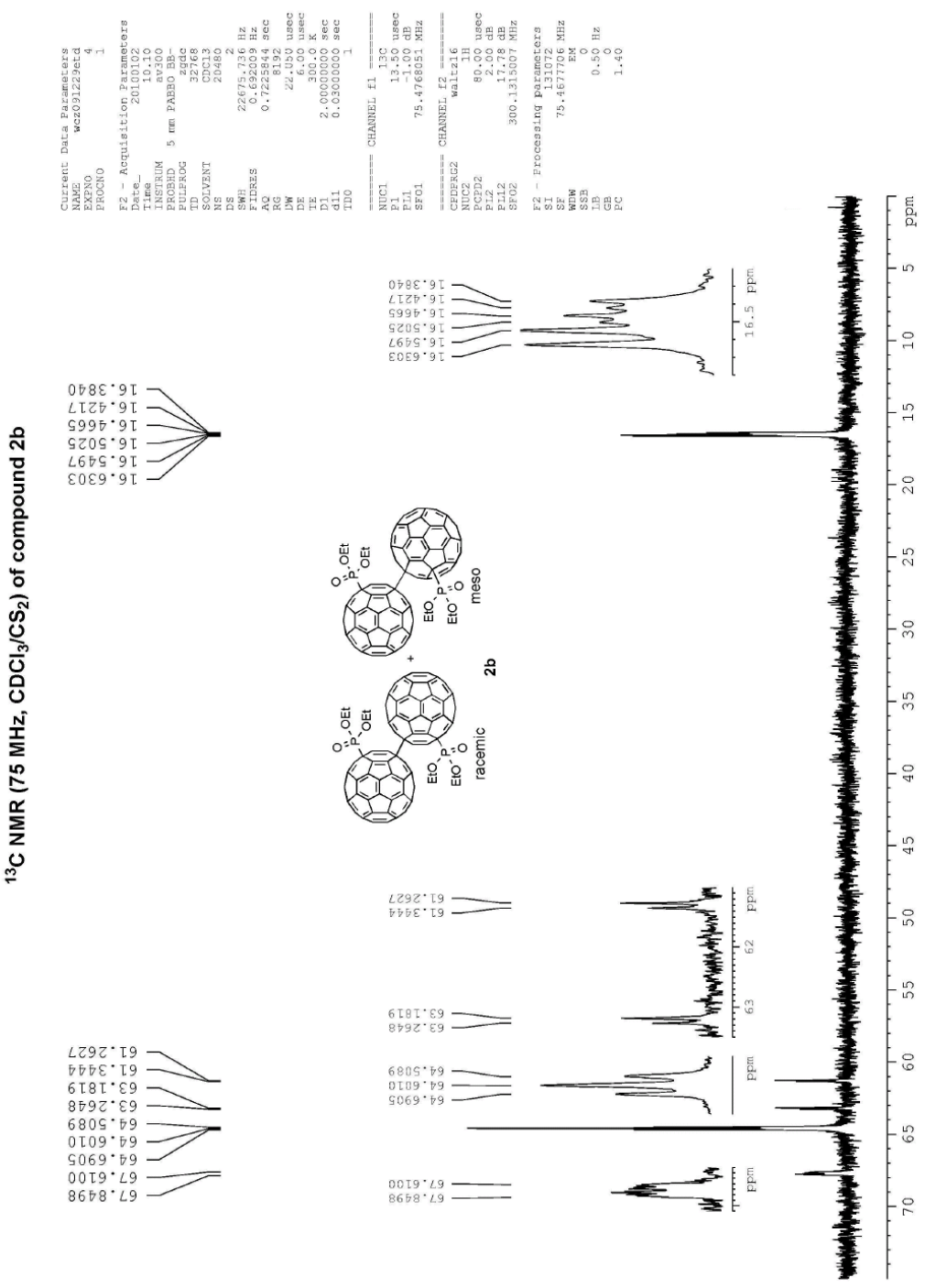

$^1$H NMR (400 MHz, $CDCl_3$) of compound 2a (minor)
NAME 106L10_wcz_0308med2
EXPNO 11
PROCNO 1
Date_ 20100308
Time 11.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 299.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 -1.00 dB
PL1W 17.70875549 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.259
4.241
4.213
4.124
4.096
1.04
1.03
1.00
1.02
*
ppm

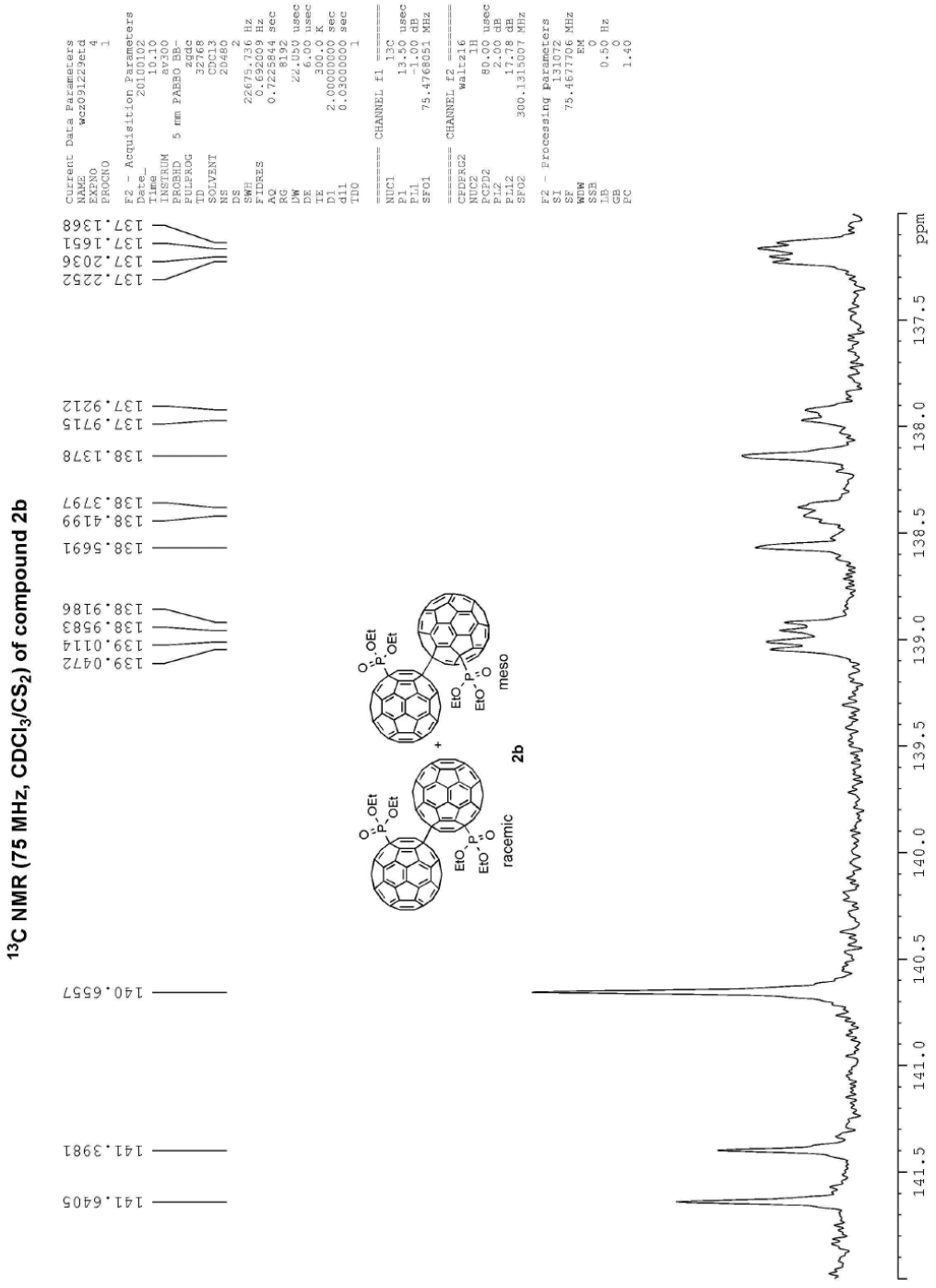

$^1$H NMR (300 MHz, $CDCl_3/CS_2$) of compound 2b
Current Data Parameters
NAME wcz100118h-etd
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100119
Time 10.57
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.73229011 sec
RG 322.5
DW 83.400 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 2.00 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 16384
SF 300.1300125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
meso
racemic
2b
ppm

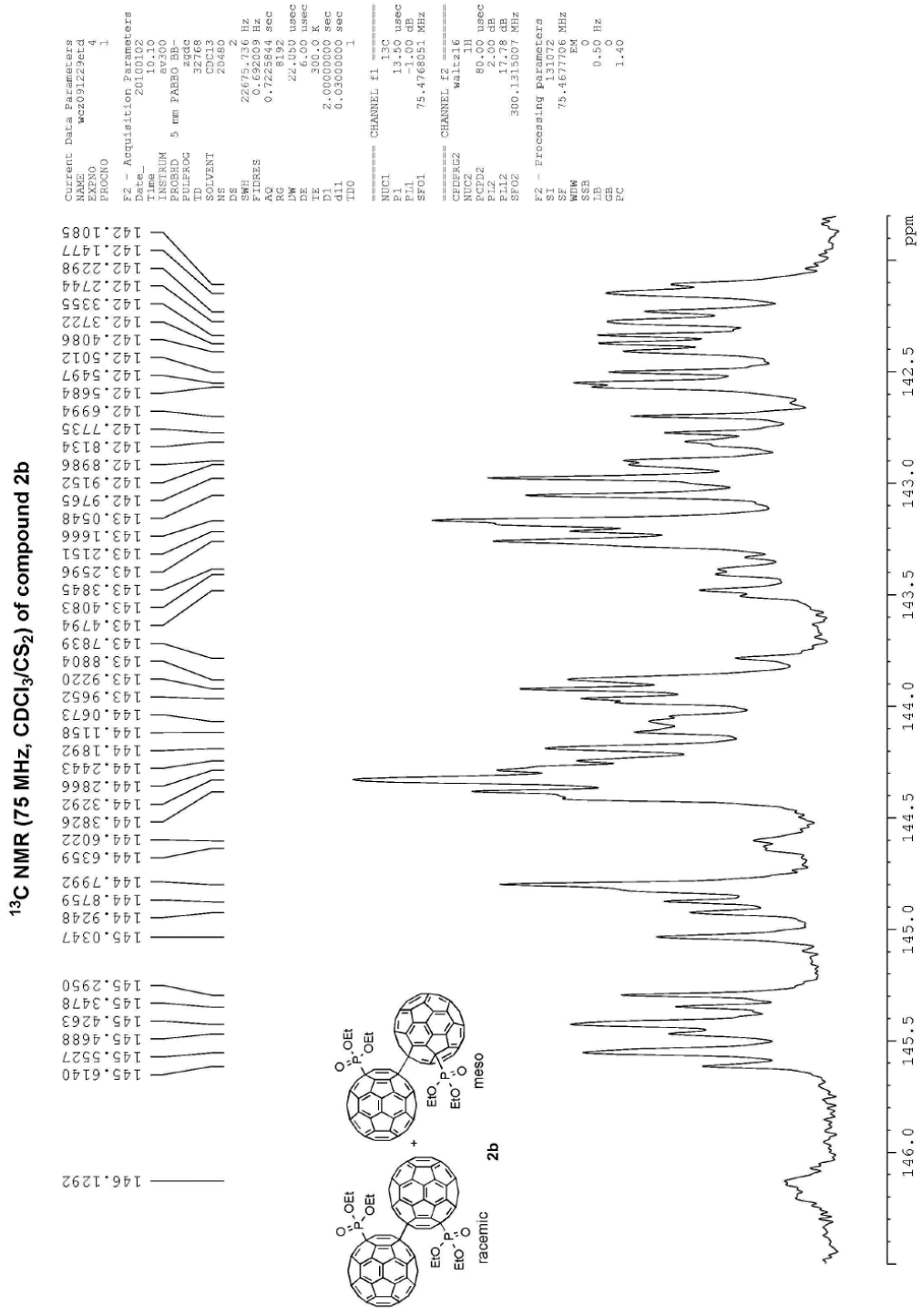
**$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2b**

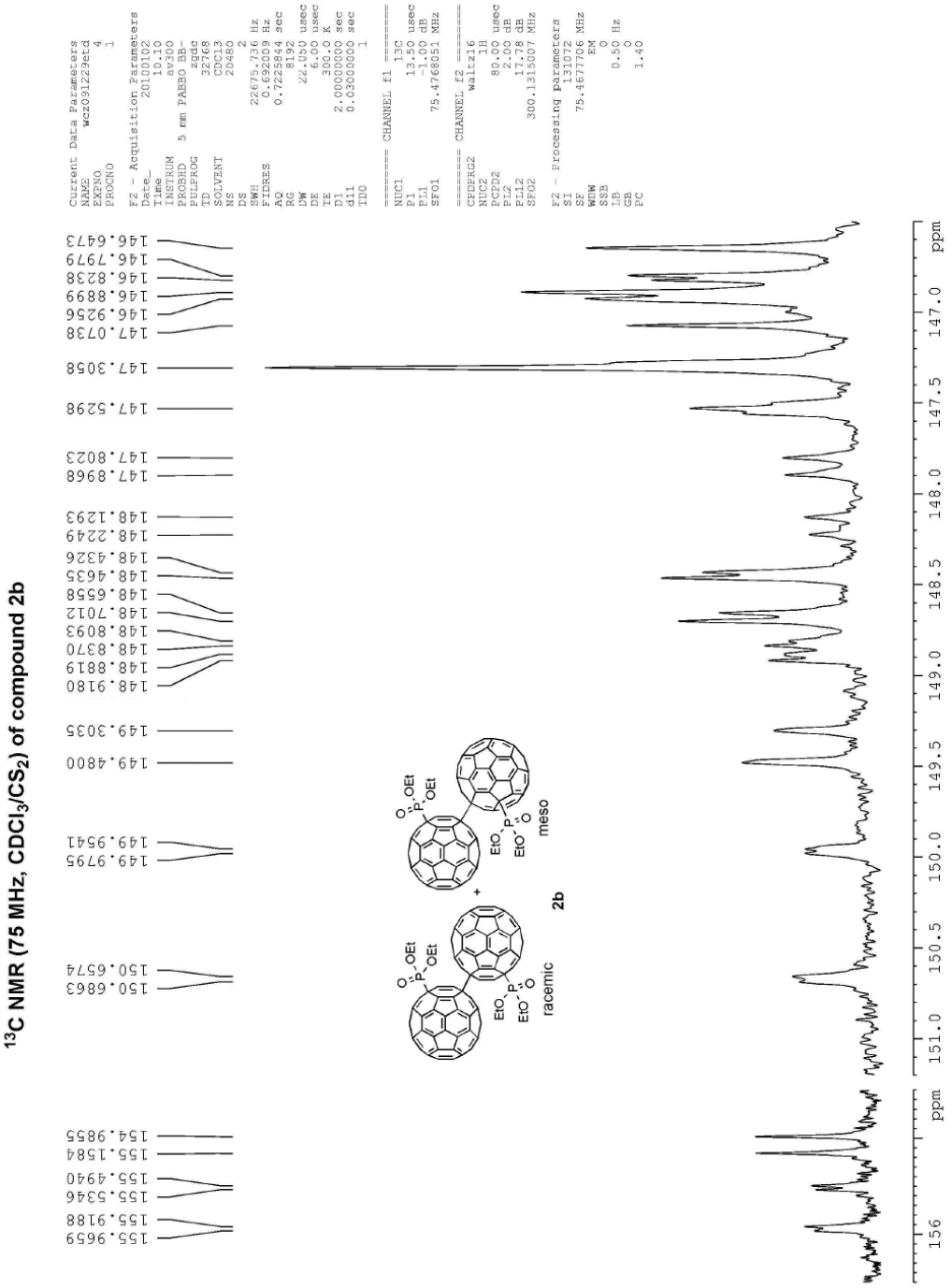


**$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2b**

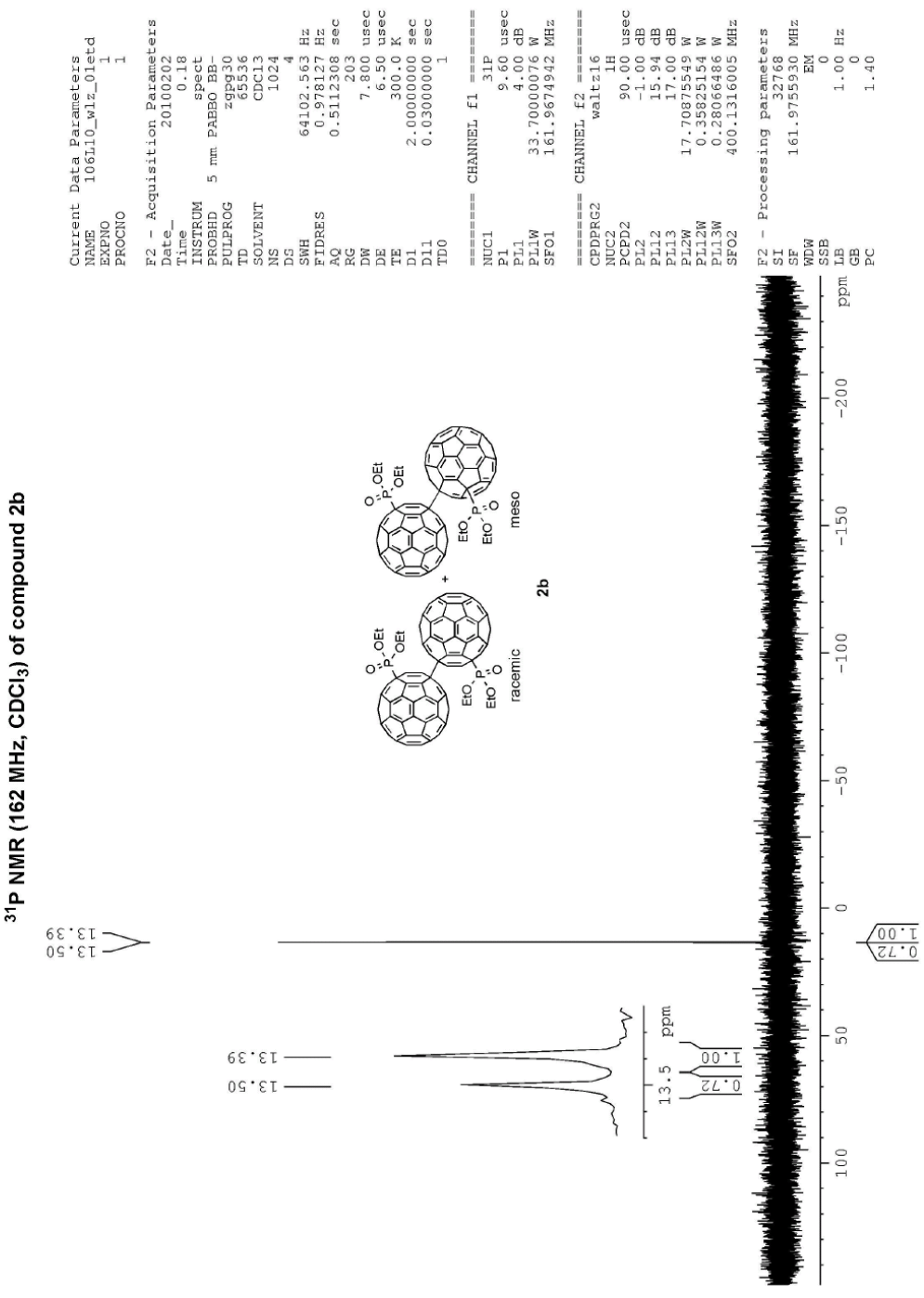


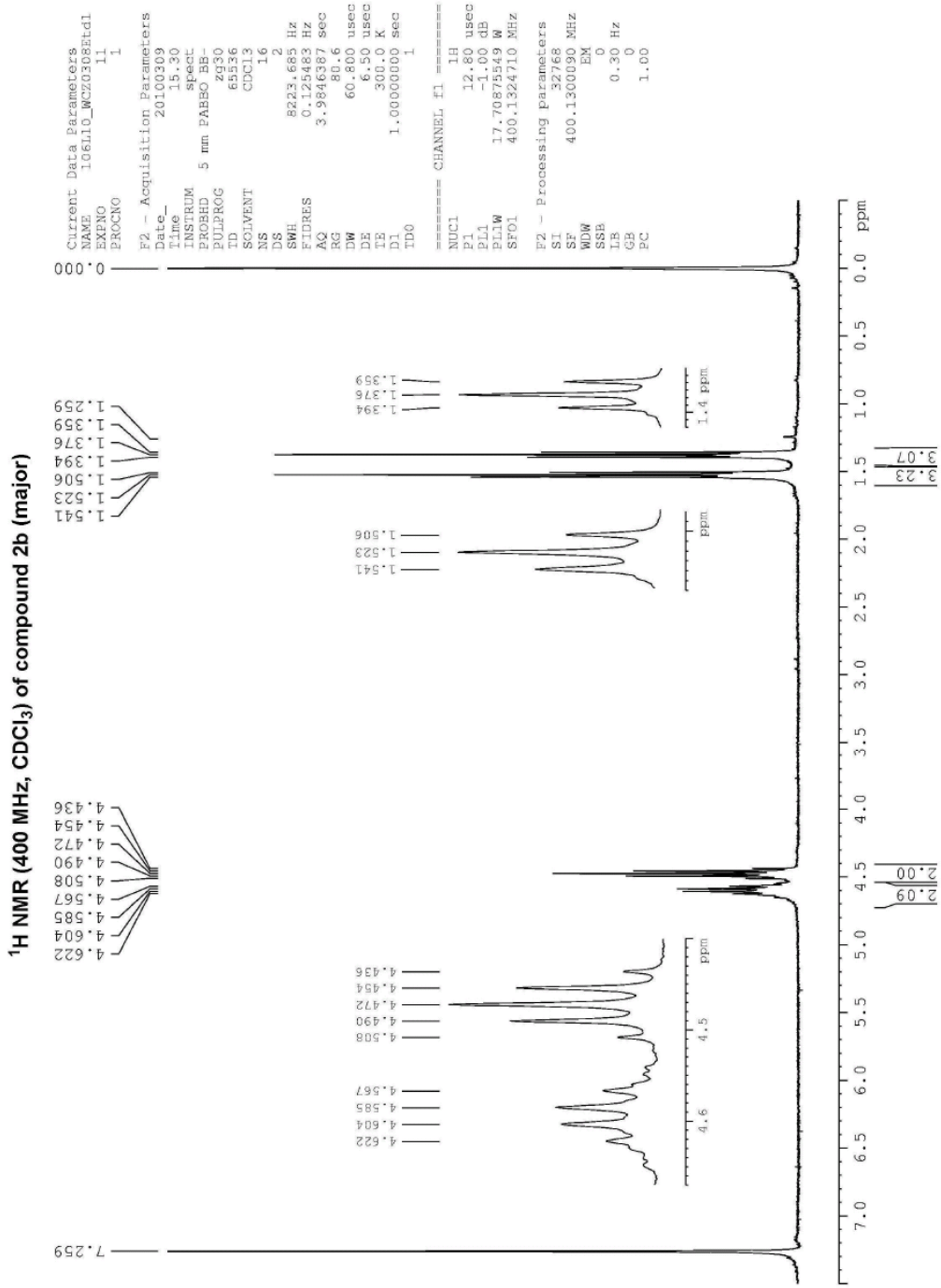

13C NMR (75 MHz, CDCl3/CS2) of compound 2b
Current Data Parameters
NAME wz2091229etd
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100102
Time 10.10
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 2048
DS 2
SWH 22675.736 Hz
FIDRES 0.692209 Hz
AQ 0.7225344 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.50 usec
PL1 1.00 dB
SFO1 75.4768051 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.78 dB
SFO2 300.1315007 MHz
F2 - Processing parameters
SI 131072
SF 75.4677276 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
137.2252
137.2036
137.1651
137.1368
138.9212
138.9715
138.1378
138.3797
138.4199
138.5691
138.9186
138.9583
139.0114
139.0472
140.6557
141.3981
141.6405
racemic
meso
2b
141.5
141.0
140.5
140.0
139.5
139.0
138.5
138.0
137.5
ppm

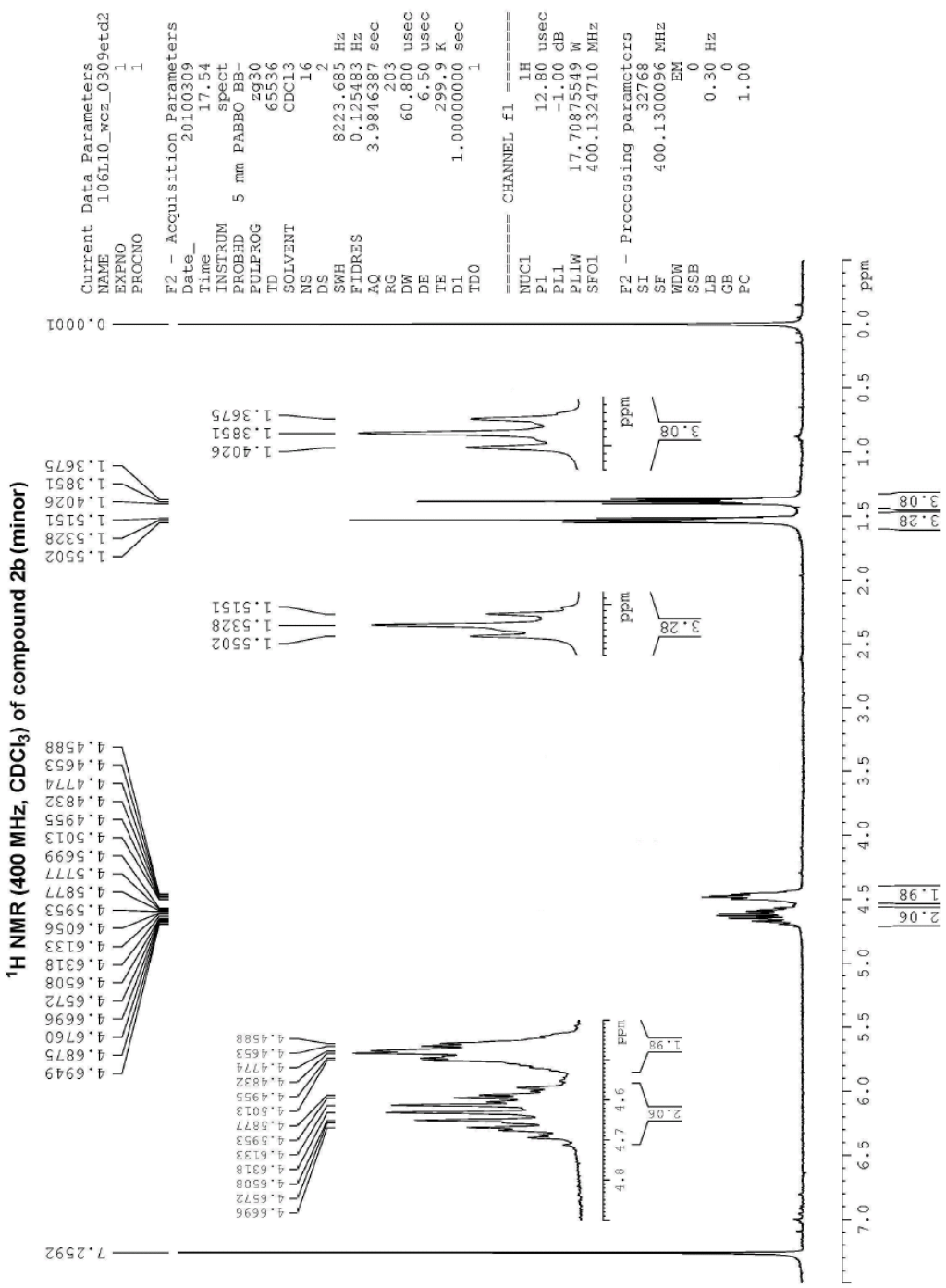

$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2b
Current Data Parameters
NAME wz2091229etd
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100102
Time 10.10
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 20480
DS 2
SWH 22675.736 Hz
FIDRES 0.692209 Hz
AQ 0.7225344 sec
RG 8192
DW 22.050 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 13.50 usec
PL1 1.00 dB
SFO1 75.4768051 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 17.78 dB
SFO2 300.1315007 MHz
F2 - Processing parameters
SI 131072
SF 75.4677876 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
racemic
2b
meso
ppm

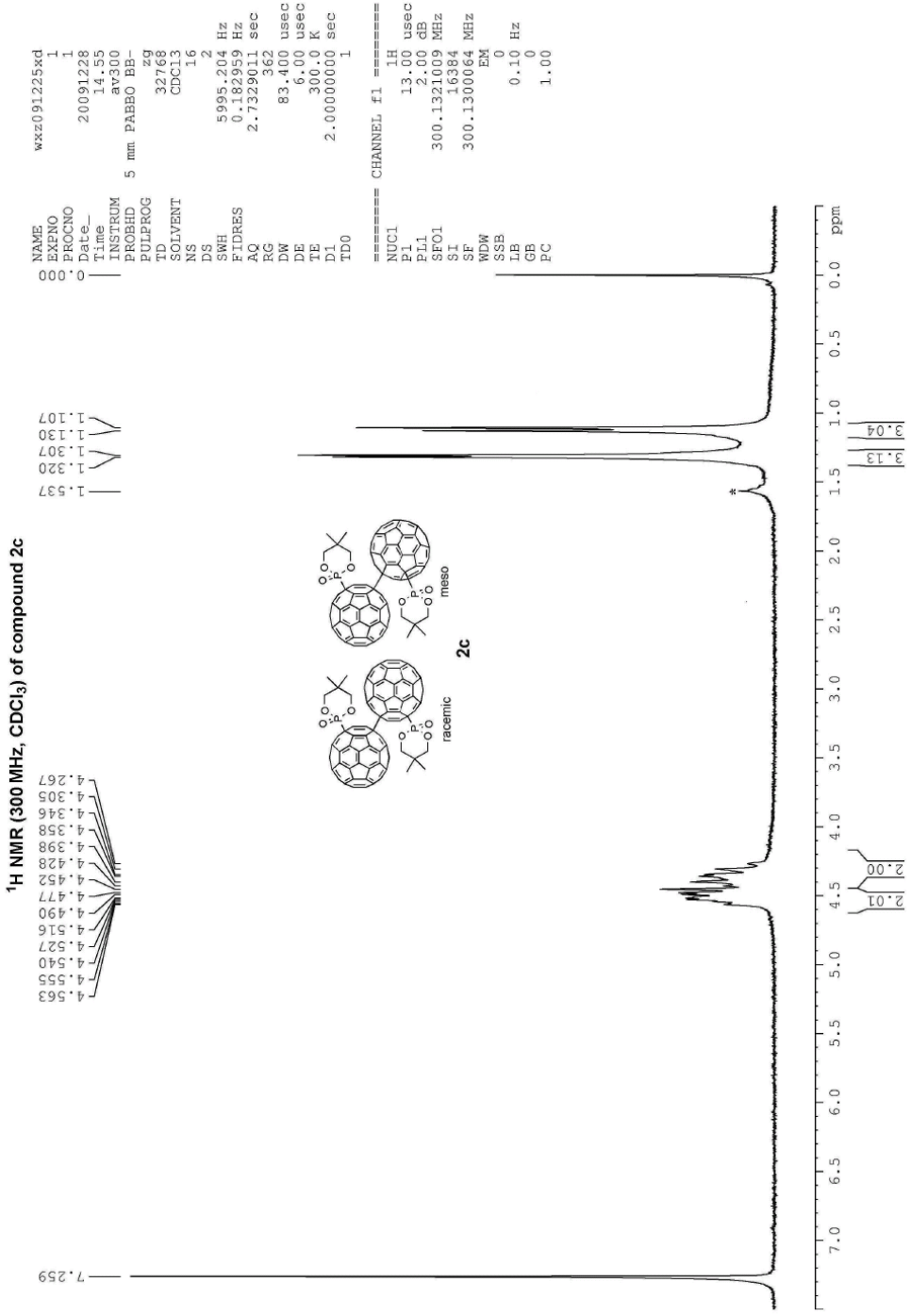

13C NMR (75 MHz, CDCl3/CS2) of compound 2b
meso
racemic
2b
ppm

**$^{31}$P NMR (162 MHz, $CDCl_3$) of compound 2b**

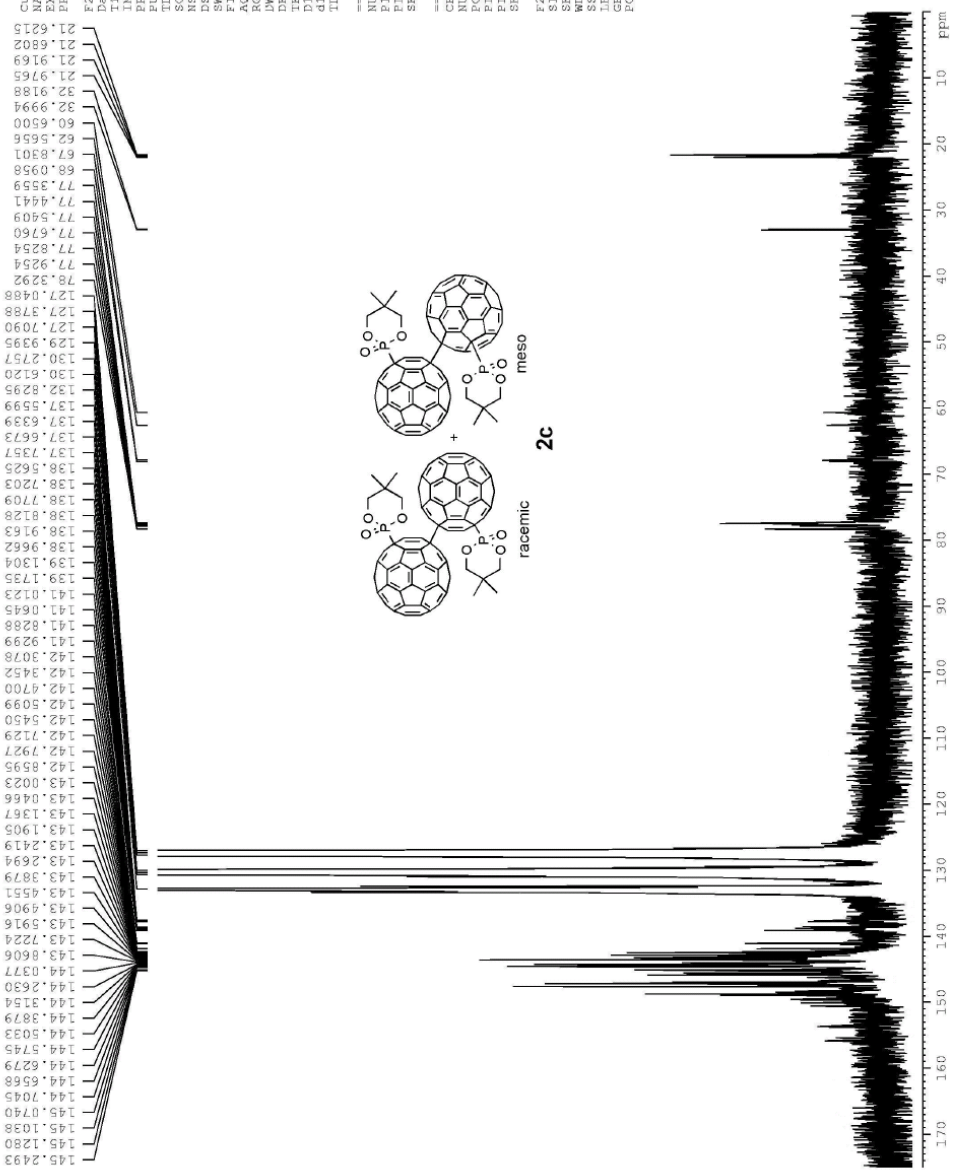



$^1$H NMR (400 MHz, $CDCl_3$) of compound 2b (major)
Current Data Parameters
NAME 106L10_WCZ0308Eld1
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100309
Time 15.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 80.6
DW 60.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 -1.00 dB
PL1W 17.70875549 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.259
4.622
4.604
4.585
4.567
4.508
4.490
4.472
4.454
4.436
1.541
1.523
1.506
1.394
1.376
1.359
1.259
2.00
2.09
3.23
3.07
ppm

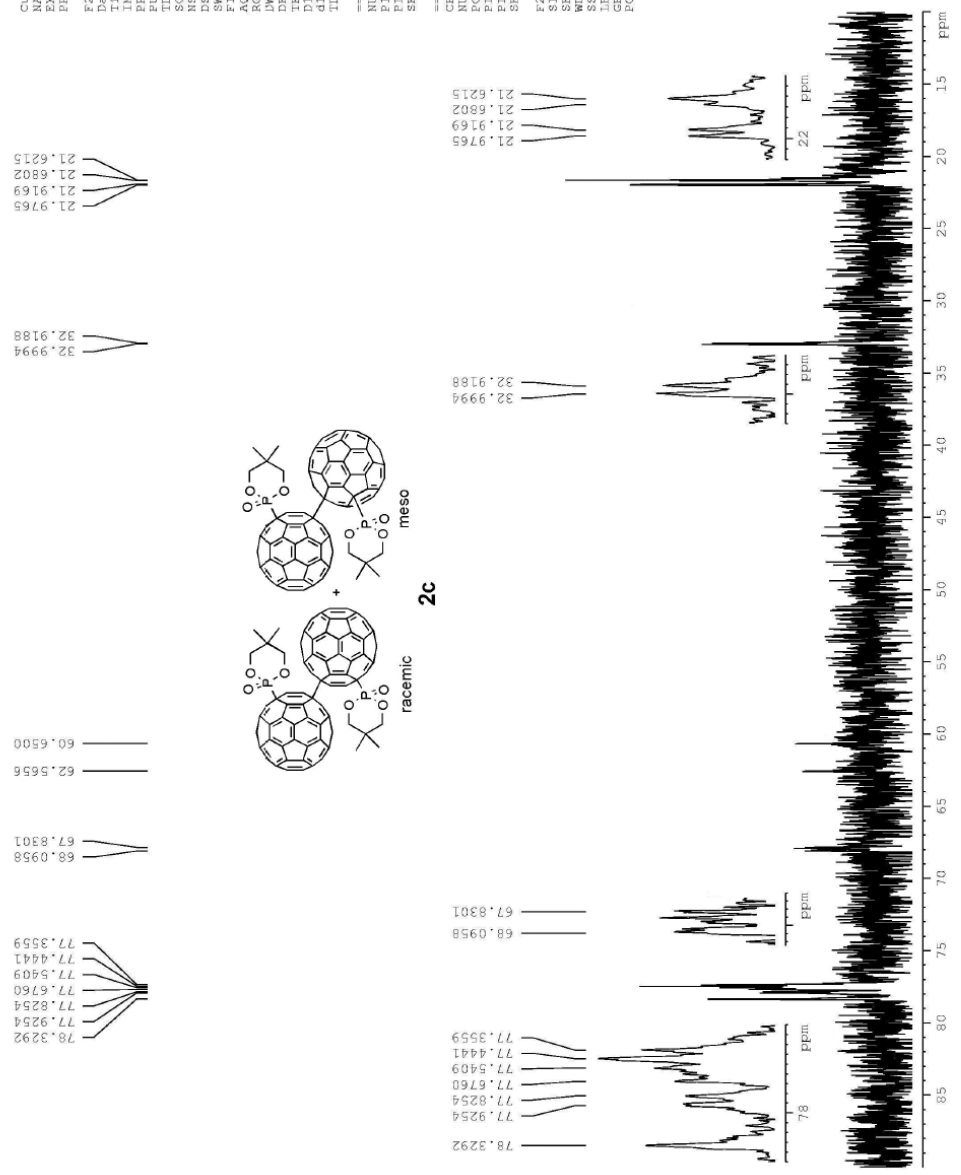

$^1$H NMR (400 MHz, $CDCl_3$) of compound 2b (minor)
Current Data Parameters
NAME 106L10_wcz_0309etd2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100309
Time 17.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.98446387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 299.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 -1.00 dB
PL1W 17.70875549 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm


$^1$H NMR (300 MHz, $CDCl_3$) of compound 2c
meso
racemic
2c
ppm

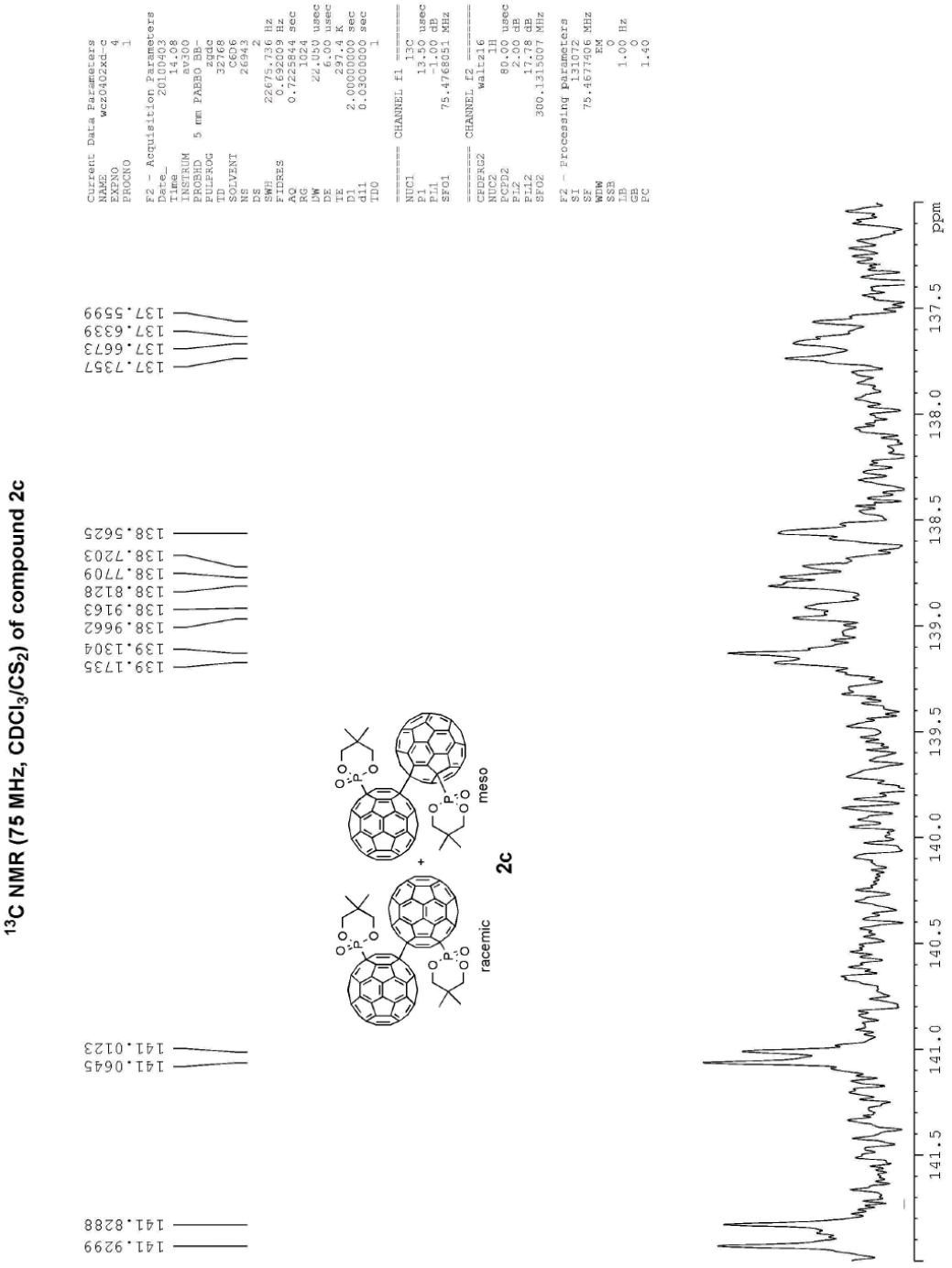
**$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2c**

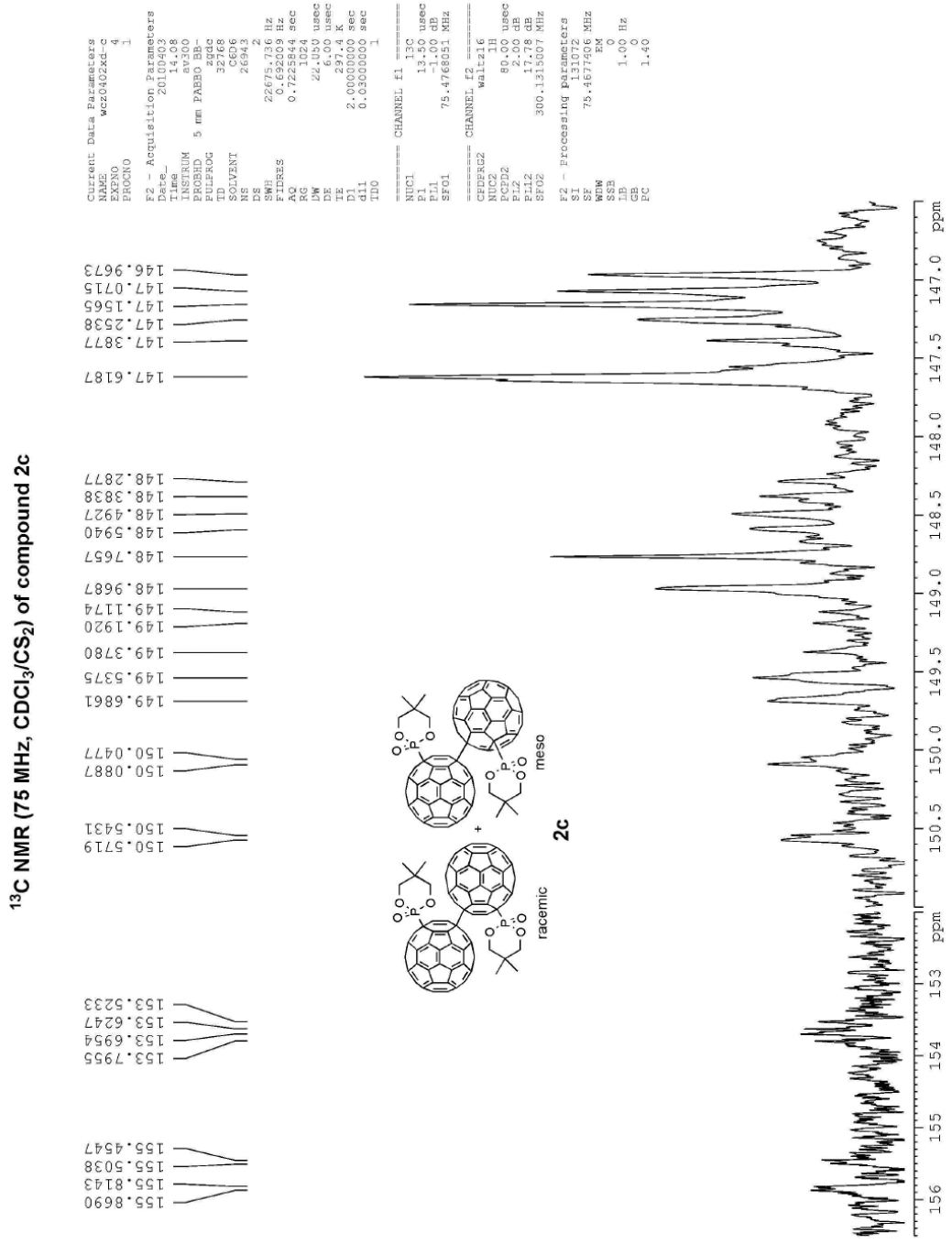


**$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2c**

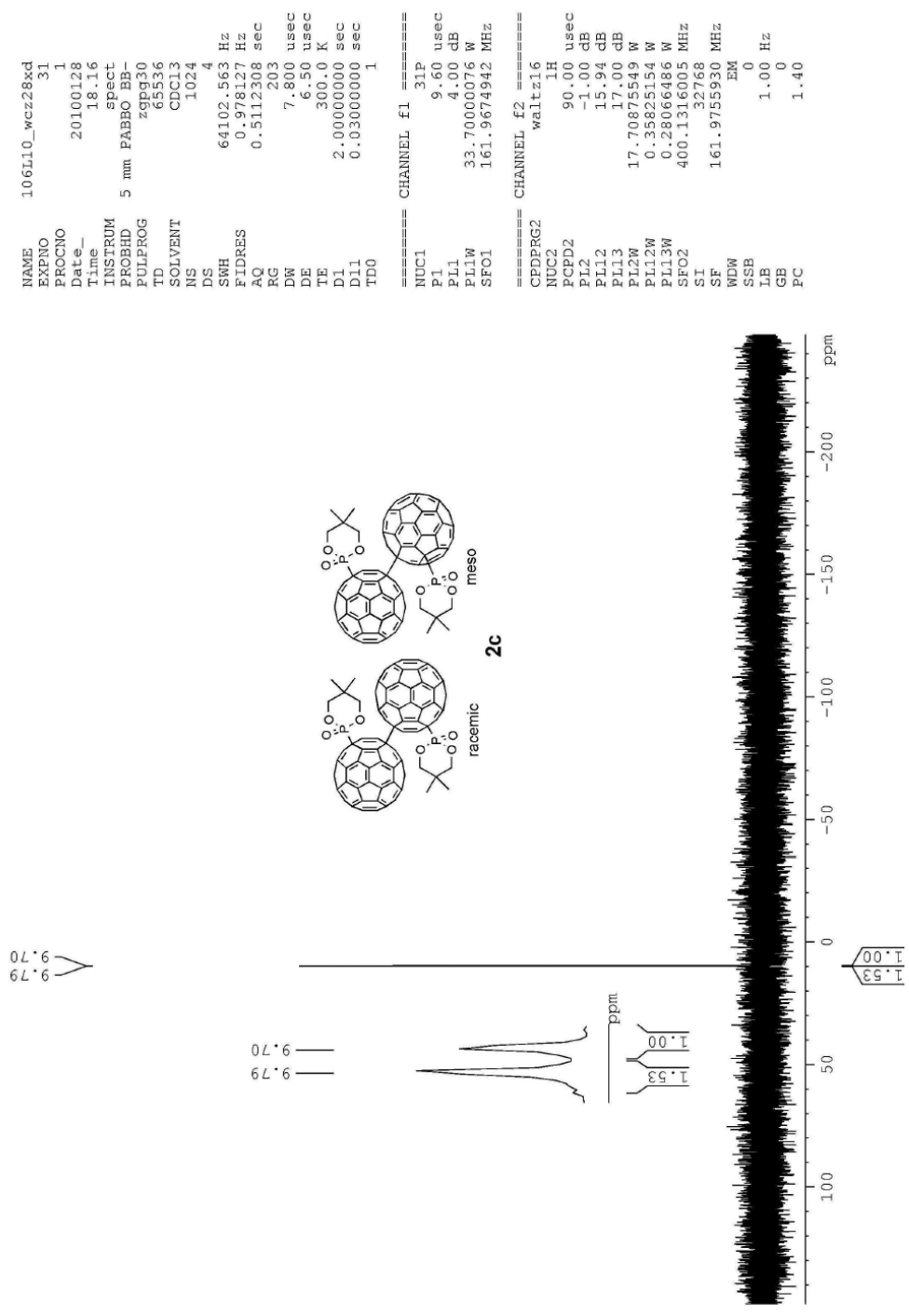


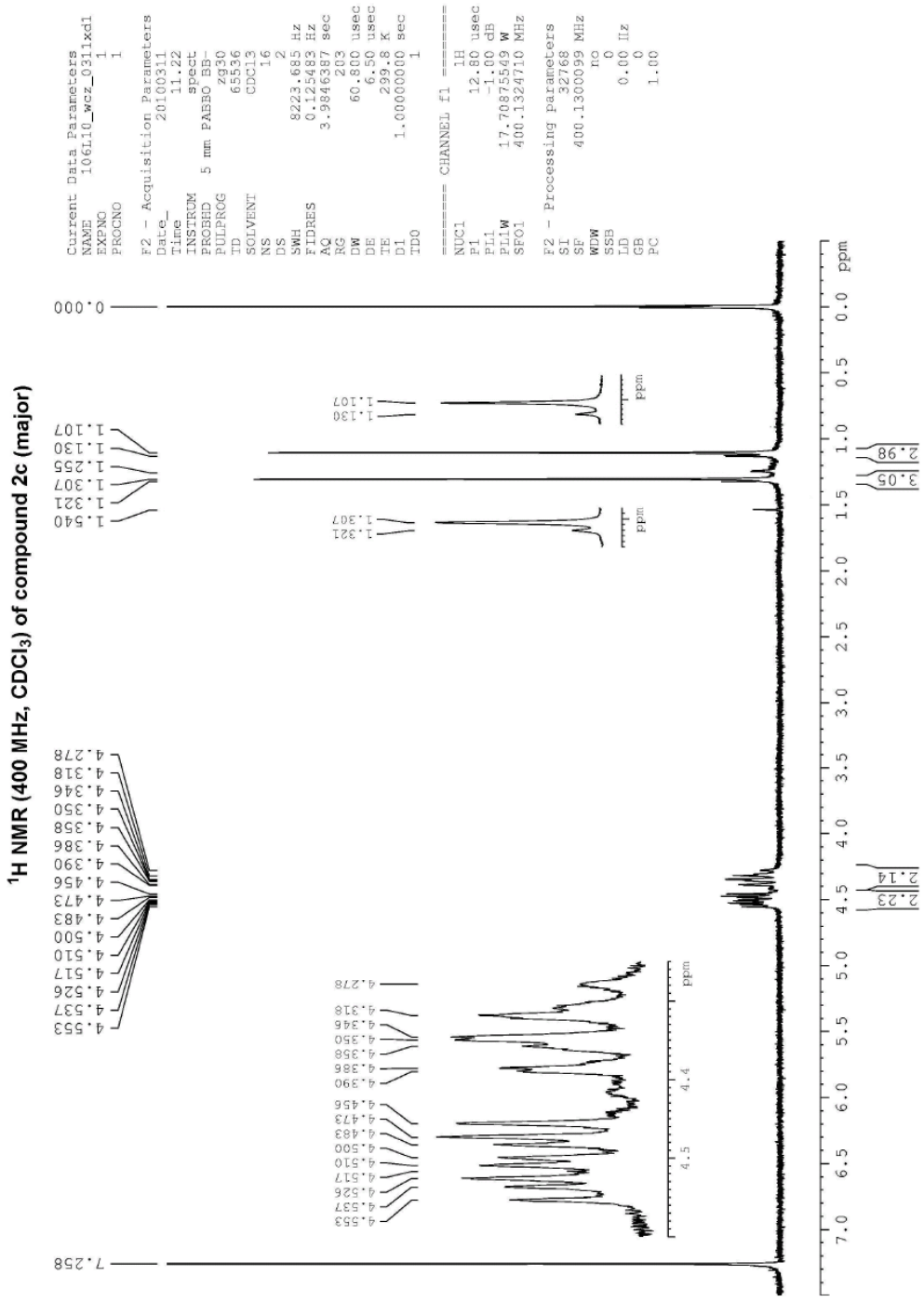
**$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2c**

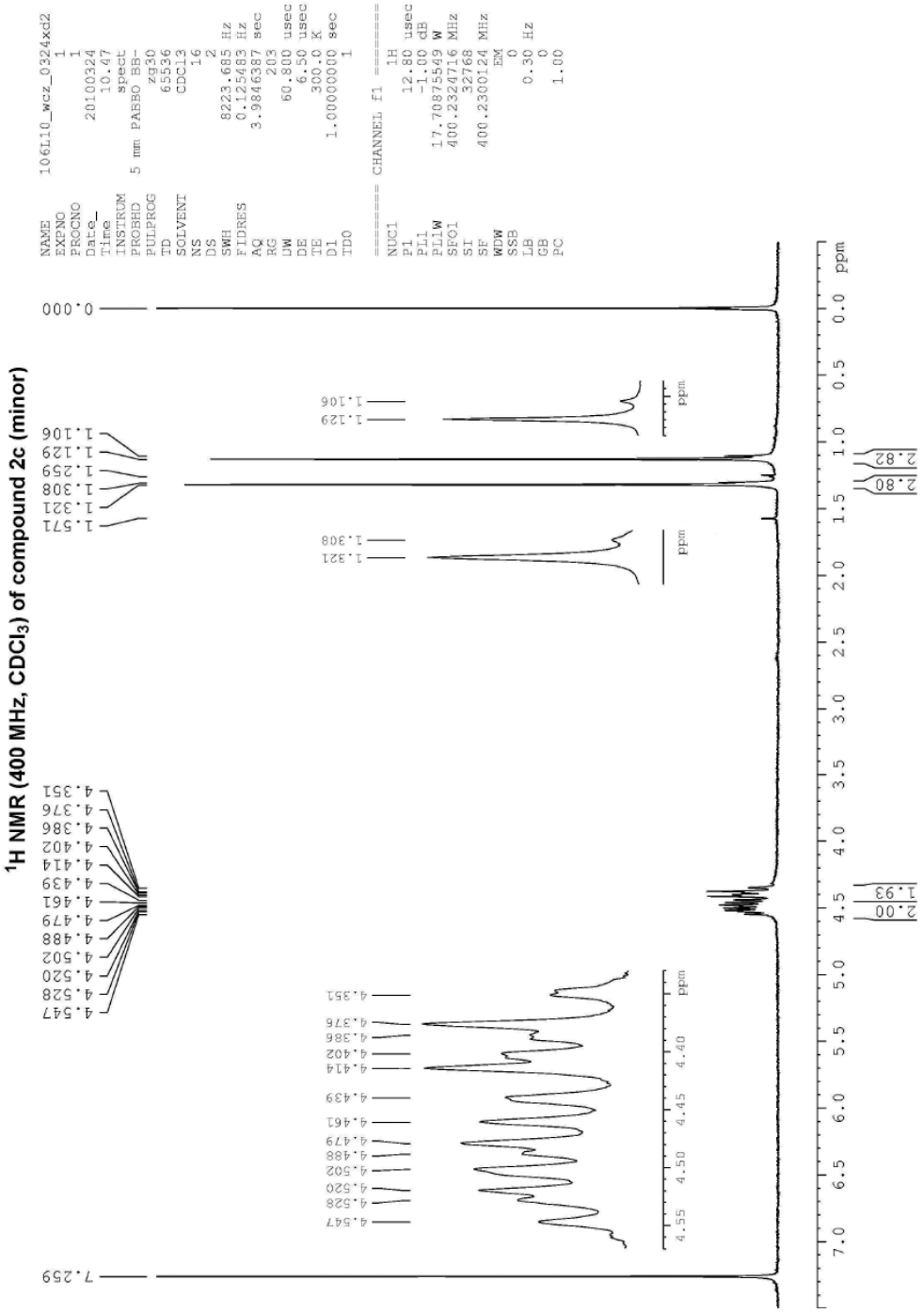



$^{13}$C NMR (75 MHz, $CDCl_3/CS_2$) of compound 2c
2c
meso
racemic
ppm

**$^{31}$P NMR (162 MHz, $CDCl_3$) of compound 2c**




$^1$H NMR (400 MHz, $CDCl_3$) of compound 2c (major)
Current Data Parameters
NAME 106l10_wcz_0311xd1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100311
Time 11.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 -1.00 dB
PL1W 17.70875549 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300099 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.258
4.553
4.537
4.526
4.517
4.510
4.500
4.483
4.473
4.456
4.390
4.386
4.358
4.350
4.346
4.318
4.278
1.540
1.321
1.307
1.255
1.130
1.107
2.98
3.05
2.23
2.14
ppm


$^1$H NMR (400 MHz, $CDCl_3$) of compound 2c (minor)
NAME 106L10_wcz_0324xd2
EXPNO 1
PROCNO 1
Date_ 20100324
Time 10.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 -1.00 dB
PL1W 17.70875549 W
SFO1 400.2324716 MHz
SI 32768
SF 400.2300124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.259
4.547
4.528
4.520
4.502
4.488
4.479
4.461
4.439
4.414
4.402
4.386
4.376
4.351
1.571
1.321
1.308
1.259
1.129
1.106
0.000
ppm
2.00
1.93
2.80
2.82