Supporting Information

Nickel-Catalyzed Oxidative C-H/N-H Annulation of N-Heteroaromatic Compounds with Alkynes

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Contents

1. General Information

^{1}H and ^{13}C NMR spectra were recorded on a JEOL ECS-400 spectrometer (JEOL, Tokyo, Japan) in $CDCl_3$ or acetone-d_6 with tetramethylsilane as the internal standard. Data are reported as follows: chemical shifts (δ) in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br s = broad singlet, m = multiplet, c = complex), coupling constant (*J*) in hertz (Hz), and integration. Infrared spectra (IR) were obtained using a JASCO FT/IR-4200 spectrometer; absorptions have been reported in reciprocal centimeters with the following relative intensitites: vs (very strong), s (strong), m (medium), w (weak). Mass spectra were obtained on a Shimadzu GCMS-QP 2014 or Shimadzu GCMS-QP 5000 instruments using ionization voltages of 70 eV. High resolution mass spectra (HRMS) were obtained on a JEOL JMS-DX303 or MS-T100LP instrument. Melying points (Mp) were determined using a Yamato melting point apparatus. Column chromatography was performed with Silicycle Silia Flash F60 (230-400 mesh, Silycycle Inc.). Most of the compounds were purified by LC-908 HPLC (GPC).

2. Materials

All chemicals were used as received.

Nickel sources: $Ni(cod)_2$ (Strem Chemicals), $Ni(OAc)_2$, $Ni(OTf)_2$ (prepared according to the literature[1]).

Ligand: 4,4'-di-tert-butyl-2,2'-bipyridyl (Aldrich), Bathophenanthroline (Kanto Chemical Co., Inc), 2-(2-Pyridyl)benzoxazole (Tokyo Chemical Industry Co., Ltd), 3,4,7,8,-tetramethyl-1,10-phenanthroline (Tokyo Chemical Industry Co., Ltd), 6,6'-dimethyl-2,2'-bipyridyl (Tokyo Chemical Industry Co., Ltd), PPh_3 (Wako Pure Chemicals Indutries, Ltd).

Indoles: 2-phenyl-1H-indole-3-carbaldehyde (Aldrich), 2-phenyl-1H-indole (Tokyo Chemical Industry Co., Ltd), 2-(p-tolyl)-1H-indole (Tokyo Chemical Industry Co., Ltd), 2-(4-fluorophenyl)-1H-indole (Tokyo Chemical Industry Co., Ltd), 2-(4-methoxyphenyl)-1H-indole (Tokyo Chemical Industry Co., Ltd), 3,5-diphenyl-1H-pyrazole (Tokyo Chemical Industry Co., Ltd).

Benzimidazoles: 2-phenylbenzimidazole (Tokyo Chemical Industry Co., Ltd).

Alkynes: diphenylacetylene (Tokyo Chemical Industry Co., Ltd).

Bases: KOMe (Aldrich), NaHMDS (Aldrich), KO^{t}Bu (Tokyo Chemical Industry Co., Ltd).

Solvents: DMSO, super dehydrated (Kanto Chemical Co., Inc), toluene, super dehydrated (Wako Pure Chemical Industries, Ltd).

[1] Y. Aihara, N. Chatani, *J. Am. Chem. Soc.* **2013**, *135*, 5308.

3. General Procedure for the Preparation of Starting Materials

(1) Synthesis of 2-Arylindoles.[2]

Acetophenone (10 mmol), phenylhydrazine (12 mmol), HOAc (2 mmol) and EtOH (10 mL) were charged in a round bottom flask and the resulting solution then refluxed at 100 °C. When the reaction reached completion (as detected by TLC), the mixture was cooled to room temperature. The solvent was removed by evaporation and the crude hydrozaone was then dissolved in toluene (10 mL). Polyphosphoric acid (PPA, 15 mmol) was added to the solution, which was then refluxed at 120 °C overnight followed by cooling. The crude mixture was quenched by adding H_2O (10 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and the solution evaporated to dryness. The resulting crude 2-phenylindole was purified by flash chromatography on silica gel (eluent: hexanes/EtOAc = 10/1) and recrystallized from EtOAc/hexane.

(2) Synthesis of 5-Methoxy-2-phenyl-1H-indole. [3]

A round bottom flask was charged with 5-methoxyindole (6 mmol), 2-norbornene (0.4 mmol), K_2CO_3 (12 mmol) and $PdCl_2(MeCN)_2$ (0.6 mmol, 10 mol%). A solution of H_2O (15 mmol) in DMA (30 mL) was added, followed by iodobenzene (12 mmol). The solution was stirred overnight at 70 °C. When the reaction reached completion, the solution was cooled to room temperature, diluted with EtOAc (20 mL), and filtered. The filtrate was washed with H_2O (3 × 10 mL) and brine and the organic phase was then concentrated by evaporation. The resulting crude indole preparation was purified by flash chromatography on silica gel (eluent: hexane/EtOAc = 10/1) and recrystallized from EtOAc/hexane to afford 5-methoxy-2-phenyl-iH-indole.

(3) Synthesis of 2-(4-(Trifluoromethyl)phenyl)-1H-benzo[d]imidazole and 2-(4-Methoxyphenyl)-1H-benzo[d]imidazole.[4]

Iodobenzene diacetate (6 mmol) was added to a mixture of o-phenylenediamine (3 mmol) and benzaldehyde (3 mmol) at room temerature and the resulting mixture was stirred for a few minutes. The crude mixture was washed with a saturated aqueous solution of Na_2CO_3 and then extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and the solution evaporated to dryness. The resulting crude benz[d]imidazole was purified by flash chromatography on silica gel (eluent: hexanes/EtOAc = 1/1) and recrystallized from EtOAc.

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[2] Lian, X.-L.; Lei, H.; Quan, X.-J.; Ren, Z.-H.; Wang, Y.-Y.; Guan, Z.-H. *Chem. Commun.* **2013**, *49*, 8196.

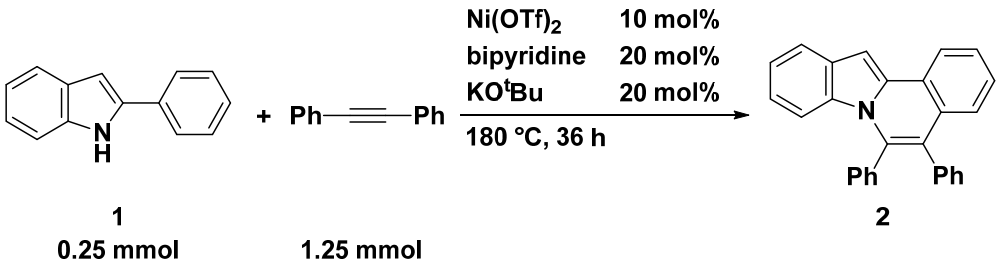
[3] Gao, Y.; Zhu, W.; Yin, L.; Dong, B.; Fu, J.; Ye, .; Xue, F.; Jiang, C. *Tetrahedron Lett.* **2017**, *58*, 2213.

[4] L.-H. Du and X.-P. Luo, *Syhth. Commun.* **2010**, 2880.

(3) Synthesis of 2-Phenyl-1H-Pyrrole.[5]

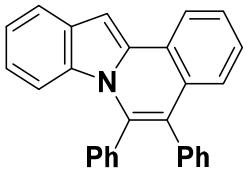
A round bottom flask was charged with diphenyliodonium bromide (4.5 mmol), NaOH (6.75 mmol) and pyrrole (22.5 mL). The solution was stirred at 80 °C for 10 h, after which, it was cooled to room temperature. The pyrrole was removed in vacuo, the mixture was diluted with EtOAc (20 mL), and washed with H_2O (3 × 10 mL) and brine. After concentrating the solution in vacuo, the resulting crude product was purified by flash chromatography on silica gel (eluent: hexans/EtOAc = 10/1) and Gel Permeation Chromatography (GPC).

4. General procedure for the Ni-catalyzed oxidative annulation



To an oven-dried 5 mL screw-capped vial in a glove box, 2-phenyl-1H-indole (**1a**, 48.3 mg, 0.25 mmol), diphenylacetylene (227 mg, 1.25 mmol), $Ni(OTf)_2$ (8.9 mg, 0.025 mmol), 4,4'-di-*tert*-butyl-2,2'-bipyridine (13.4 mg, 0.05 mmol), and KO^tBu (5.7 mg, 0.05 mmol) were added. The mixture was stirred for 36 h at 180 °C and then allowed to cool to room temperature. The resulting mixture was filtered through a celite pad and the filtrate was concentrated in vacuo. The residue was purified by column chromatography on silica gel (hexane/chloroform=3/1), followed by GPC to afford the desired product **2a** (48.1 mg, 52% yield) as a green solid. Both ^1H and ^{13}C NMR spectra showed that the product is apparently pure, as attached, but it was not possible to remove the color from the product, even after repeated recrystalization.

5,6-diphenylindolo[2,1-a]isoquinoline (2a)[6]

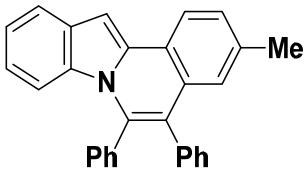


Green solid. R_f = 0.26 (hexane/chloroform 3:1). Yield = 52 %, m = 48.1 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 5.98-6.01 (m, 1H), 6.80-6.84 (m, 1H), 7.15-7.40 (m, 14H), 7.48 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.78 (d, *J* = 7.8 Hz, 1H), 8.28 (d, *J* = 7.8 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 94.3, 114.7, 120.2, 120.3, 121.5, 121.7, 123.4, 125.5, 126.2, 126.8, 127.1, 127.4, 127.9, 128.7, 128.8, 129.7, 130.3, 130.9, 131.9, 132.8, 135.4, 136.0, 136.1, 136.8.; HRMS Calcd for $C_{28}H_{20}N$ $(M+H)^+$: 370.1590; Found: 370.1583.

3-methyl-5,6-diphenylindolo[2,1-a]isoquinoline (2b)

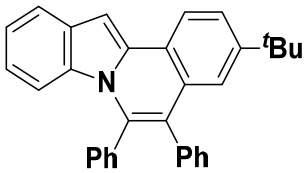
[5] Wen, J.; Zhang, R.-Y.; Chen, S.-Y.; Zhang, J.; Yu, X.-Q. *J. Org. Chem.* **2012**, *77*, 766.

[6] Ackermann, L.; Wang, L.; Lygin, A. V. *Chem. Sci.* **2012**, *3*, 177.



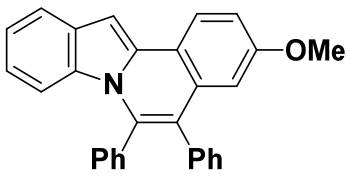
Green solid, Mp = 241-242 °C. R_f = 0.23 (hexane/chloroform 3:1). Yield = 50 %, m = 48.2 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 2.34 (s, 3H), 5.96 (d, *J* = 8.7 Hz, 1H), 6.78 (dd, *J* = 7.8, 7.3 Hz, 1H), 6.93 (s, 1H), 7.16-7.34 (m, 13H), 7.77 (d, *J* = 7.8 Hz, 1H), 8.20 (d, *J* = 7.8 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 21.9, 93.5, 114.6, 119.9, 120.2, 121.4, 121.7, 123.1, 123.5, 126.2, 126.8, 127.9, 128.6, 128.7, 128.8, 129.9, 130.3, 131.0, 132.0, 132.7, 135.5, 136.2, 136.3, 136.9, 137.5. **IR** (ATR): 3057 w, 1612 w, 1544 w, 1485 w, 1442 w, 1380 w, 1340 w, 1299 w, 1249 w, 1151 w, 1101 w, 1071 w, 1024 w, 843 w, 816 w, 759 w, 696 w. **MS** (EI+): 384 (32), 383 (M^+, 100). **HRMS** (EI+) Calcd for $C_{29}H_{21}N$: 383.1674; Found: 383.1677.

3-(tert-butyl)-5,6-diphenylindolo[2,1-a]isoquinoline (2c)



Green solid, Mp = 262 °C. R_f = 0.31 (hexane/chloroform 3:1). Yield = 52 %, m = 54.9 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 1.24 (s, 9H), 5.97 (d, *J* = 8.3 Hz, 1H), 6.79 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.15-7.26 (m, 7H), 7.30-7.36 (m, 6H), 7.58 (d, *J* = 8.3 Hz, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 8.24, (d, *J* = 8.3 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 31.3, 35.0, 93.6, 114.7, 119.9, 120.2, 121.6, 121.9, 122.6, 123.1, 123.3, 125.0, 126.8, 127.9, 128.7, 128.8, 129.9, 130.1, 131.0, 131.9, 132.8, 135.6, 136.0, 136.2, 136.9, 150.6. **IR** (ATR): 2959 w, 1602 w, 1547 w, 1484 w, 1443 w, 1418 w, 1336 w, 1260 w, 1156 w, 1124 w, 1072 w, 1020 w, 894 w, 829 w, 788 w, 755 m, 696 w. **MS** (EI+): 426 (34), 425 (M^+, 100), 410 (18), 395 (15). **HRMS** (EI+) Calcd for $C_{32}H_{27}N$: 425.2143; Found: 425.2136.

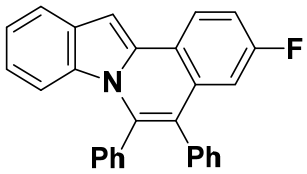
3-methoxy-5,6-diphenylindolo[2,1-a]isoquinoline (2d)



Green solid, Mp = 210-212 °C. R_f = 0.11 (hexane/chloroform 3:1). Yield = 67 %, m = 66.7 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 3.71 (s, 3H), 5.95 (d, *J* = 8.7 Hz, 1H), 6.59 (s, 1H), 6.77 (dd, *J* = 7.8, 7.8 Hz, 1H), 7.10-7.36 (m, 13H), 7.75 (d, *J* = 8.3 Hz, 1H), 8.22, (d, *J* = 8.7 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 55.4, 92.7, 109.3, 114.6, 115.2, 119.3, 119.7, 120.0, 121.3, 121.7, 125.1, 126.9, 128.0, 128.7, 128.8, 130.1, 130.9, 131.9, 132.0, 132.6, 135.5, 136.3, 136.6, 136.8, 159.1. ; **IR** (ATR): 1606 w, 1485 w, 1444 w, 1290 w,

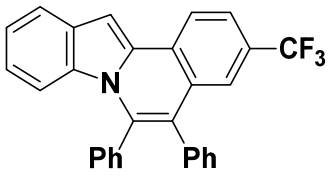
1173 w, 1028 w, 824 w, 774 w, 726 w, 697 w. **MS** (EI+): 400 (31), 399 (M^+, 100). **HRMS** (EI+) Calcd for $C_{29}H_{21}NO$: 399.1632; Found: 399.1621.

3-fluoro-5,6-diphenylindolo[2,1-a]isoquinoline (2e)[6]



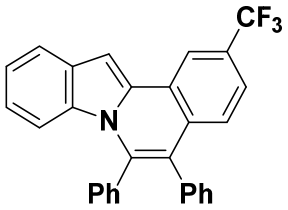
Green solid. R_f = 0.26 (hexane/chloroform 3:1). Yield = 62 %, m = 59.5 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 5.96 (d, *J* = 8.7 Hz, 1H), 6.78-6.83 (m, 2H), 7.14-7.36 (m, 13H), 7.77 (d, *J* = 7.8 Hz, 1H), 8.25 (dd, *J* = 8.7, 5.5 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 94.0, 111.8 (d, J_{CF} = 23), 114.7, 115.3, (d, J_{CF} = 23), 120.3, 120.9, 122.0, 125.5 (d, J_{CF} = 9), 127.2, 128.2, 128.8, 129.0, 129.8, 130.8, 131.8, 132.4 (d, J_{CF} = 8), 132.7, 135.1, 135.5, 136.3, 137.2, 162.1 (d, J_{CF} = 244).; HRMS Calcd for $C_{28}H_{19}FN$ $(M+H)^+$: 388.1496; Found: 388.1487.

5,6-diphenyl-3-(trifluoromethyl)indolo[2,1-a]isoquinoline (2f) [6]



Green solid. R_f = 0.34 (hexane/chloroform 3:1). Yield = 41 %, m = 45.0 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 5.98 (d, *J* = 9.2 Hz, 1H), 6.86 (dd, *J* = 7.8, 7.8 Hz, 1H), 7.13-7.15 (m ,2H), 7.19-7.38 (m, 10H), 7.47 (s, 1H), 7.68 (d, *J* = 8.3 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 8.33 (d, *J* = 8.7 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 96.2, 114.8, 120.7, 121.0, 121.2, 122.2, 123.3 (q, J_{CF} = 4), 123.4 (q, J_{CF} = 3), 123.9, 124.3 (q, J_{CF} = 270), 127.3, 128.0, 128.2, 128.9, 129.0 (q, J_{CF} = 32), 129.1, 129.6, 130.3, 130.7, 131.8, 133.0, 134.8, 135.0, 135.8, 137.5; HRMS Calcd for $C_{19}H_{20}N_3O$ $(M+H)^+$:438.1464; Found: 438.1427.

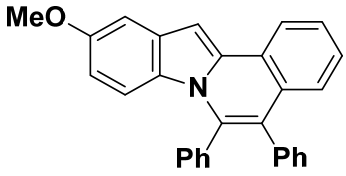
5,6-diphenyl-2-(trifluoromethyl)indolo[2,1-a]isoquinoline (2g)



Yellow solid, Mp = 193-194 °C. R_f = 0.37 (hexane/chloroform 3:1). Yield = 73%, m = 79.5 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 5.99 (d, *J* = 9.0 Hz, 1H), 6.86 (dd, *J* = 7.9, 7.9 Hz, 1H), 7.15-7.39 (m, 12H), 7.50-7.52 (m, 2H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.83 (s, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 95.6, 114.8, 120.6

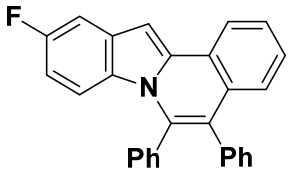
(d, J_{CF} = 4), 120.7, 120.8, 121.0, 122.2, 123.5 (d, J_{CF} = 4 Hz), 124.4 (*q*, J_{CF} = 271 Hz), 125.5, 126.9, 127.2, 128.2, 128.8 (*q*, J_{CF} = 32 Hz), 128.9, 129.2, 129.7, 130.6, 131.8, 132.8, 132.9, 134.9, 135.1, 136.2, 138.2. ;**IR** (ATR): 3058 w, 1620 w, 1549 w, 1493 w, 1445 w, 1429 m, 1384 w, 1335 m, 1313 m, 1284 w, 1243 w, 1171 w, 1146 m, 1121 m, 1072 m, 1053 w, 1023 w, 938 w, 894 w, 833 w, 789 w, 759 m, 699 m. ; **MS** (EI+): 438 (31), 437 (M^+, 100), 436 (11).; **HRMS** (EI+) Calcd for $C_{29}H_{18}F_3N$: 437.1391; Found: 437.1389.

10-methoxy-5,6-diphenylindolo[2,1-a]isoquinoline (2h) [6]



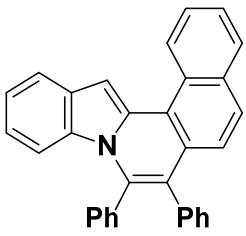
Green solid. R_f = 0.17 (hexane/chloroform 3:1). Yield = 48 %, m = 47.6 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 3.85 (s, 3H), 5.85 (d, *J* = 9.2 Hz, 1H), 6.46 (d, *J* = 9.4 Hz, 1H), 7.14-7.38 (m, 14H), 7.50 (dd, *J* = 7.4, 7.4 Hz, 1H), 8.28 (d, *J* = 8.2 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 55.6, 93.9, 100.9, 110.6, 115.5, 121.1, 123.3, 125.2, 126.2, 126.9, 127.0, 127.3, 127.9, 128.0, 128.8, 128.9, 130.2, 130.6, 130.9, 131.9, 135.3, 135.9, 136.6, 136.8, 155.2.; HRMS(EI+) Calcd for $C_{29}H_{21}NO$: 399.1623; Found: 399.1628.

10-fluoro-5,6-diphenylindolo[2,1-a]isoquinoline (2i) [6]



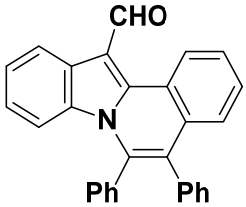
Green solid. R_f = 0.31 (hexane/chloroform 3:1). Yield = 62 %, m = 60.3 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 5.88 (dd, *J* = 9.6, 4.6 Hz, 1H), 6.51-6.58 (m, 1H), 7.15-7.39 (m, 14H), 7.49-7.53 (m, 1H), 8.28 (d, *J* = 7.8 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 94.1 (d, J_{CF} = 4 Hz), 104.5 (d, J_{CF} = 23 Hz), 108.7 (d, J_{CF} = 26 Hz), 115.6 (d, J_{CF} = 9 Hz), 121.7, 123.5, 125.0, 126.4, 127.0, 127.3, 127.8, 128.0, 128.9, 129.0, 129.5, 130.3, 130.4 (d, J_{CF} = 10 Hz), 130.9, 131.9, 135.1, 135.8, 136.6, 137.5, 158.7 (d, J_{CF} = 237 Hz). ; HRMS Calcd for $C_{28}H_{19}FN$ $(M+H)^+$: 388.1496; Found: 388.1474.

7,8-diphenylbenzo[h]indolo[2,1-a]isoquinoline (2j) [6]



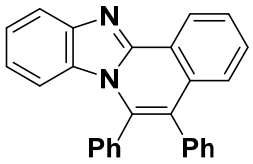
Green solid. R_f = 0.26 (hexane/chloroform 3:1). Yield = 47 %, m = 48.8 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 6.10 (d, *J* = 8.7 Hz, 1H), 6.86 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.19-7.36 (m, 12H), 7.63 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.73 (d, *J* = 8.7 Hz, 1H), 7.80 (dd, *J* = 7.1, 7.1 Hz, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 8.01 (s, 1H), 9.35 (d, *J* = 8.7 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 99.4, 115.0, 120.3, 120.4, 121.3, 122.1, 122.2, 124.3, 125.8, 126.1, 126.9, 127.4, 128.1, 128.8, 129.0, 129.6, 130.3, 130.8, 131.8, 132.1, 132.9, 135.0, 135.7, 136.7, 137.3.; HRMS(EI+) Calcd for $C_{32}H_{21}N$: 419.1674; Found: 419.1667.

5,6-diphenylindolo[2,1-a]isoquinoline-12-carbaldehyde (2k) [6]



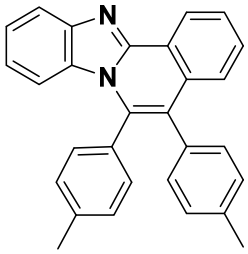
Green solid. R_f = 0.03 (hexane/chloroform 3:1). Yield = 49 %, m = 48.2 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 6.02 (d, *J* = 8.7 Hz, 1H), 6.89-6.93 (m, 1H), 7.15-7.42 (m, 12H), 7.56-7.60 (m, 1H), 7.67-7.72 (m, 1H), 8.65 (d, *J* = 8.2 Hz, 1H), 9.15 (d, *J* = 8.2 Hz, 1H), 10.99 (s, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 115.3, 121.0, 122.7, 124.6, 124.9, 125.7, 126.8, 127.4, 127.9, 128.2, 128.2, 129.0, 129.4, 130.1, 130.9, 131.5, 132.7, 133.2, 134.6, 135.9, 136.1, 141.3, 184.8.; HRMS(EI+) Calcd for $C_{29}H_{19}NO$:397.1467; Found: 397.1472.

5,6-diphenylbenzo[4,5]imidazo[2,1-a]isoquinoline (4a)



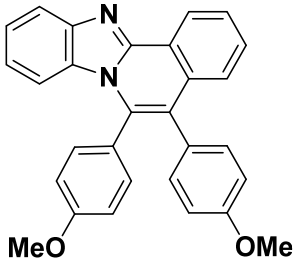
R_f 0.28 (Hexane/EtOAc = 150/50/3). Yield = 95%, m = 87.7 mg. Wihte Solid. ^{1}H NMR (CDCl3, 399.78 MHz) δ 6.01 (d, *J* = 8.5 Hz, 1H), 6.94 (*t*, *J* = 7.9 Hz, 1H), 7.20-7.31(m, 5H), 7.32-7.45 (m, 7H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 8.00 (d, *J* = 8.3 Hz, 1H), 9.01 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (CDCl3, 100.53 MHz) δ 114.14, 119.40, 121.33, 122.66, 123.69, 124.23, 125.12, 126.37, 127.27, 127.83, 128.01, 128.74, 129.25, 130.00, 130.60, 131.07, 131.45, 132.65, 133.61, 135.06, 135.54, 143.81, 147.52; HRMS Calcd for $C_{27}H_{19}N_2$ $(M+H)^+$: 371.1543; Found: 371.1532.

5,6-di-*p*-tolylbenzo[4,5]imidazo[2,1-a]isoquinoline (4b)



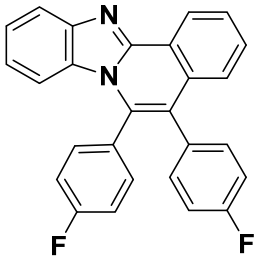
R_f 0.13 (toluene /EtOAc/$CHCl_3$ = 100/5/2). Yield = 88%, m = 85.1 mg. Wihte Solid. Mp = 265-266 °C. ^{1}H NMR (CDCl3, 399.78 MHz) δ 2.33 (s, 3H), 2.42 (s, 3H), 6.03 (d, *J* = 8.5 Hz, 1H), 6.91-6.97 (m, 1H), 7.06-7.12 (m, 4H), 7.20 (dd, *J* = 10.8, 8.5 Hz, 4H), 7.32-7.39 (m, 2H), 7.54-7.58 (m, 1H), 7.65-7.69 (m, 1H), 7.98 (d, *J* = 8.2 Hz, 1H), 8.99 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (CDCl3, 100.53 MHz) δ21.3, 21.5, 114.3, 119.4, 121.2, 122.7, 123.6, 124.1, 125.0, 126.4, 127.6, 128.7, 129.5, 129.8, 130.4, 130.8, 131.2, 131.3, 132.6, 132.9, 135.2, 136.7, 139.0, 144.0, 147.7; IR (ATR) 3025 w, 2947 w, 1627 w, 1609 w, 1529 w, 1503 m, 1475 w, 1446 s, 1369 w, 1351 w, 1334 w, 1305 w, 1292 w, 1275 w, 1255 w, 1216 w, 1182 w, 1157 w, 1111 w, 1021 w, 828 w, 818 w, 757 s, 740 s, 700 w, 662 w ; MS(DI) *m/z* (relative intensity, %) 398 ($M^{+\cdot}$, 100), 397 (23), 184 (11); HRMS Calcd for $C_{29}H_{22}N_2(M+H)^+$: 399.1856; Found: 399.1842.

5,6-di-*p*-methoxyphenylbenzo[4,5]imidazo[2,1-a]isoquinoline (4c)



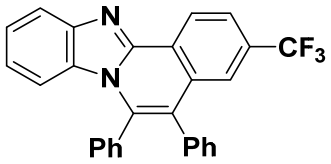
R_f 0.17 (Hexane/EtOAc = 3/1). Yield = 91%, m = 96.8 mg. Wihte Solid. Mp = 263-264 °C. ^{1}H NMR (CDCl3, 399.78 MHz) δ 3.81 (s, 3H), 3.87 (s, 3H), 6.13 (d, *J* = 8.5 Hz, 1H), 6.83 (dt, *J* = 8.7, 2.7 Hz, 2H), 6.92 (dt, *J* = 8.7, 2.7 Hz, 2H), 6.97 (ddd, *J* = 8.3, 7.1, 1.1 Hz, 1H), 7.11 (dt, *J* = 8.7, 2.7 Hz, 2H), 7.24 (dt, *J* = 8.7, 2.7 Hz, 2H), 7.38 (t, *J* = 8.2 Hz, 2H), 7.58 (td, *J* = 7.5, 1.4 Hz, 1H), 7.68 (td, *J* = 7.5, 1.2 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 8.99 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (CDCl3, 100.53 MHz) δ 55.15, 55.25, 113.47, 114.12, 114.27, 119.43, 121.19, 122.77, 123.53, 124.07, 126.18, 126.37, 127.61, 127.94, 129.83, 131.22, 131.80, 132.48, 133.06, 135.21, 144.08, 147.74, 158.47, 159.85; IR (ATR) 2359 m, 1739 s, 1609 m, 1503 s, 1444 s, 1367 s, 1291 m, 1249 s, 1219 s, 1031 m, 833 m, 771 s; MS *m/z* (relative intensity, %) 431.15 (32), 430 (M^+, 100), 97 (13), 95 (10), 84 (12), 83 (13), 81 (21), 73 (13), 71 (14), 69 (41), 60 (12), 57 (23), 55 (19); HRMS Calcd for $C_{29}H_{23}N_2O_2$ $(M+H)^+$: 431.1754; Found: 431.1753.

5,6-bis(4-fluorophenyl)benzo[4,5]imidazo[2,1-*a*]isoquinoline (4d)



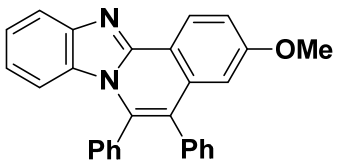
R_f 0.03 (Hexane/EtOAc = 3/1). Yield = 81%, m = 80.1 mg. Wihte Solid. Mp = 276 ℃. ^{1}H NMR (CDCl3, 399.78 MHz) δ 6.08 (d, *J* = 7.8 Hz, 1H), 6.96-7.02 (m, 3H), 7.09-7.18 (m, 4H), 7.29-7.33 (m, 3H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.70 (t, *J* = 7.8 Hz, 1H), 9.00 (d, *J* = 8.2 Hz, 1H); ^{13}C NMR (CDCl3, 100.53 MHz, quant) δ113.82, 115.20, 115.41, 116.07, 116.28, 119.62, 121.55, 122.77, 123.16, 124.40, 125.21, 126.16, 128.11, 129.58, 130.14, 130.92, 131.30, 132.41, 132.48 (d, *J* = 8.6 Hz), 132.48 (d, *J* = 8.6 Hz), 132.99 (d, *J* = 7.7 Hz), 132.99 (d, *J* = 7.7 Hz), 134.30, 143.87, 147.47, 161.95 (d, *J* = 247.3 Hz), 162.95 (d, *J* = 251.1 Hz); IR (ATR) 1064 w, 1502 s, 1446 m, 1227 s, 1158 w, 836 m, 771 m, 738 m; MS (DI) *m/z* (relative intensity, %) 407 (M^++1, 29), 406 (M^+, 100), 405 (34), 310 (11); HRMS Calcd for $C_{27}H_{17}N_2F_2$ $(M+H)^+$: 407.1354; Found: 407.1349.

5,6-diphenyl-3-(trifluoromethyl)benzo[4,5]imidazo[2,1-a]isoquinoline (4e)



R_f 0.15 (Toluene/EtOAc/$CHCl_3$ = 100/5/2). Yield = 88%, m = 94.0 mg. Wihte Solid. ^{1}H NMR (CDCl3, 399.78 MHz) δ 6.03 (d, *J* = 8.7 Hz, 1H), 6.99 (t, *J* = 7.8 Hz, 1H), 7.21 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.29-7.36 (m, 5H), 7.39-7.48 (m, 4H), 7.61 (s, 1H), 8.02 (d, *J* = 8.3 Hz, 1H), 9.14 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (CDCl3, 100.53 MHz) δ114.28, 119.81, 121.99, 123.15, 123.45 (d, *J* = 4.1 Hz), 123.83 (d, *J* = 3.1 Hz), 123.86 (q, *J* = 272.6 Hz), 124.60, 125.05, 125.89, 127.72, 128.29, 128.86, 129.50, 130.37, 131.08, 133.18, 134.55, 136.51, 144.07, 146.52; HRMS Calcd for $C_{29}H_{23}N_2O_2$ $(M+H)^+$: 439.1417; Found: 439.1406.

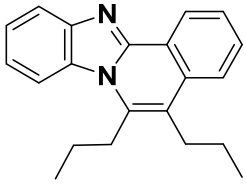
3-methoxy-5,6-diphenylbenzo[4,5]imidazo[2,1-a]isoquinoline (4f)



R_f 0.17 (toluene/EtOAc/$CHCl_3$ = 50/5/1). Yield = 63%, m = 59.7 mg. Wihte Solid. ^{1}H NMR (CDCl3, 399.78 MHz) δ 3.75 (s, 3H), 5.96 (d, *J* = 8.5 Hz, 1H), 6.73 (d, *J* = 2.5 Hz, 1H), 6.89 (td, *J* = 8.5, 1.1 Hz, 1H), 7.19-7.44 (m, 12H), 7.95 (d, *J* = 8.2 Hz, 1H), 8.92 (d, *J* = 9.0 Hz, 1H); ^{13}C NMR (CDCl3, 100.53 MHz, quant.) δ 161.02, 147.79, 144.03, 135.56, 135.56, 134.59, 133.66, 131.37, 131.37, 131.04, 130.53, 130.53, 129.20,

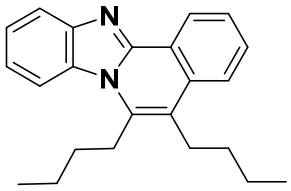
128.70, 128.70, 128.06, 128.06, 127.29, 126.99, 124.05, 123.30, 120.82, 119.04, 116.57, 116.40, 113.96, 108.75, 55.31; HRMS(DART) Calcd for $C_{28}H_{21}ClN_2O$ $(M+H)^+$: 401.1648; Found: 401.1636.

5,6-dipropylbenzo[4,5]imidazo[2,1-a]isoquinoline (4g)



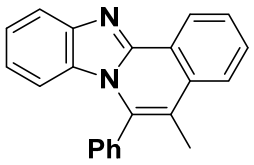
R_f 0.29 (Hexane/EtOAc = 3/1). Yield = 59%, 44.3 mg. Wihte Solid. Mp = 140 °C. ^{1}H NMR (CDCl3, 399.78 MHz) δ 1.15 (t, *J* = 7.3 Hz, 3H), 1.25 (t, *J* = 7.3 Hz, 3H), 1.69-1.78 (m, 2H), 1.87-1.97 (m, 2H), 2.98 (t, *J* = 8.1 Hz, 2H), 3.38 (t, *J* = 8.1 Hz, 2H), 7.38 (t, *J* = 8.2 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.71 (t, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.2 Hz, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 8.2 Hz, 1H), 8.94 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (CDCl3, 100.53 MHz) δ 13.82, 14.46, 21.53, 23.78, 29.53, 31.01, 114.25, 118.75, 119.84, 121.62, 122.67, 123.44, 124.01, 125.61, 126.81, 130.00, 130.71, 131.55, 135.70, 144.05, 147.91; IR (ATR) 2959 m, 2871 w, 1523 m, 1455 m, 1373 w, 1338 w, 1286 w, 912 w, 760 m, 736 s; MS (DI) *m/z* (relative intensity, %) 303 (14), 302 (M+, 59), 274 (22), 273 (100), 258 (11), 257 (32); HRMS Calcd for $C_{21}H_{23}N_2(M+H)^+$: 303.1856; Found: 303.1851.

5,6-dibutylbenzo[4,5]imidazo[2,1-a]isoquinoline (4h)



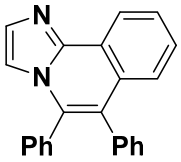
R_f 0.23 (Hexane/EtOAc = 5/1). Yield = 66%, m = 63.0 mg. Pale yellow viscous gel. ^{1}H NMR (CDCl3, 399.78 MHz) δ 1.03-1.10 (m, 6H), 1.54-1.74 (m, 6H), 1.84-1.92 (m, 2H), 2.99 (t, *J* = 8.1 Hz, 2H), 3.41 (t, *J* = 8.2 Hz, 2H), 7.38 (td, *J* = 7.8, 1.1 Hz, 1H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.71 (td, *J* = 7.6, 1.4 Hz, 1H), 7.88 (d, *J* = 8.3 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 8.93 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (CDCl3, 100.53 MHz) δ 13.95, 13.98, 22.67, 23.16, 27.16, 28.92, 30.25, 32.65, 114.33, 118.68, 119.90, 121.57, 122.72, 123.39, 123.96, 125.57, 126.99, 130.75, 131.55, 135.80, 144.20, 148.02; IR (ATR) 2956 m, 2927 w, 2870 w, 1630 w, 1523 m, 1452 m, 1375 w, 1337 m, 1282 m, 1254 w, 760 m, 734 s; MS *m/z* (relative intensity, %)331 (25), 330 (M+, 97), 288 (20), 287 (78), 257 (24), 246 (20), 245 (100), 243 (12), 232 (15); HRMS Calcd for $C_{23}H_{27}N_2(M+H)^+$: 331.2169; Found:331.2164.

5,6-dipropylbenzo[4,5]imidazo[2,1-a]isoquinoline (4i)



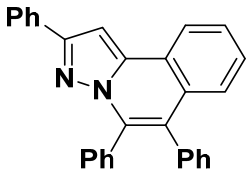
R_f 0.29 (Hexane/EtOAc = 3/1). Yield = 78%, m = 58.3 mg. Pale Yellow Solid. ^{1}H NMR (CDCl3, 399.78 MHz) δ 2.31 (s, 3H), 5.93 (dd, *J* = 9.6, 0.9 Hz, 1H), 6.91 (ddd, *J* = 8.7, 6.9, 0.5 Hz, 1H), 7.34 (ddd, *J* = 8.0, 7.3, 0.9 Hz, 1H), 7.78 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.62-7.78 (m, 5H), 7.93 (td, *J* = 9.2, 1.4 Hz, 2H), 8.97 (dd, *J* = 8.2, 1.4 Hz, 1H) ; ^{13}C NMR (CDCl3, 100.53 MHz) δ 14.48, 113.80, 115.54, 119.36, 121.06, 123.02, 123.86, 124.02, 125.35, 127.64, 129.51, 129.74, 130.06, 130.20, 131.06, 132.30, 134.25, 134.48, 143.85, 147.48 ; IR (ATR) 3058 w, 1633 w, 1560 w, 1525 m, 1479 w, 1447 s, 1376 m, 1335 w, 1304 w, 1282 w, 1252 w, 1163 w, 1014 w, 910 w, 792 w, 758 s, 737 s, 702 s; MS (DI) *m/z* (relative intensity, %) 309 (24), 308 (M+, 100), 307 (39), 306 (14), 305 (15), 147 (24); HRMS Calcd for $C_{22}H_{17}N_2$ $(M+H)^+$: 309.1386; Found: 309.1379.

5,6-dipropylbenzo[4,5]imidazo[2,1-a]isoquinoline (6)



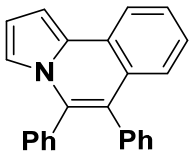
R_f 0.20 (Hexane/EtOAc/$CHCl_3$ = 150/50/3). Yield = 81%, m = 67.5 mg. Pale Yellow Solid. ^{1}H NMR (CDCl3, 399.78 MHz) δ 7.19-7.21 (m, 3H), 7.23-7.35(m, 6H), 7.40 (d, *J* = 8.2 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.56 (s, 1H), 7.66 (t, *J* = 7.4 Hz, 1H), 8.80 (brs, 1H) ; ^{13}C NMR (CDCl3, 100.53 MHz, quant.) δ 113.90, 123.14, 123.16, 124.42, 126.40, 127.26, 127.80, 128.01, 128.01, 128.01, 128.60, 128.60, 128.81, 130.16, 130.16, 130.56, 130.80, 131.38, 131.38, 133.34, 133.43, 135.88, 143.03 ; HRMS Calcd for $C_{24}H_{19}ClN_2$ $(M+H)^+$: 321.1386; Found: 321.1340.

2,5,6-triphenylpyrazolo[5,1-a]isoquinoline (8)

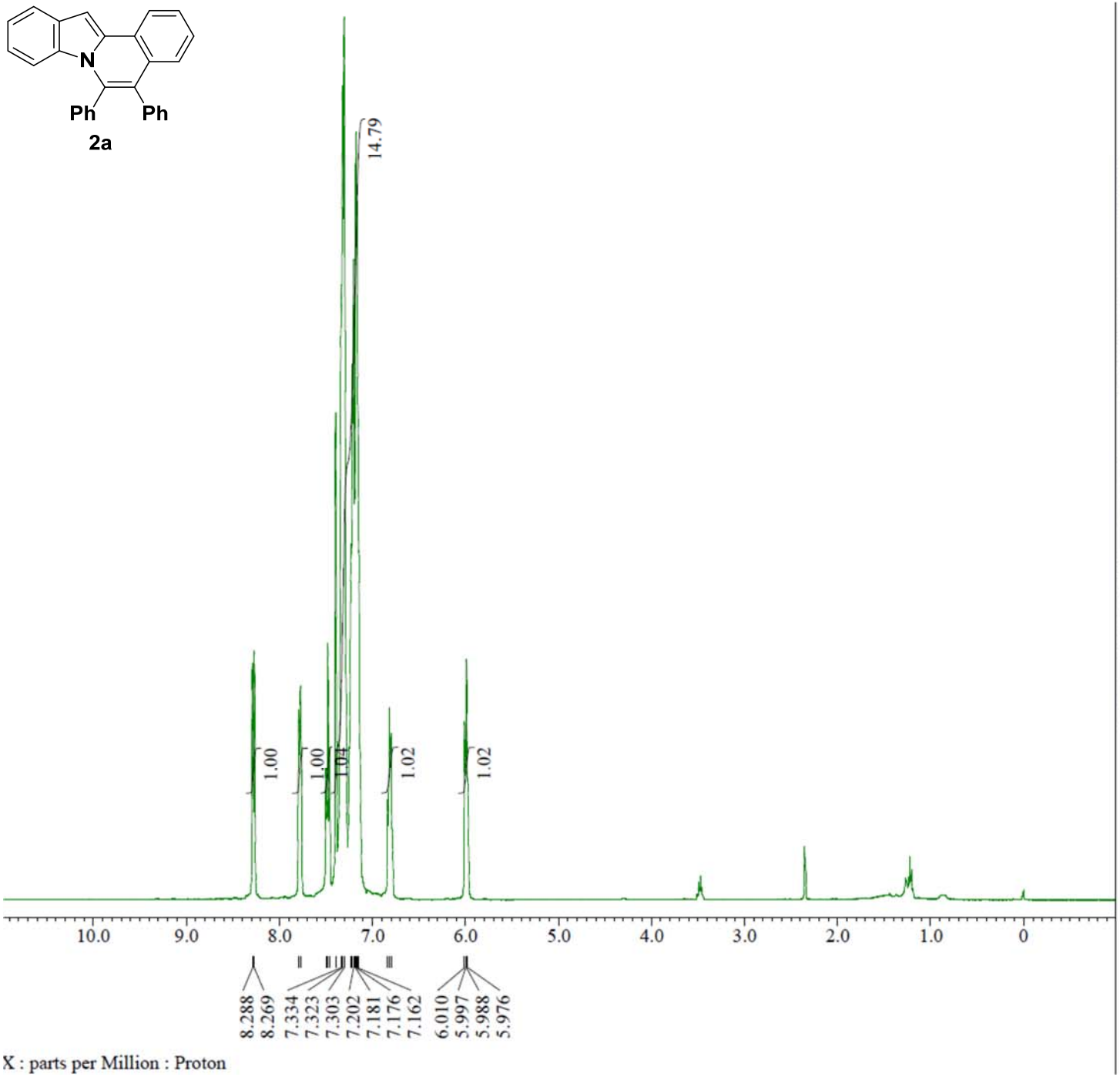


White solid, Mp = 186-188 °C. R_f = 0.50 (hexane/diethyl ether 3:1). Yield = 92 %, m = 92.0 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 7.19-7.42 (m, 16H), 7.53-7.57 (m, 1H), 7.92 (d, *J* = 7.3 Hz, 2H), 8.20 (d, *J* = 7.8 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 94.7, 123.7, 123.9, 124.0, 126.5, 126.9, 127.2, 127.4, 127.6, 127.8, 128.1, 128.2, 128.2, 128.7, 130.1, 131.5, 131.8, 133.1, 133.5, 136.5, 136.5, 140.0, 152.3. **IR** (ATR): 3059 w, 1623 w, 1600 w, 1538 w, 1488 w, 1455 m, 1389 w, 1341 w, 1277 w, 1179 w, 1074 w, 1028 w, 952 w, 916 w, 863 w, 693 s. **MS** (EI+): 397 (27), 396 (M^+, 97), 395 (100), 198 (11). **HRMS** (EI+) Calcd for $C_{29}H_{20}N_2$: 396.1626; Found: 396.1631.

5,6-diphenylpyrrolo[2,1-a]isoquinoline (10)



Yellow solid, Mp = 216-217 °C. R_f = 0.60 (hexane/diethyl ether 3:1). Yield = 61 %, m = 48.7 mg. **^{1}H NMR** (399.78 MHz, $CDCl_3$): δ 6.65-6.67 (m, 1H), 6.86-6.87 (m, 1H), 7.08 (d, *J* = 4.1 Hz, 1H), 7.15-7.37 (m, 12H), 7.44-7.48 (m, 1H), 8.13 (d, *J* = 7.8 Hz, 1H); **^{13}C NMR** (100.53 MHz, $CDCl_3$): δ 100.3, 111.5, 115.1, 122.0, 122.5, 125.4, 125.9, 126.5, 126.9, 127.2, 128.0, 128.3, 128.5, 128.6, 130.5, 130.6, 131.7, 134.2, 134.4, 137.0. **IR** (ATR): 3056 w, 1601 w, 1484 w, 1444 w, 1371 w, 1335 w, 1261 w, 1148 w, 1109 w, 1071 w, 1025 w, 698 w. **MS** (EI+): 320 (25), 319 (M^+, 100), 318 (66), 317 (19). **HRMS** (EI+) Calcd for $C_{24}H_{17}N$: 319.1361; Found: 319.1361.

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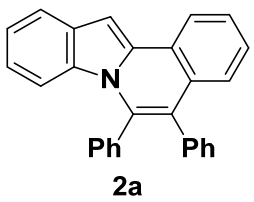
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 26
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```



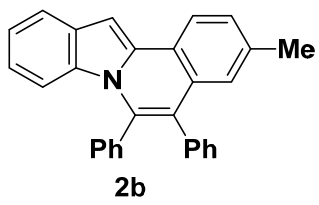
2a


```
Filename          = AO-1123 GPC_Carbon-1-1.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1123 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 13-MAR-2018 04:35:13
Revision_Time     = 13-MAR-2018 10:07:42
Current_Time      = 16-MAR-2018 19:12:33

Comment           = AO-1123 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```



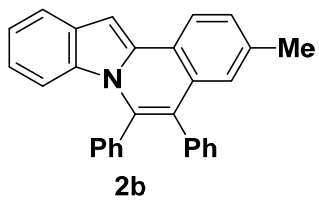
2b


```
Filename          = AO-1163 GPC_Proton-2-1.jd
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1163 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 26-FEB-2018 21:25:03
Revision_Time     =  6-MAR-2018 12:42:07
Current_Time      = 16-MAR-2018 19:17:59

Comment           = AO-1163 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 30
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```



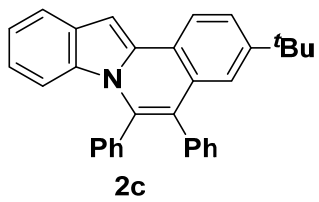
2b


```
Filename          = AO-1163 GPC_Carbon-1-1.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1163 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 27-FEB-2018 09:04:29
Revision_Time     = 27-FEB-2018 13:03:14
Current_Time      = 16-MAR-2018 19:17:45

Comment           = AO-1163 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```



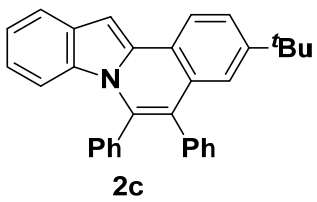
2c


```
Filename          = AO-1176 GPC_Proton-2-1.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1176 GPC
Solvent           = CHLOROFORM-D
Creation_Time     =  6-MAR-2018 10:20:07
Revision_Time     =  6-MAR-2018 12:47:11
Current_Time      = 16-MAR-2018 19:19:37

Comment           = AO-1176 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```



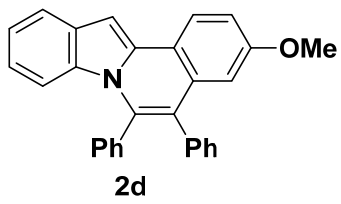
2c


```
Filename          = AO-1176 GPC_Carbon-1-1.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1176 GPC
Solvent           = CHLOROFORM-D
Creation_Time     =  6-MAR-2018 04:05:16
Revision_Time     =  6-MAR-2018 12:47:55
Current_Time      = 16-MAR-2018 19:19:19

Comment           = AO-1176 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```



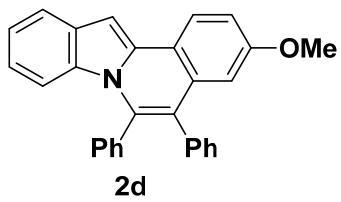
2d


```
Filename          = AO-1131 GPC_Proton-1-1.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1131 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 21-DEC-2017 15:45:40
Revision_Time     =  6-MAR-2018 12:51:15
Current_Time      = 16-MAR-2018 19:13:27

Comment           = AO-1131 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18365952[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45794685[Hz]
X_Sweep           = 7.5030012[kHz]
X_Sweep_Clipped   = 6.00240096[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 44
Temp_Get          = 17.9[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18365952[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18365952[s]
```



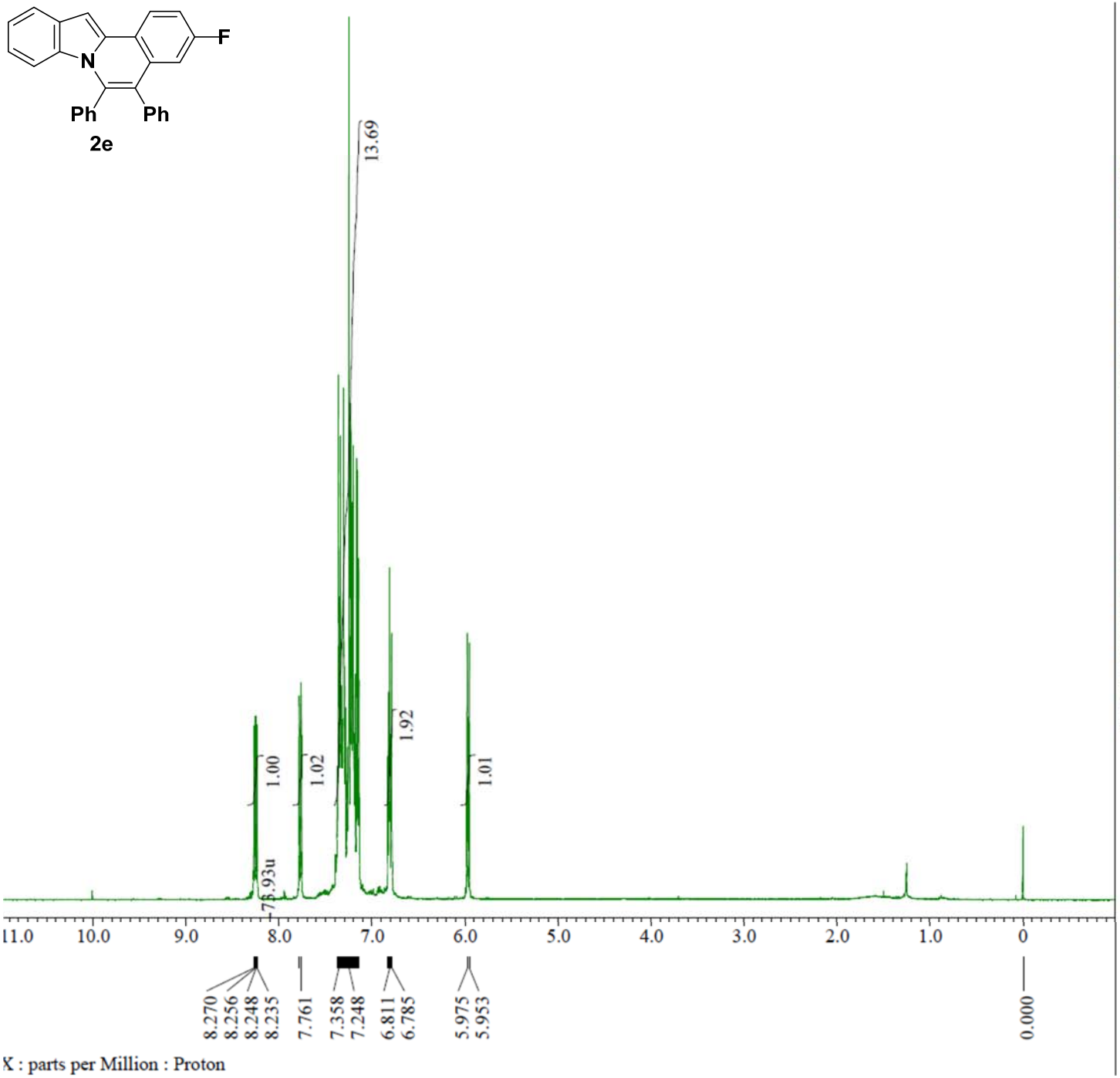
2d


```
Filename          = AO-1131 GPC_Carbon-1-1.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1131 GPC
Solvent           = CHLOROFORM-D
Creation_Time     =  6-MAR-2018 02:05:35
Revision_Time     =  6-MAR-2018 12:49:38
Current_Time      = 16-MAR-2018 19:13:12

Comment           = AO-1131 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```

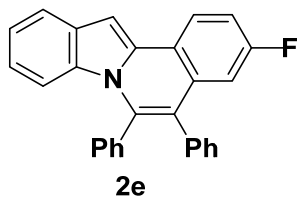



```
Filename          = AO-1134 GPC_Proton-3-1.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1134 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 22-FEB-2018 18:23:24
Revision_Time     =  6-MAR-2018 12:54:30
Current_Time      = 16-MAR-2018 19:13:52

Comment           = AO-1134 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```



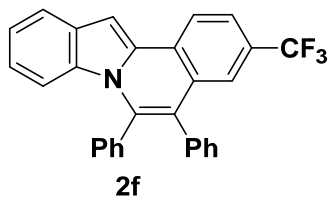
2e


```
Filename          = AO-1134 GPC_Carbon-2-1.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1134 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 23-FEB-2018 02:04:31
Revision_Time     = 23-FEB-2018 10:03:27
Current_Time      = 16-MAR-2018 19:14:07

Comment           = AO-1134 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```



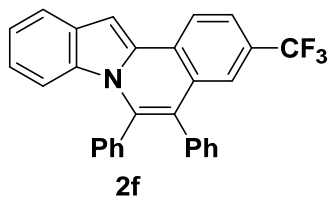
2f


```
Filename          = AO-1189 GPC_Proton-1-1.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1189 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 23-FEB-2018 17:39:11
Revision_Time     =  6-MAR-2018 12:34:54
Current_Time      = 16-MAR-2018 19:20:17

Comment           = AO-1189 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```



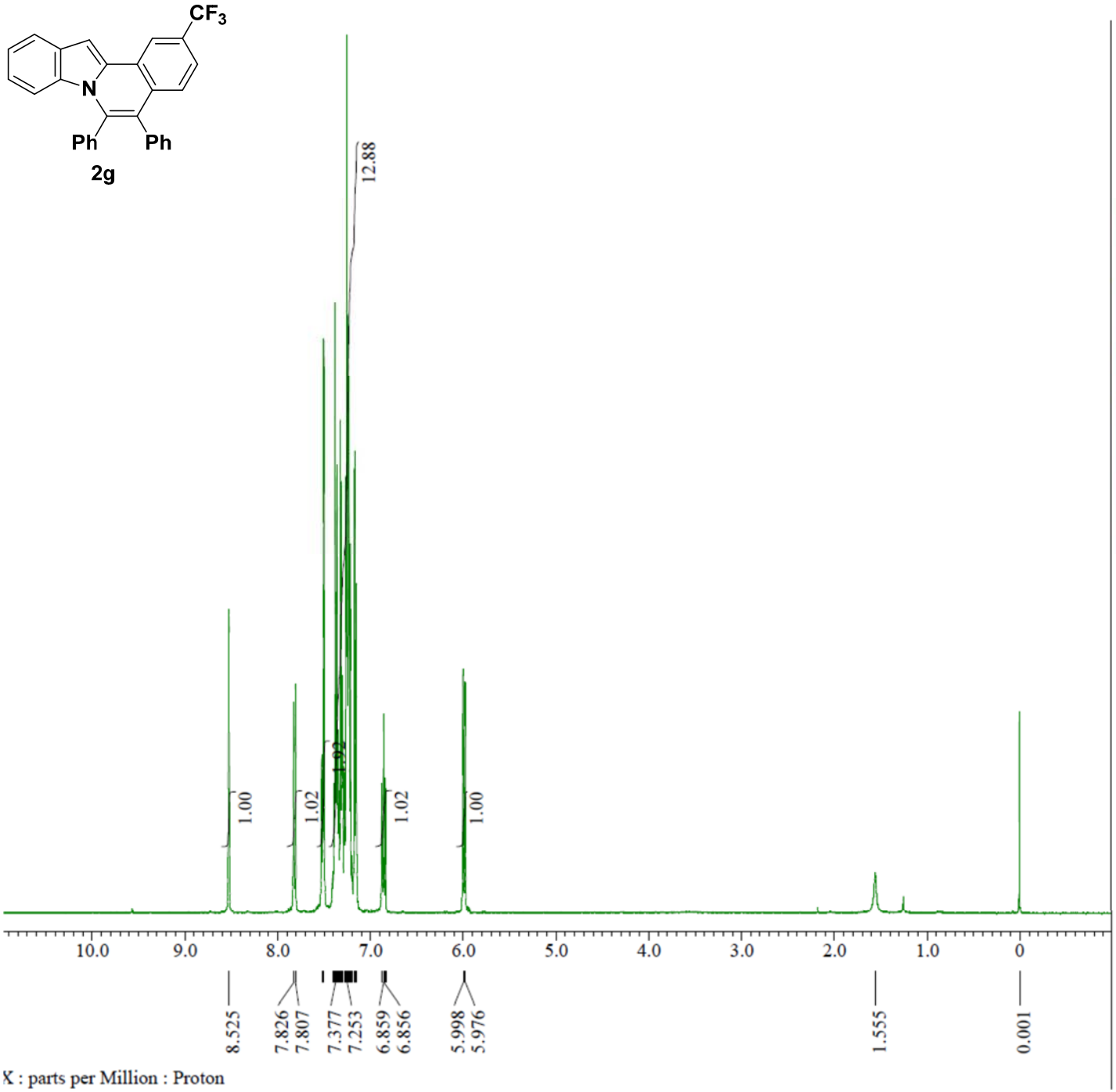
2f


```
Filename          = AO-1189 GPC_Carbon-1-1.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1189 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 24-FEB-2018 03:03:57
Revision_Time     =  6-MAR-2018 12:36:19
Current_Time      = 16-MAR-2018 19:19:57

Comment           = AO-1189 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```

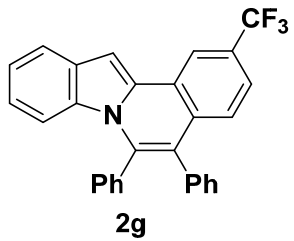



```
Filename          = AO-1174_Proton-1-1.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1174
Solvent           = CHLOROFORM-D
Creation_Time     =  6-MAR-2018 19:56:07
Revision_Time     =  7-MAR-2018 10:21:59
Current_Time      = 16-MAR-2018 19:18:53

Comment           = AO-1174
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 30
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```



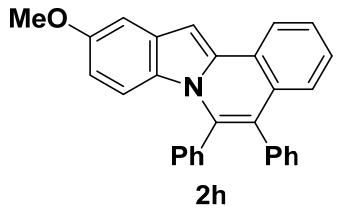
2g


```
Filename          = AO-1174_Carbon-1-1.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1174
Solvent           = CHLOROFORM-D
Creation_Time     =  7-MAR-2018 02:05:40
Revision_Time     =  7-MAR-2018 09:52:14
Current_Time      = 16-MAR-2018 19:18:34

Comment           = AO-1174
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```



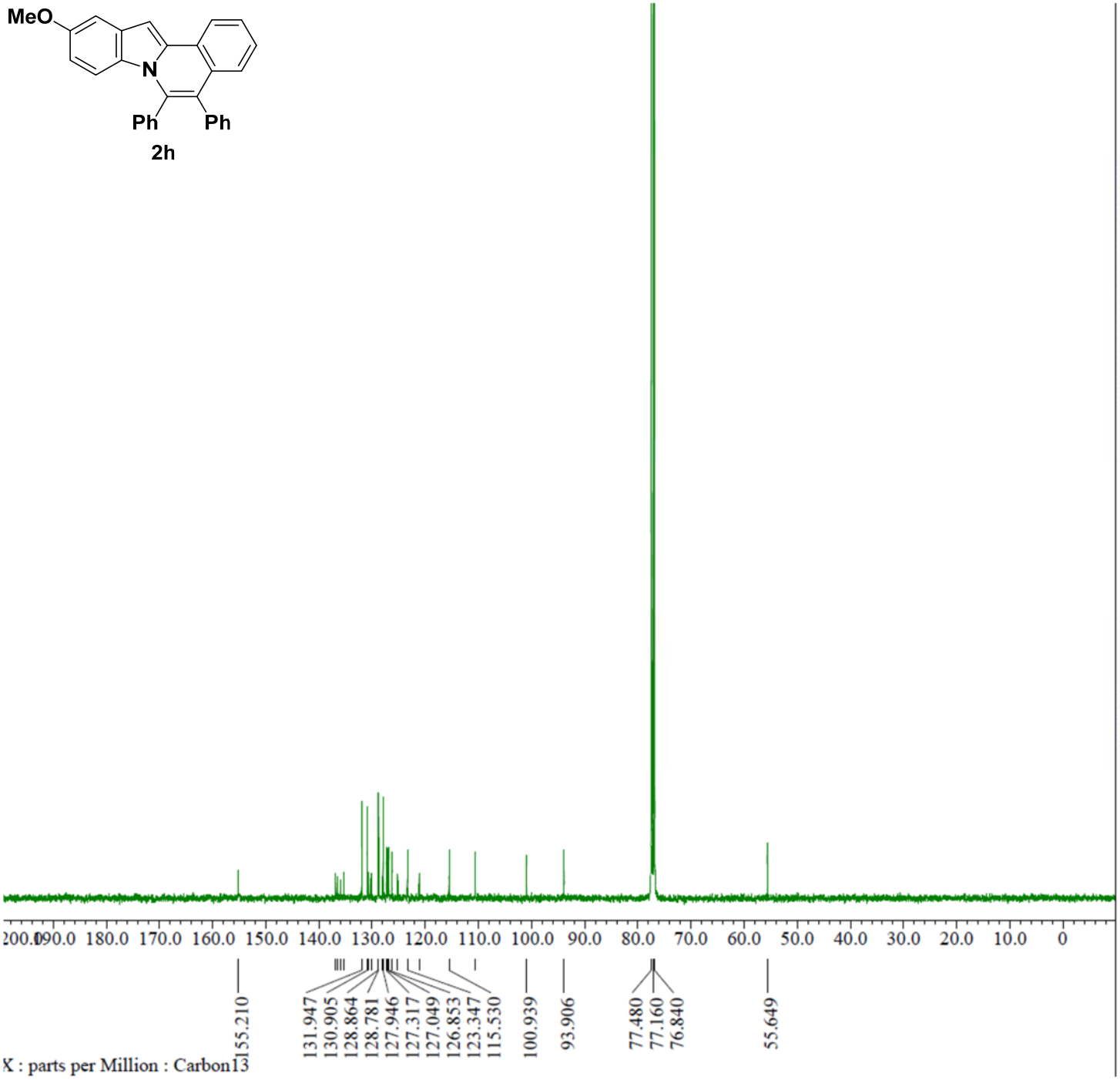
2h


```
Filename          = AO-1156 GPC_Proton-2-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1156 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 22-FEB-2018 19:22:28
Revision_Time     = 23-FEB-2018 10:28:52
Current_Time      = 16-MAR-2018 19:15:23

Comment           = AO-1156 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```

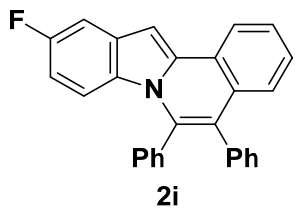



```
Filename          = AO-1156 GPC_Carbon-1-1.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1156 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 23-FEB-2018 05:05:16
Revision_Time     = 23-FEB-2018 10:02:30
Current_Time      = 16-MAR-2018 19:15:51

Comment           = AO-1156 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```



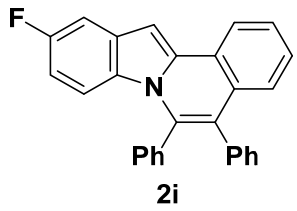
2i


```
Filename          = AO-1151 GPC_Proton-1-1.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1151 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 22-FEB-2018 19:16:29
Revision_Time     = 23-FEB-2018 10:06:05
Current_Time      = 16-MAR-2018 19:14:50

Comment           = AO-1151 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```



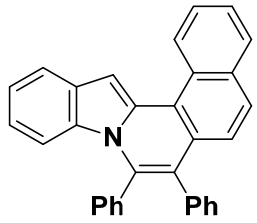
2i


```
Filename          = AO-1151 GPC_Carbon-1-1.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1151 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 23-FEB-2018 04:04:34
Revision_Time     = 23-FEB-2018 10:00:37
Current_Time      = 16-MAR-2018 19:14:29

Comment           = AO-1151 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```



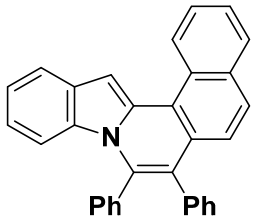
2i


```
Filename          = AO-1160 GPC_Proton-2-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1160 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 26-FEB-2018 21:19:05
Revision_Time     =  9-MAR-2018 16:02:55
Current_Time      = 16-MAR-2018 19:17:19

Comment           = AO-1160 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```



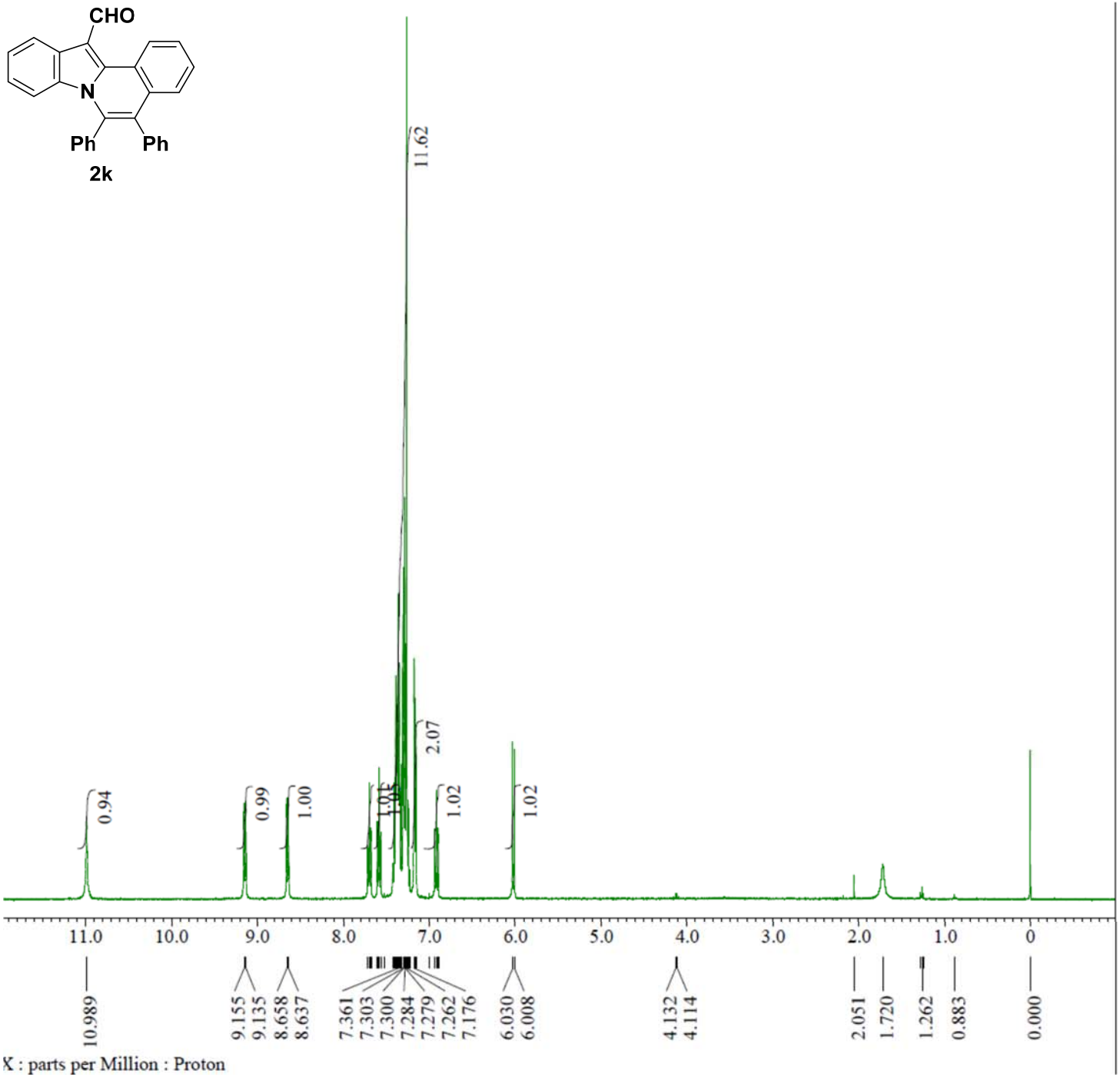
2i


```
Filename          = AO-1160 GPC_Carbon-1-1.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1160 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 27-FEB-2018 08:05:35
Revision_Time     = 27-FEB-2018 13:03:51
Current_Time      = 16-MAR-2018 19:17:05

Comment           = AO-1160 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```

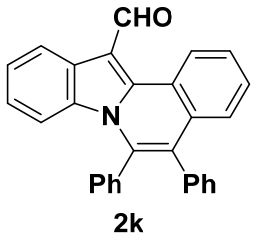



```
Filename          = AO-1158 GPC_Proton-1-1.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1158 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 22-FEB-2018 18:29:36
Revision_Time     = 23-FEB-2018 10:04:50
Current_Time      = 16-MAR-2018 19:16:41

Comment           = AO-1158 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```



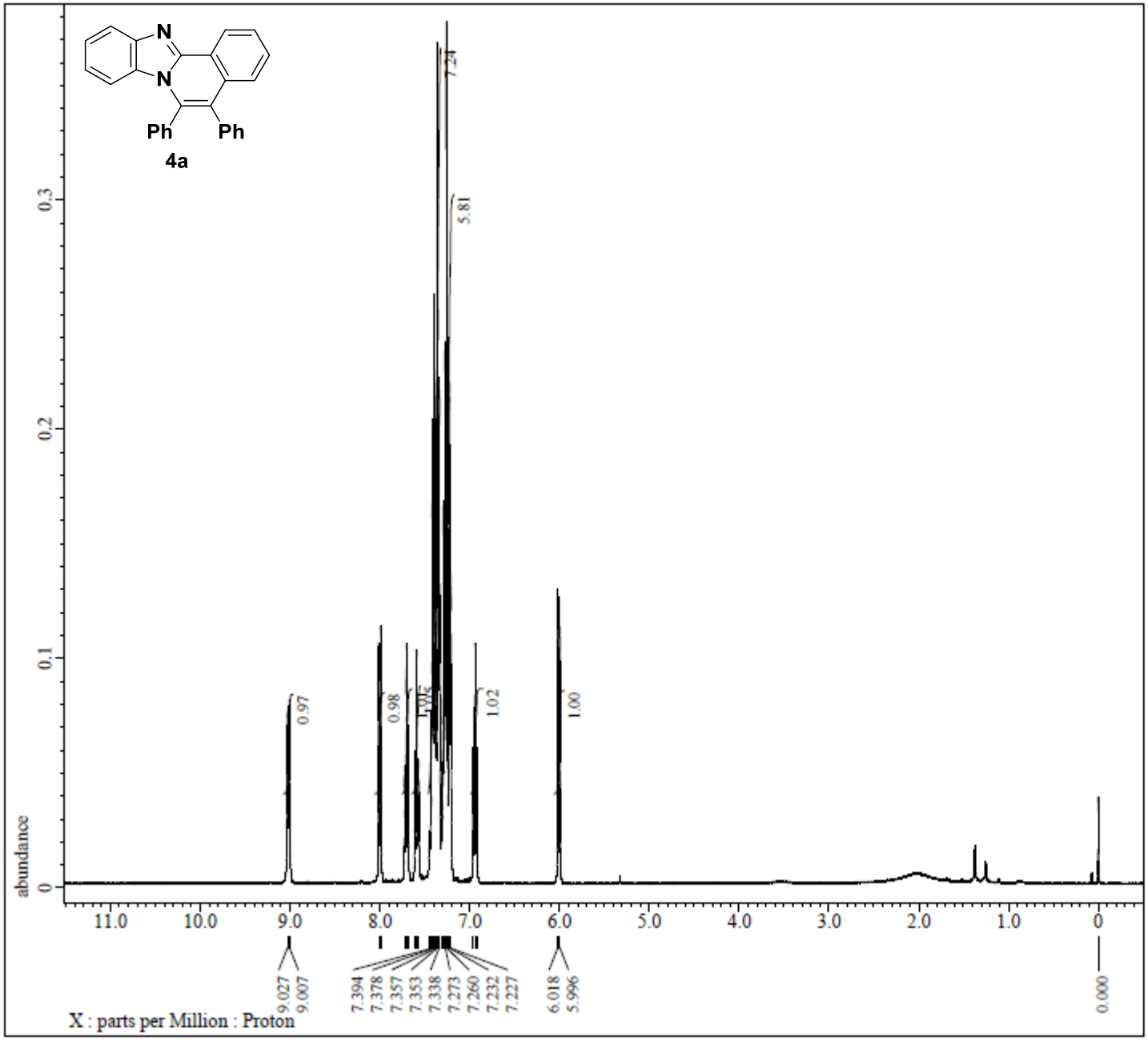
2k


```
Filename          = AO-1158 GPC_Carbon-2-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1158 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 24-FEB-2018 02:05:27
Revision_Time     = 12-MAR-2018 14:19:57
Current_Time      = 16-MAR-2018 19:16:22

Comment           = AO-1158 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = TRUE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```



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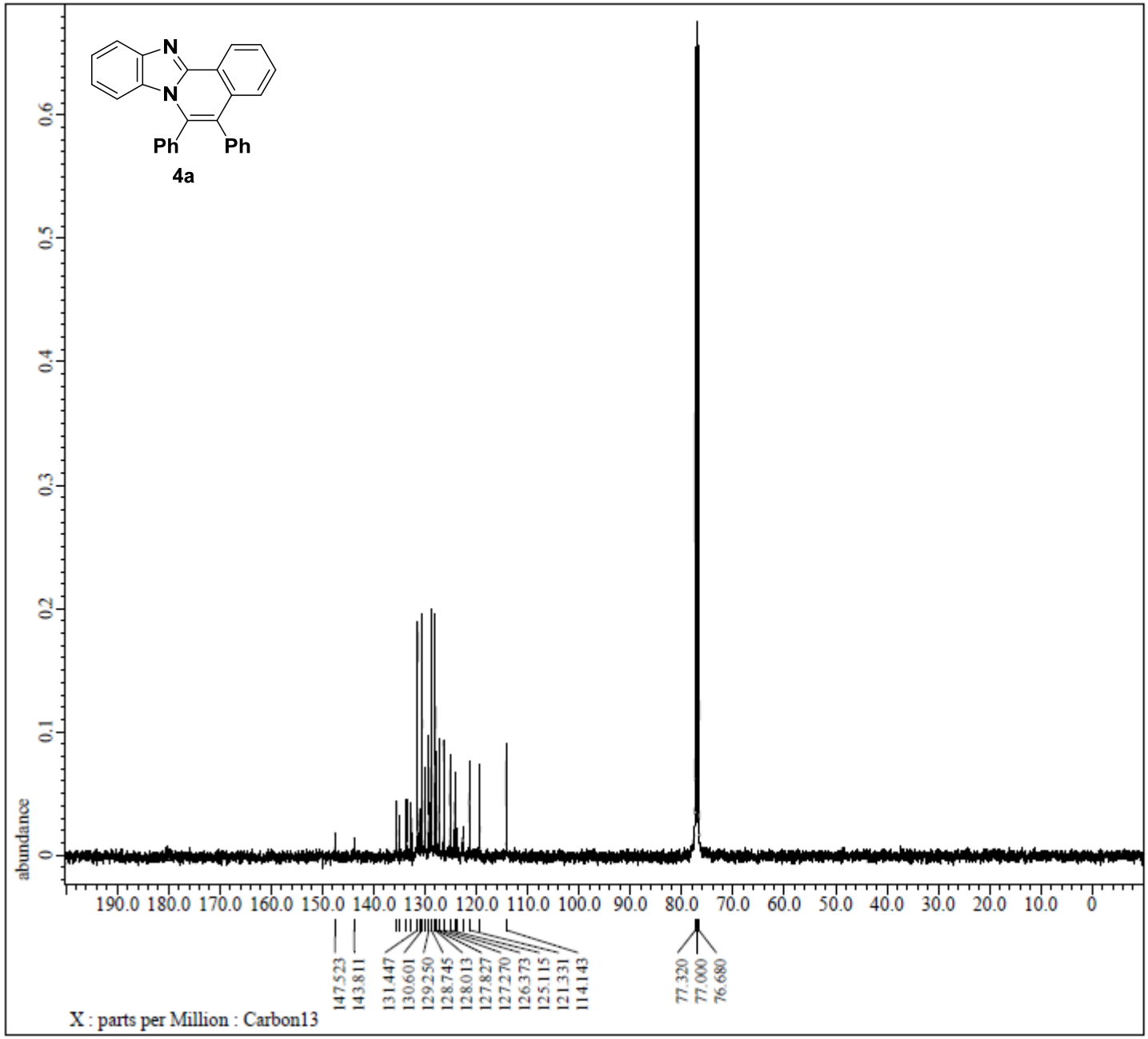
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = AS_283 column b_Proton-1-2
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AS_283 column b
Solvent           = CHLOROFORM-D
Creation_Time     =  5-JUN-2018 21:56:06
Revision_Time     =  6-JUN-2018 14:58:11
Current_Time      = 25-OCT-2018 08:54:44

Comment           = AS_283 column b
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 4.36207616[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 32768
X_Prescans        = 1
X_Resolution      = 0.22924863[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 34
Temp_Get          = 19.7[dC]
X_90_Width        = 11.5[us]
X_Acq_Time        = 4.36207616[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.75[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



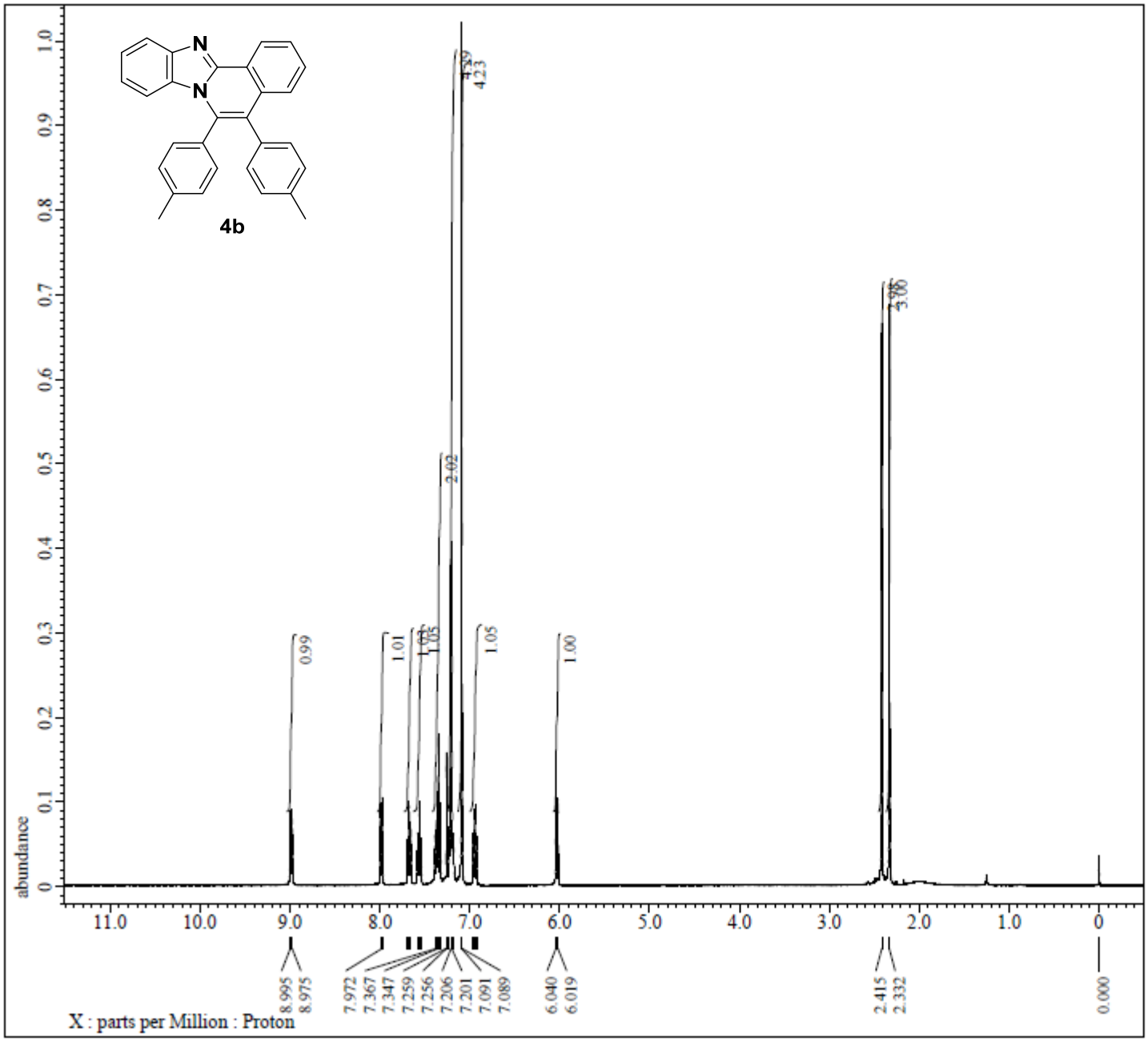

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = AS_283 column b_Carbon-2-3
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AS_283 column b
Solvent           = CHLOROFORM-D
Creation_Time     =  8-JUN-2018 02:08:40
Revision_Time     = 25-OCT-2018 09:01:50
Current_Time      = 25-OCT-2018 09:02:11

Comment           = AS_283 column b
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-EC8400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 20[dC]
X_90_Width        = 14.5[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.83333333[us]
Irr_Atn_Dec       = 21.5[dB]
Irr_Atn_Noe       = 21.5[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



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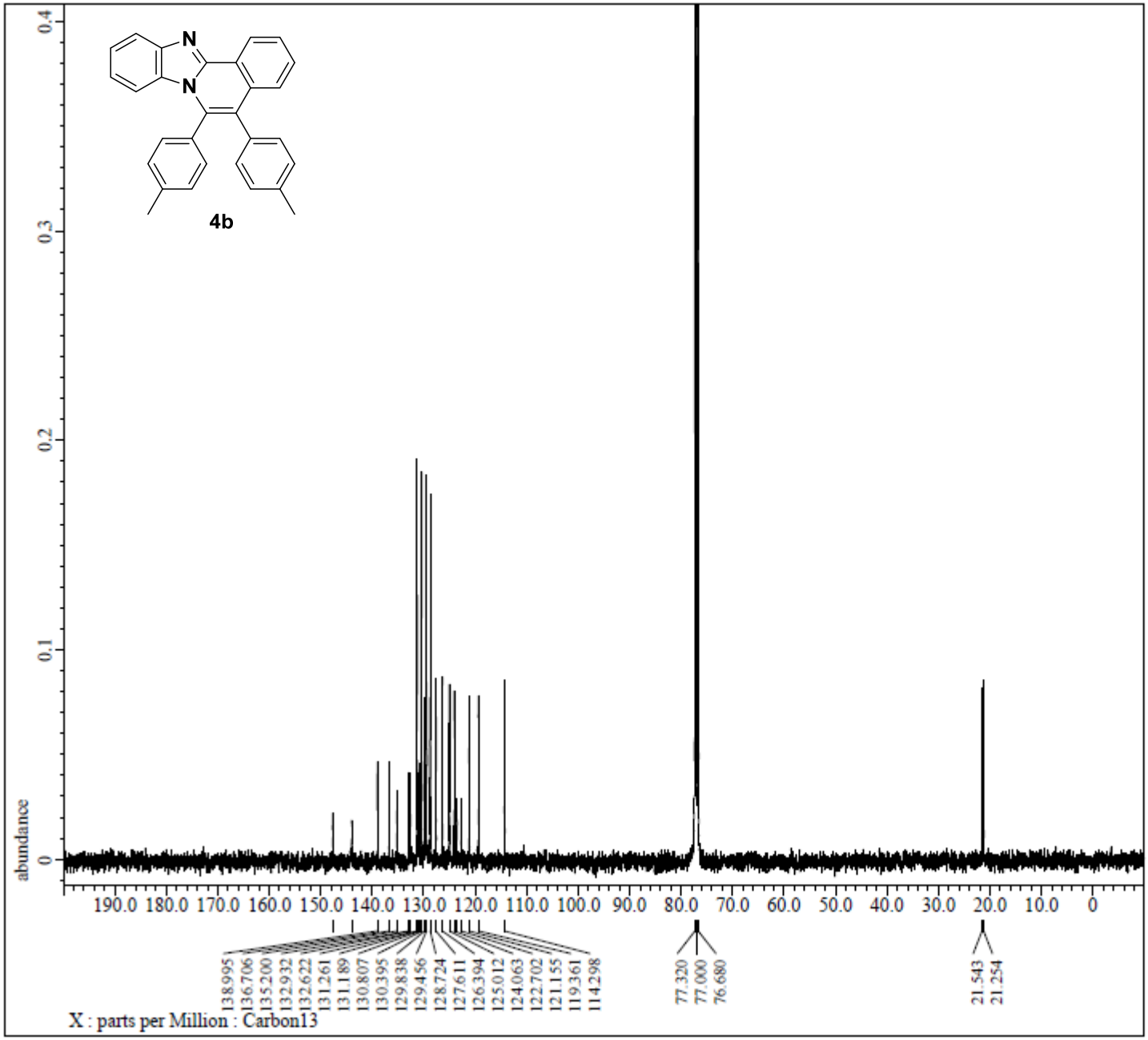
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = AS_329 column f15-18 rc_Pr
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AS_329 column f15-18 rc
Solvent           = CHLOROFORM-D
Creation_Time     = 17-MAY-2018 10:04:02
Revision_Time     = 17-MAY-2018 10:31:26
Current_Time      = 25-OCT-2018 09:12:20

Comment           = AS_329 column f15-18 rc
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 4.36207616[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 32768
X_Prescans        = 1
X_Resolution      = 0.22924863[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 32
Temp_Get          = 19.6[dC]
X_90_Width        = 11.5[us]
X_Acq_Time        = 4.36207616[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.75[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



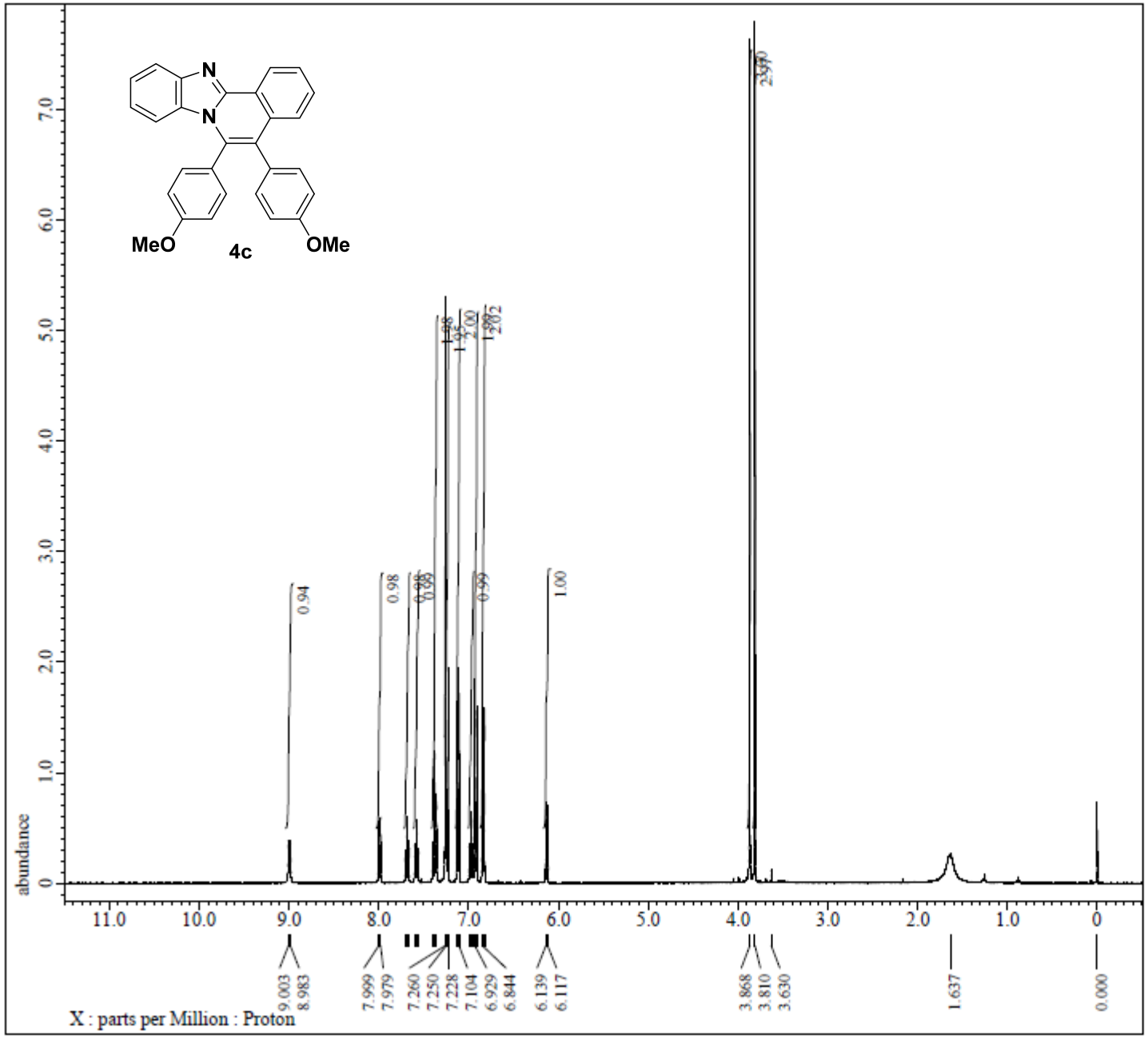
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm

Filename = AS_329 column f15-18 rc_Ca
Author = delta
Experiment = carbon.jxp
Sample_Id = AS_329 column f15-18 rc
Solvent = CHLOROFORM-D
Creation_Time = 18-MAY-2018 09:34:08
Revision_Time = 21-MAY-2018 15:16:06
Current_Time = 25-OCT-2018 09:13:41

Comment = AS_329 column f15-18 rc
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 0.96468992[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.03660252[Hz]
X_Sweep = 33.9673913[kHz]
X_Sweep_Clipped = 27.17391304[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1280
Total_Scans = 1280

Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.3[dC]
X_90_Width = 14.5[us]
X_Acq_Time = 0.96468992[s]
X_Angle = 30[deg]
X_Atn = 7[dB]
X_Pulse = 4.83333333[us]
Irr_Atn_Dec = 21.5[dB]
Irr_Atn_Noe = 21.5[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.115[ms]
Decoupling = TRUE



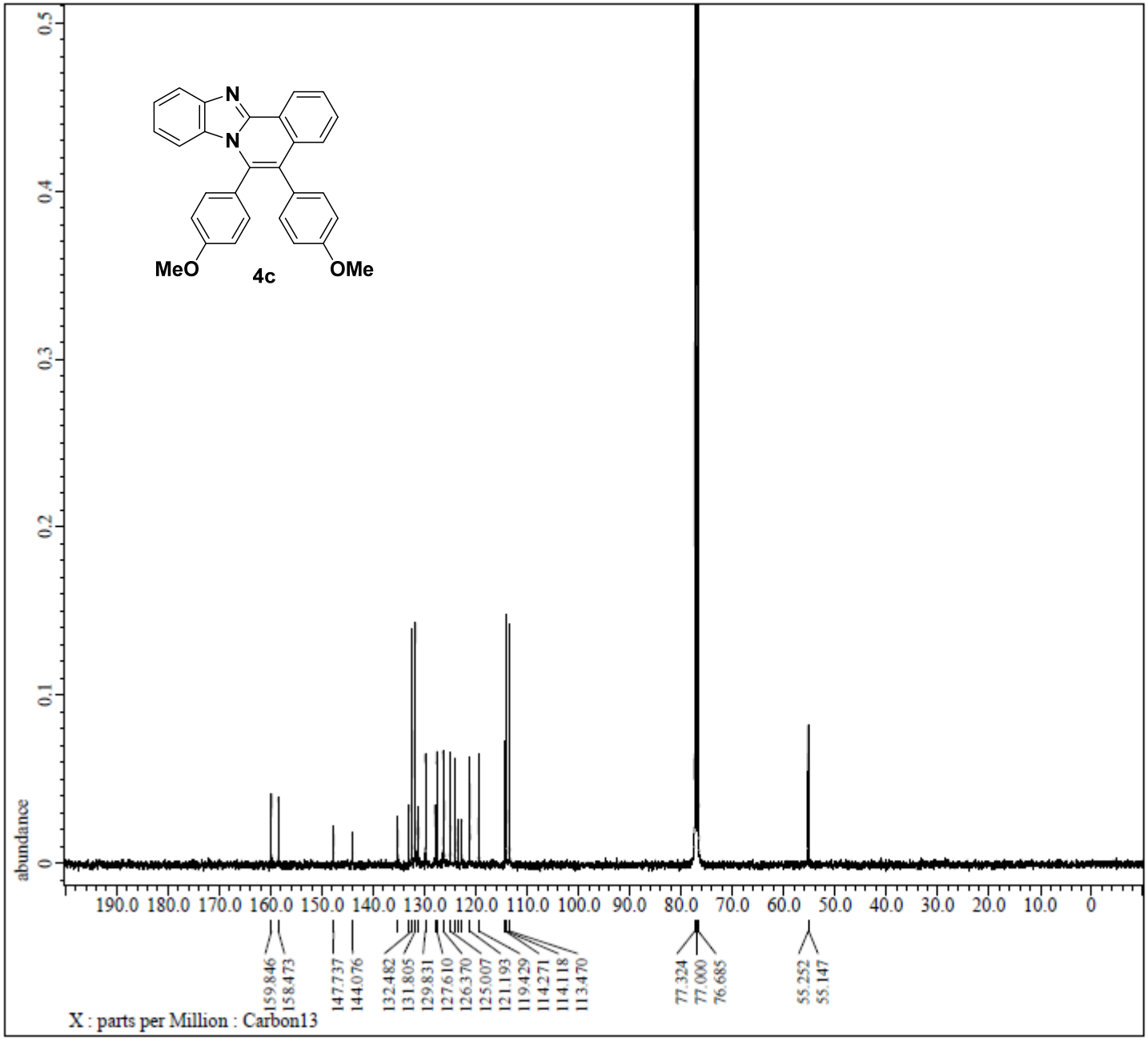

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01181[ppm], 0[ppm] )
```

```
Filename          = AS_342 column solid_Proton
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AS_342 column solid
Solvent           = CHLOROFORM-D
Creation_Time     = 26-JUL-2018 21:37:24
Revision_Time     = 26-JUL-2018 23:13:58
Current_Time      = 25-OCT-2018 09:20:42

Comment           = AS_342 column solid
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 5[s]
Recvr_Gain        = 50
Temp_Get          = 25.1[dC]
X_90_Width        = 11.5[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.75[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



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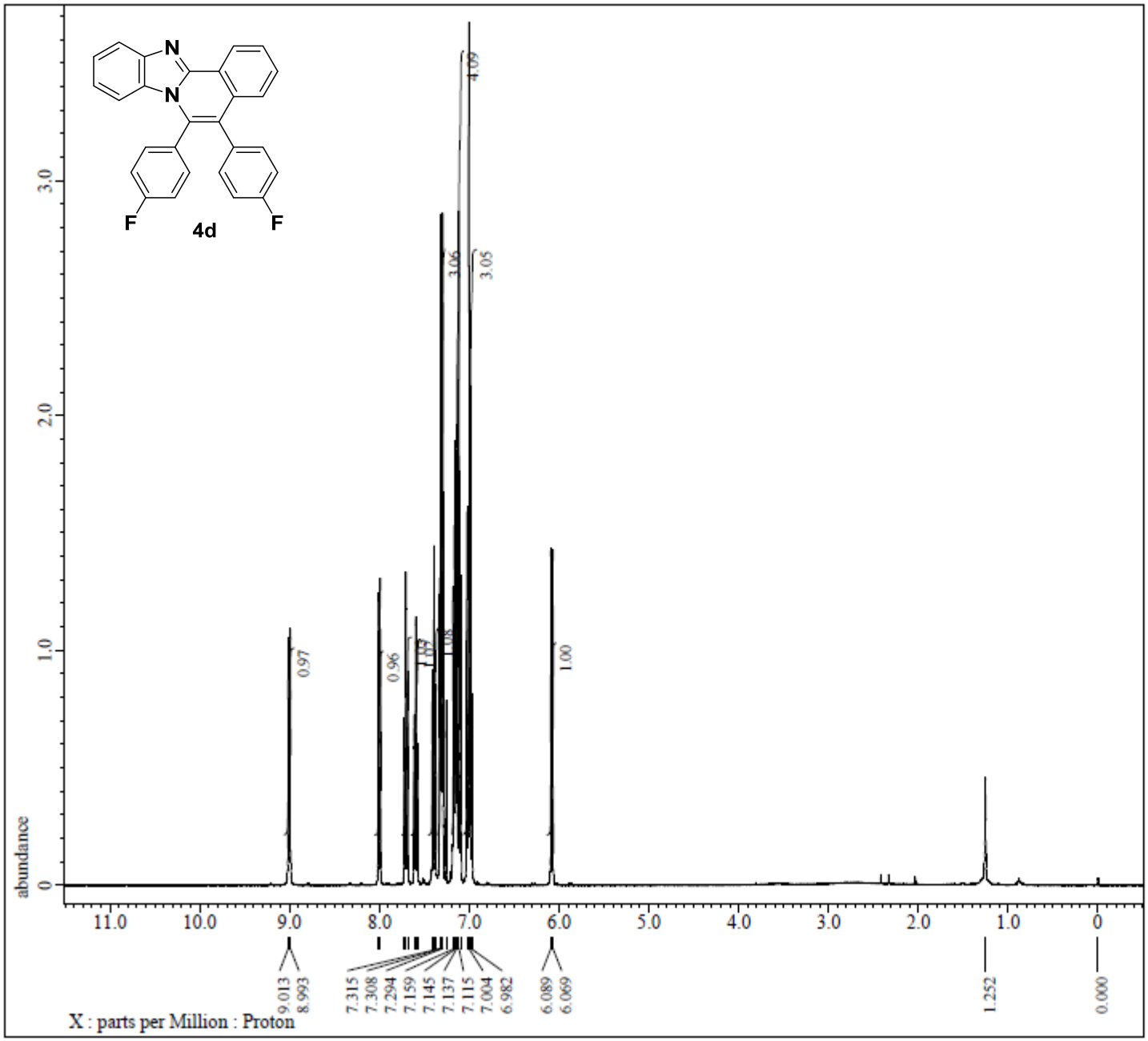
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= AS_342 rc_Carbon-2-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= AS_342 rc
Solvent	= CHLOROFORM-D
Creation_Time	= 13-SEP-2018 23:06:06
Revision_Time	= 14-SEP-2018 22:59:42
Current_Time	= 25-OCT-2018 09:19:59
Comment	= AS_342 rc
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 4096
Total_Scans	= 4096
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.2[dC]
X_90_Width	= 10.5[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 6[dB]
X_Pulse	= 3.5[us]
Irr_Atn_Dec	= 21.5[dB]
Irr_Atn_Noe	= 21.5[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE



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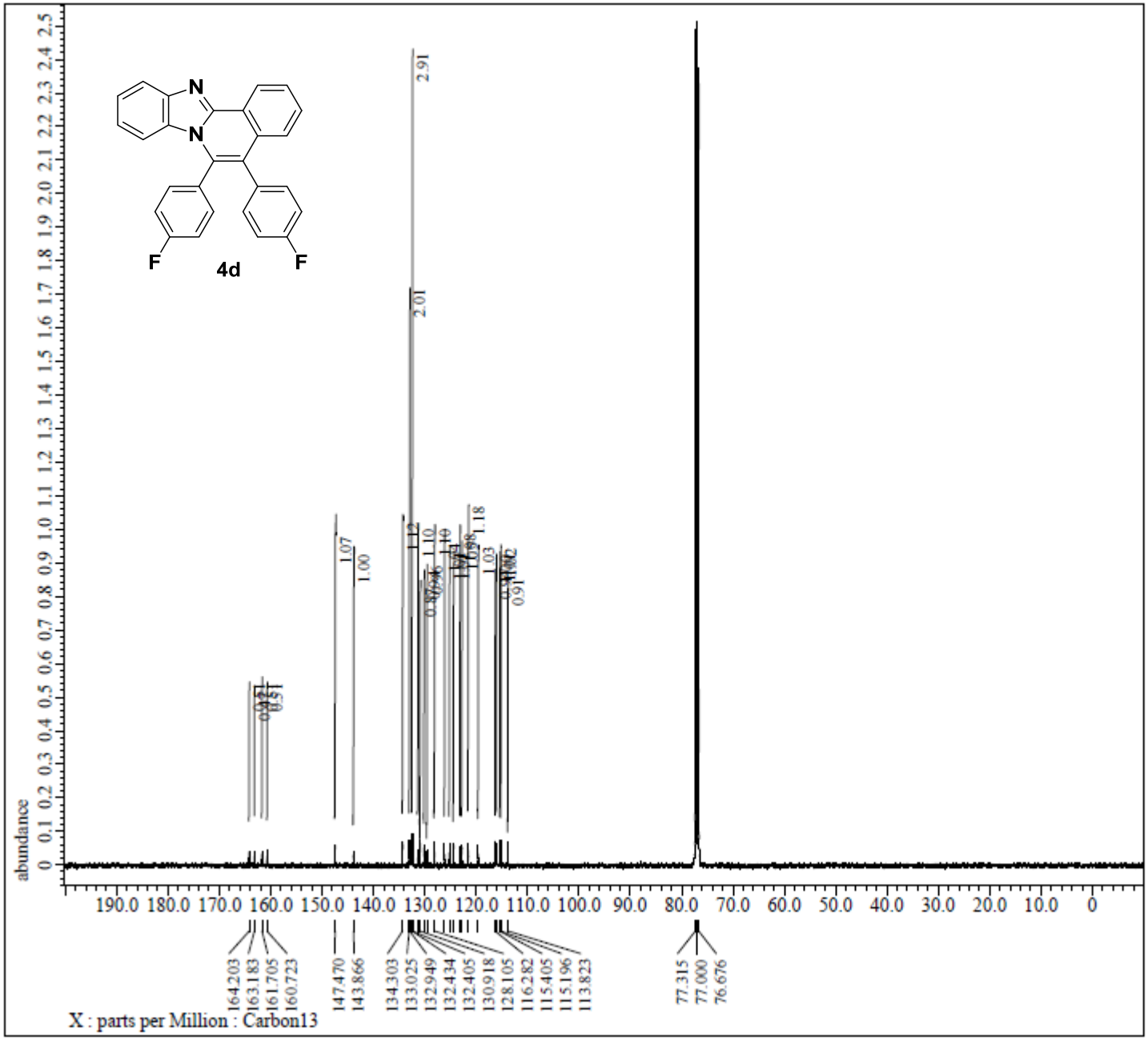
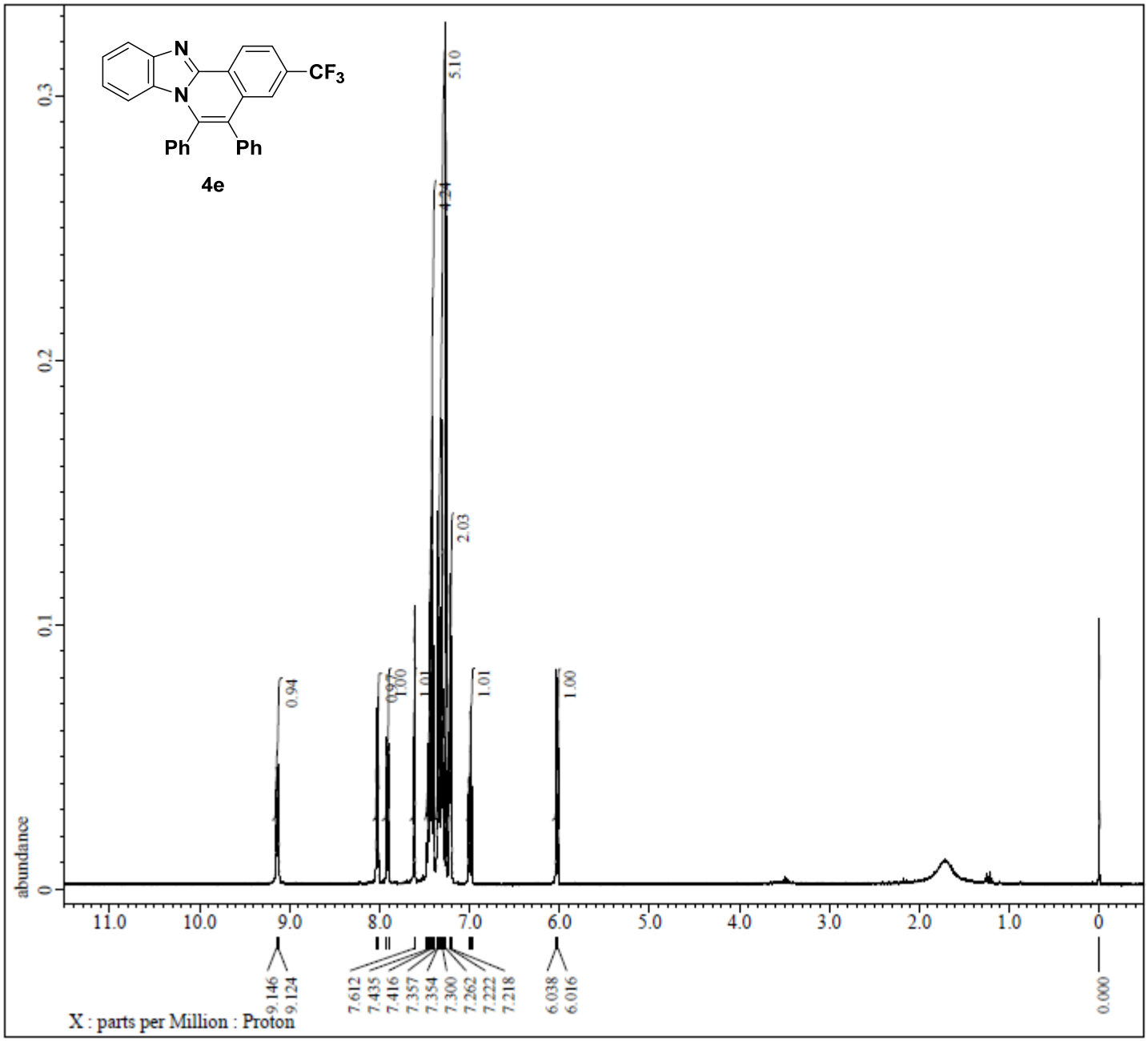
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= AS_313 column rc 1_Proton-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= AS_313 column rc 1
Solvent	= CHLOROFORM-D
Creation_Time	= 26-JUL-2018 12:40:34
Revision_Time	= 26-JUL-2018 16:32:51
Current_Time	= 25-OCT-2018 09:08:10
Comment	= AS_313 column rc 1
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 25.4[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 1.5[dB]
X_Pulse	= 5.75[us]
Irr_Mode	= Off
Tri_Mode	= Off




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= AS_313 column rc 1_Carbon-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= AS_313 column rc 1
Solvent	= CHLOROFORM-D
Creation_Time	= 27-JUL-2018 05:06:23
Revision_Time	= 27-JUL-2018 10:51:08
Current_Time	= 25-OCT-2018 09:07:31
Comment	= AS_313 column rc 1
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 30[s]
Recvr_Gain	= 60
Temp_Get	= 23.3[dC]
X_90_Width	= 10.5[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 6[dB]
X_Pulse	= 3.5[us]
Irr_Atn_Dec	= 21.5[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]



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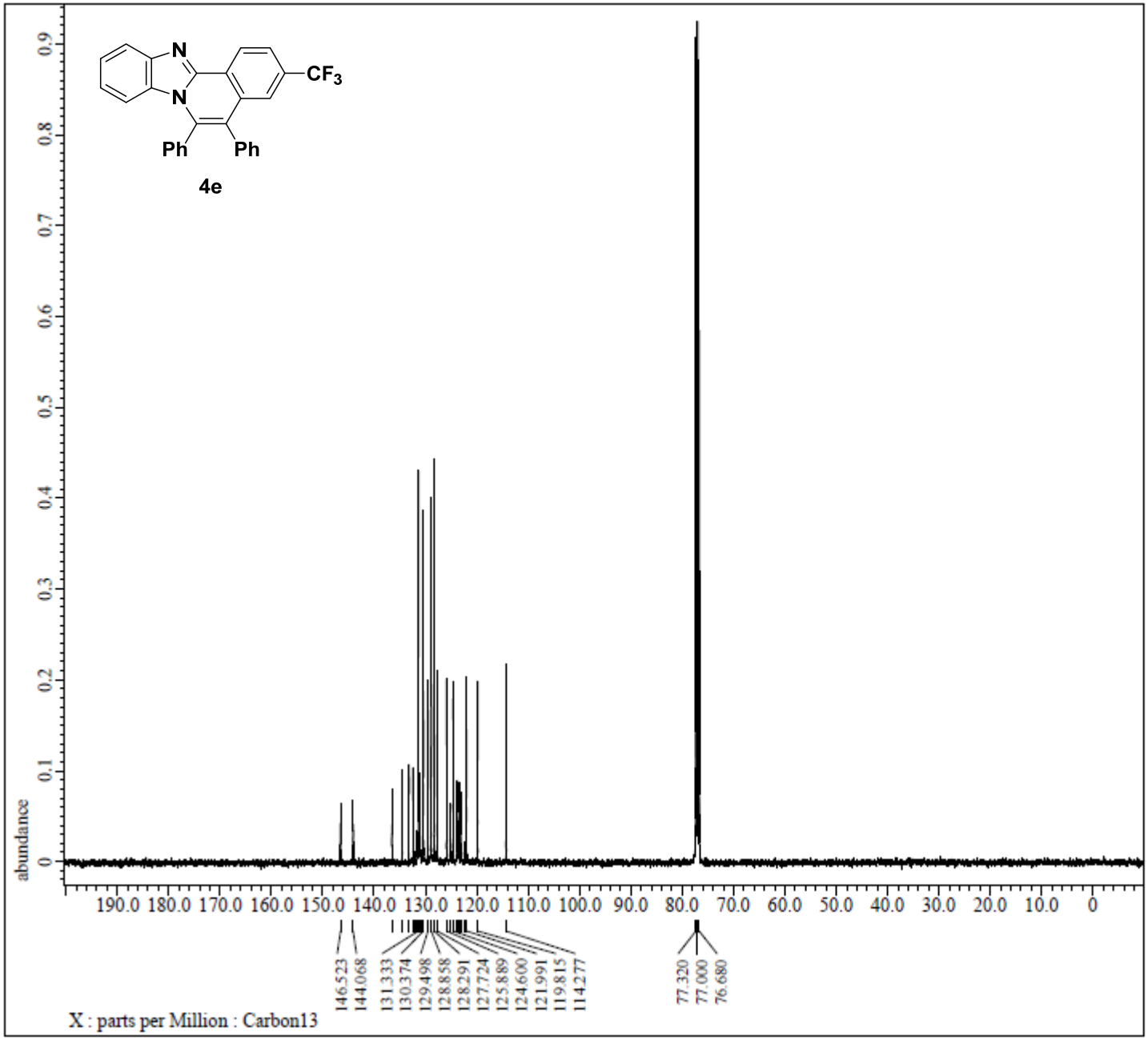
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= AS_328 column F1_Proton-1-
Author	= delta
Experiment	= proton.jxp
Sample_Id	= AS_328 column F1
Solvent	= CHLOROFORM-D
Creation_Time	= 6-JUN-2018 14:58:46
Revision_Time	= 25-OCT-2018 09:16:33
Current_Time	= 25-OCT-2018 09:16:41
Comment	= AS_328 column F1
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 4.36207616[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.22924863[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 34
Temp_Get	= 19.2[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 4.36207616[s]
X_Angle	= 45[deg]
X_Atn	= 1.5[dB]
X_Pulse	= 5.75[us]
Irr_Mode	= Off
Tri_Mode	= Off



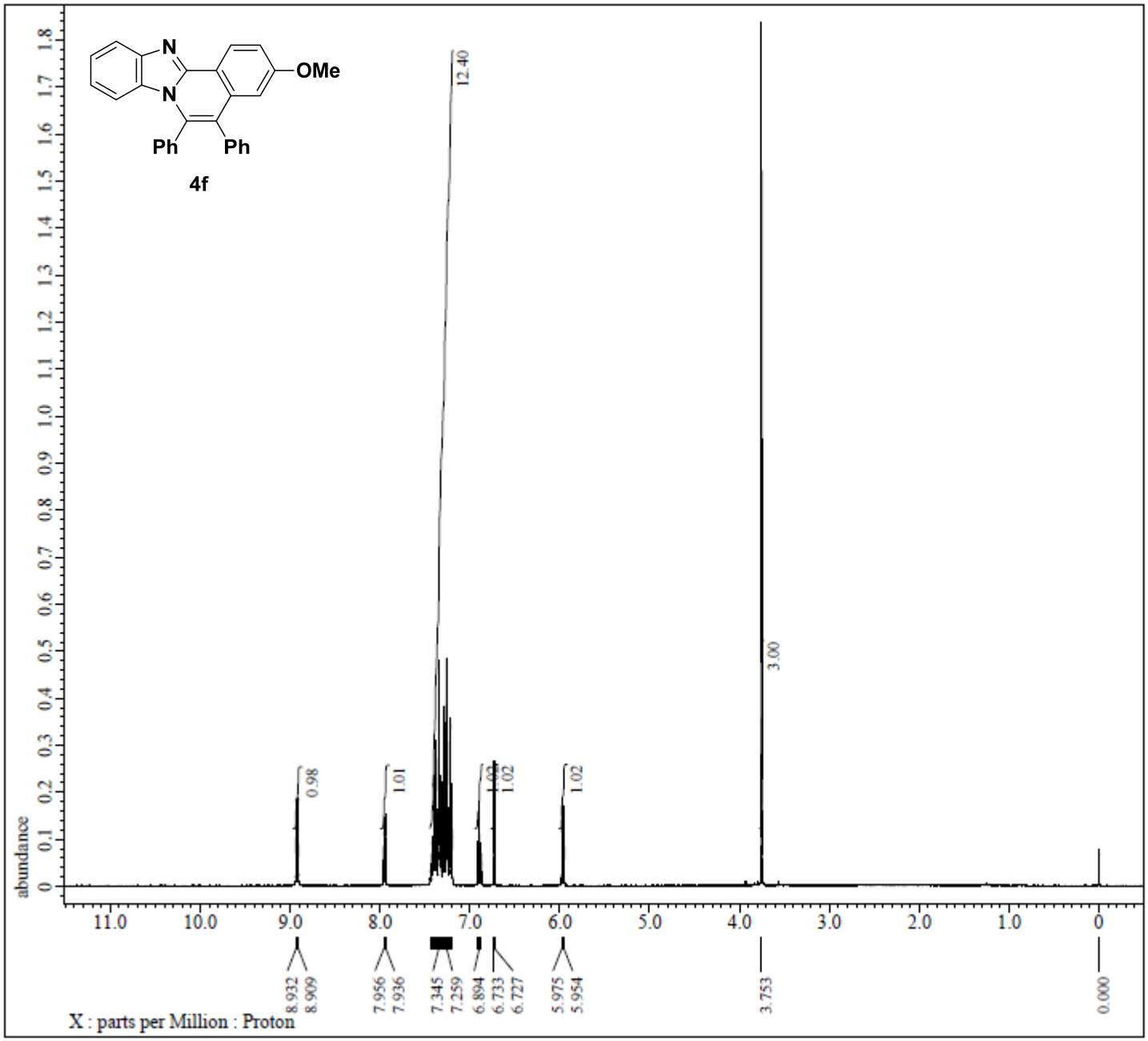

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = AS_328 column f11-12_Carbo
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AS_328 column f11-12
Solvent           = CHLOROFORM-D
Creation_Time     = 11-MAY-2018 02:08:05
Revision_Time     = 25-OCT-2018 09:15:27
Current_Time      = 25-OCT-2018 09:15:42

Comment           = AS_328 column f11-12
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

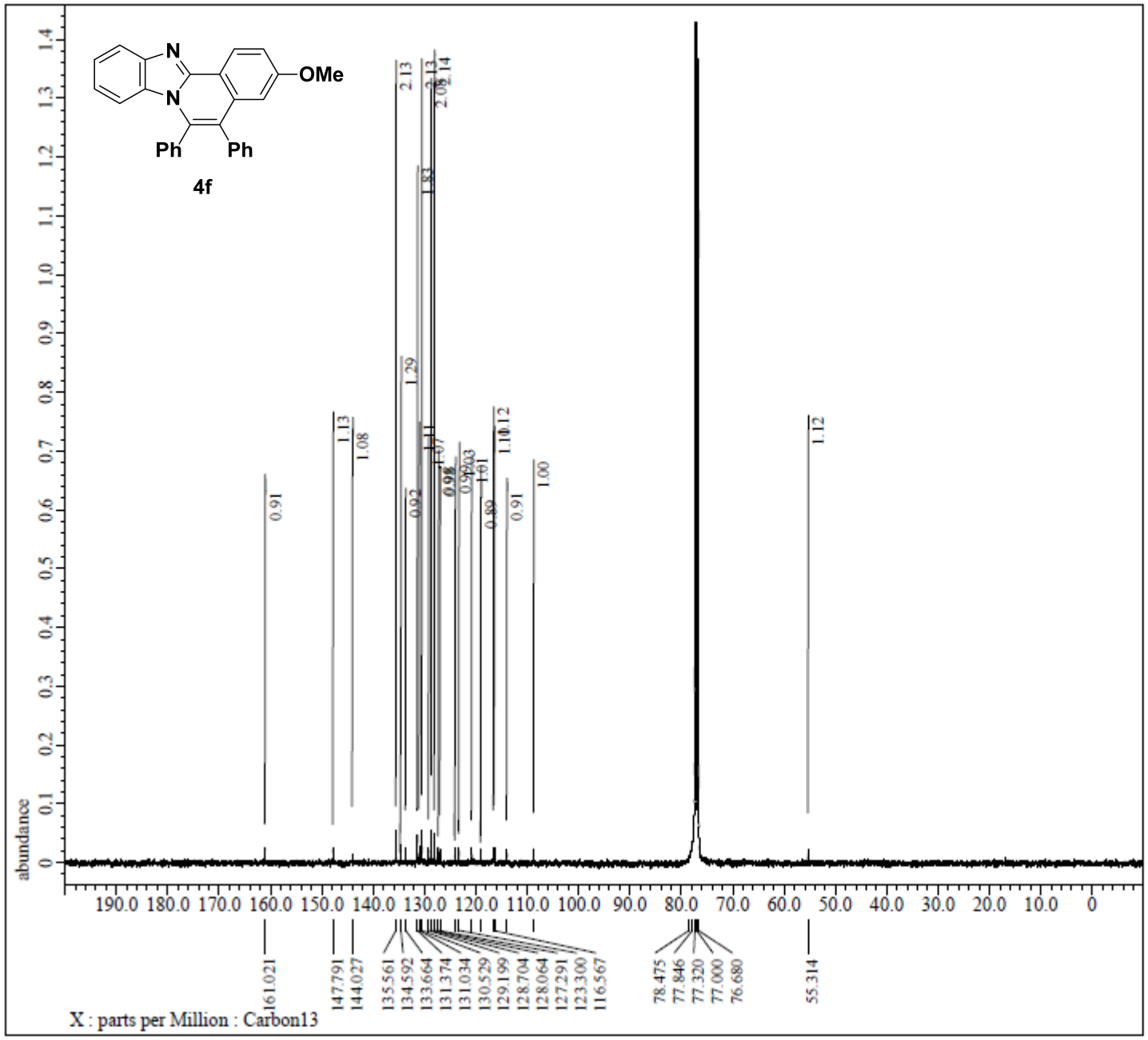
Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 17.5[dC]
X_90_Width        = 14.5[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.83333333[us]
Irr_Atn_Dec       = 21.5[dB]
Irr_Atn_Noe       = 21.5[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
```



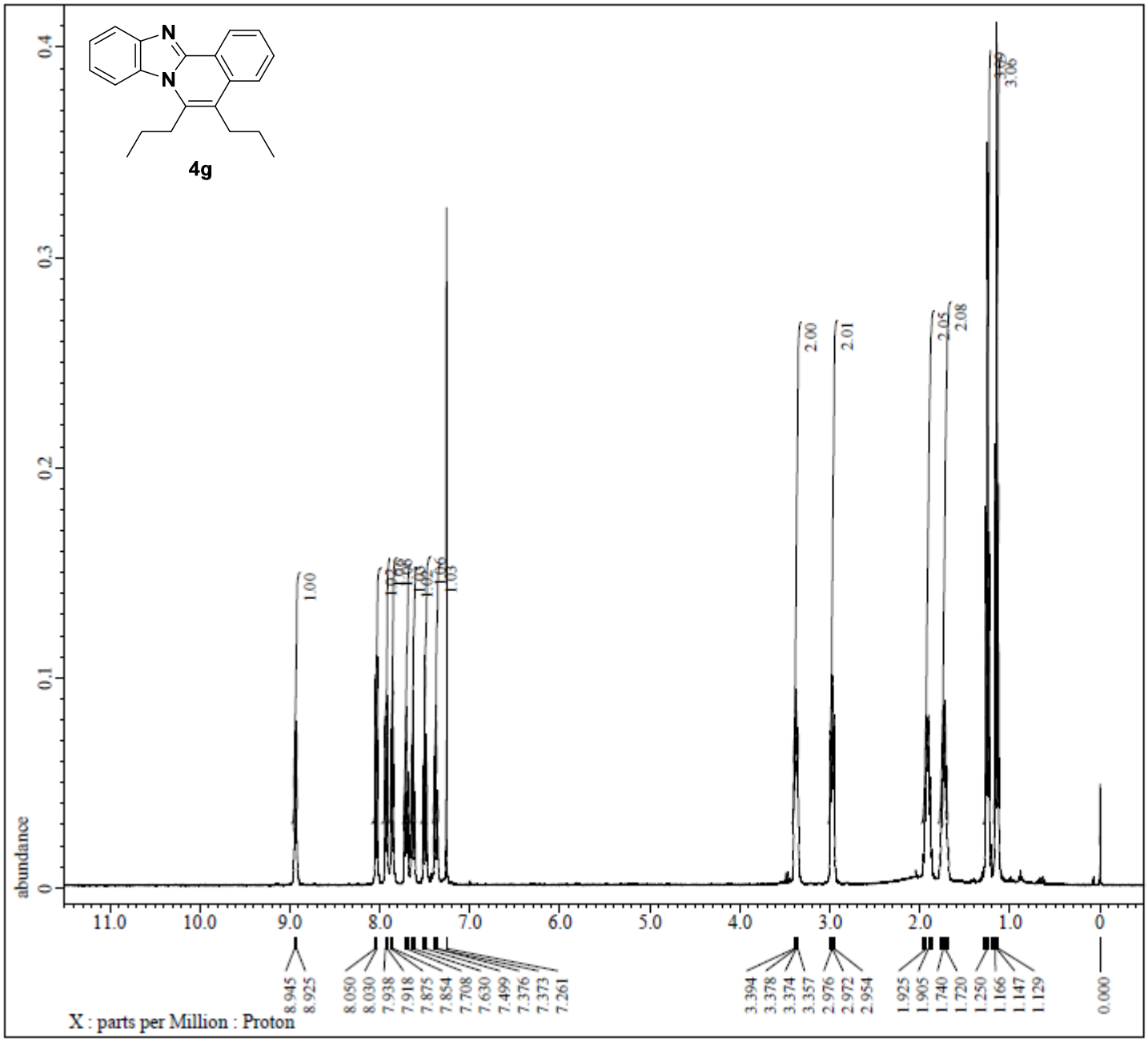

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= AS_321 column 2 column 1 f
Author	= delta
Experiment	= proton.jxp
Sample_Id	= AS_321 column 2 column 1 f
Solvent	= CHLOROFORM-D
Creation_Time	= 16-MAY-2018 21:25:32
Revision_Time	= 17-MAY-2018 21:13:25
Current_Time	= 25-OCT-2018 09:09:51
Comment	= AS_321 column 2 column 1 f
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 4.36207616[s]
X_Domain	= 1H
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 0.22924863[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 32
Temp_Get	= 20.2[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 4.36207616[s]
X_Angle	= 45[deg]
X_Atn	= 1.5[dB]
X_Pulse	= 5.75[us]
Irr_Mode	= Off
Tri_Mode	= Off




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= AS_321 column 2 f10-13_Car
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= AS_321 column 2 f10-13
Solvent	= CHLOROFORM-D
Creation_Time	= 26-MAY-2018 01:07:58
Revision_Time	= 29-MAY-2018 10:16:19
Current_Time	= 25-OCT-2018 09:11:13
Comment	= AS_321 column 2 f10-13
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 0.96468992[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.03660252[Hz]
X_Sweep	= 33.9673913[kHz]
X_Sweep_Clipped	= 27.17391304[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 30[s]
Recvr_Gain	= 60
Temp_Get	= 18.9[dC]
X_90_Width	= 14.5[us]
X_Acq_Time	= 0.96468992[s]
X_Angle	= 30[deg]
X_Atn	= 7[dB]
X_Pulse	= 4.83333333[us]
Irr_Atn_Dec	= 21.5[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]



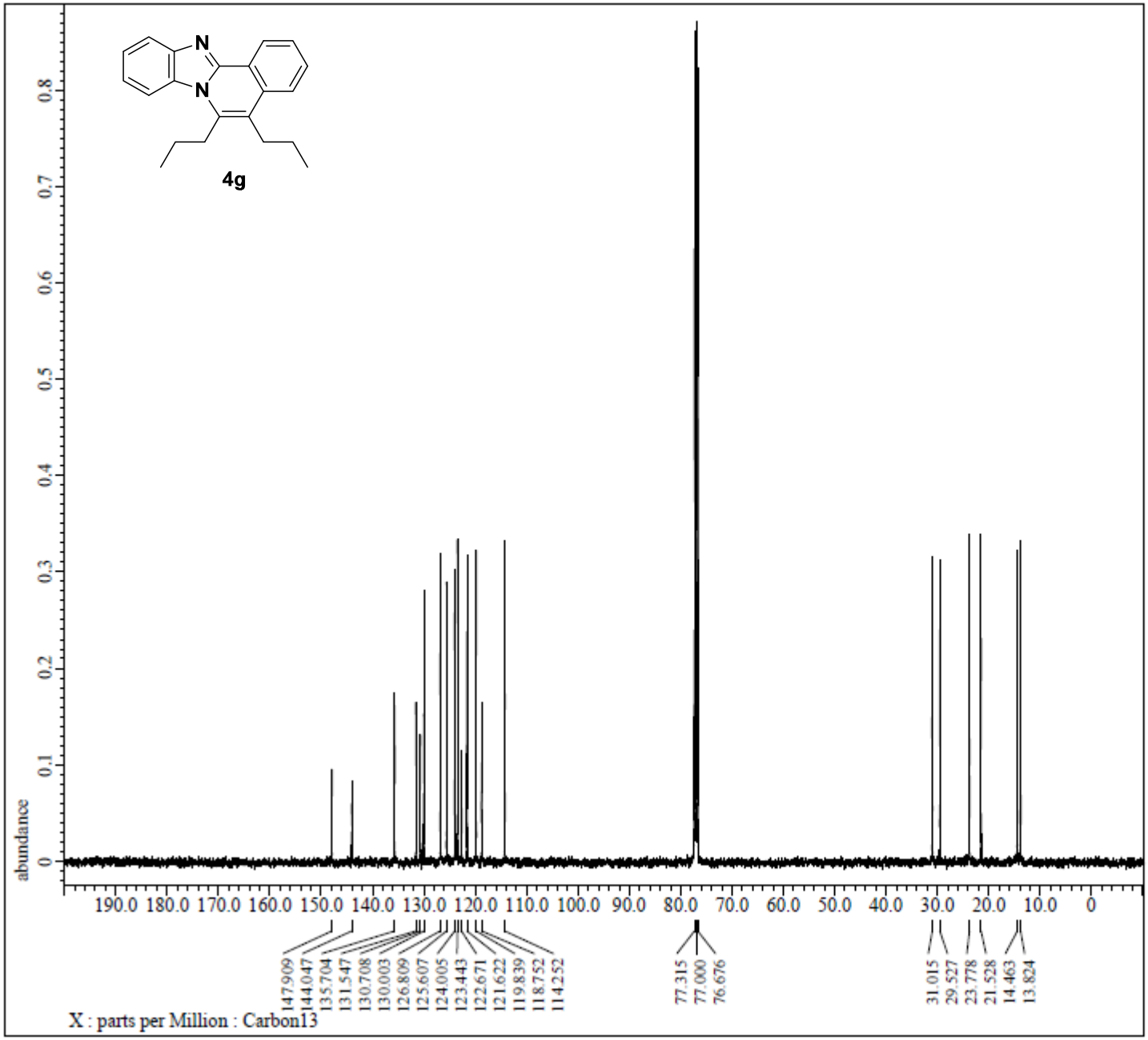

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01525[ppm], 0[ppm] )
```

```
Filename          = AS_338 column F1_Proton-1-
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AS_338 column F1
Solvent           = CHLOROFORM-D
Creation_Time     =  4-JUN-2018 10:59:15
Revision_Time     = 18-JUL-2018 15:35:34
Current_Time      = 25-OCT-2018 09:28:17

Comment           = AS_338 column F1
Data_Format       = 1D COMPLEX
Dim_Size          = 52429
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 4.36207616[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 32768
X_Prescans        = 1
X_Resolution      = 0.22924863[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 32
Temp_Get          = 18.6[dC]
X_90_Width        = 11.5[us]
X_Acq_Time        = 4.36207616[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.75[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



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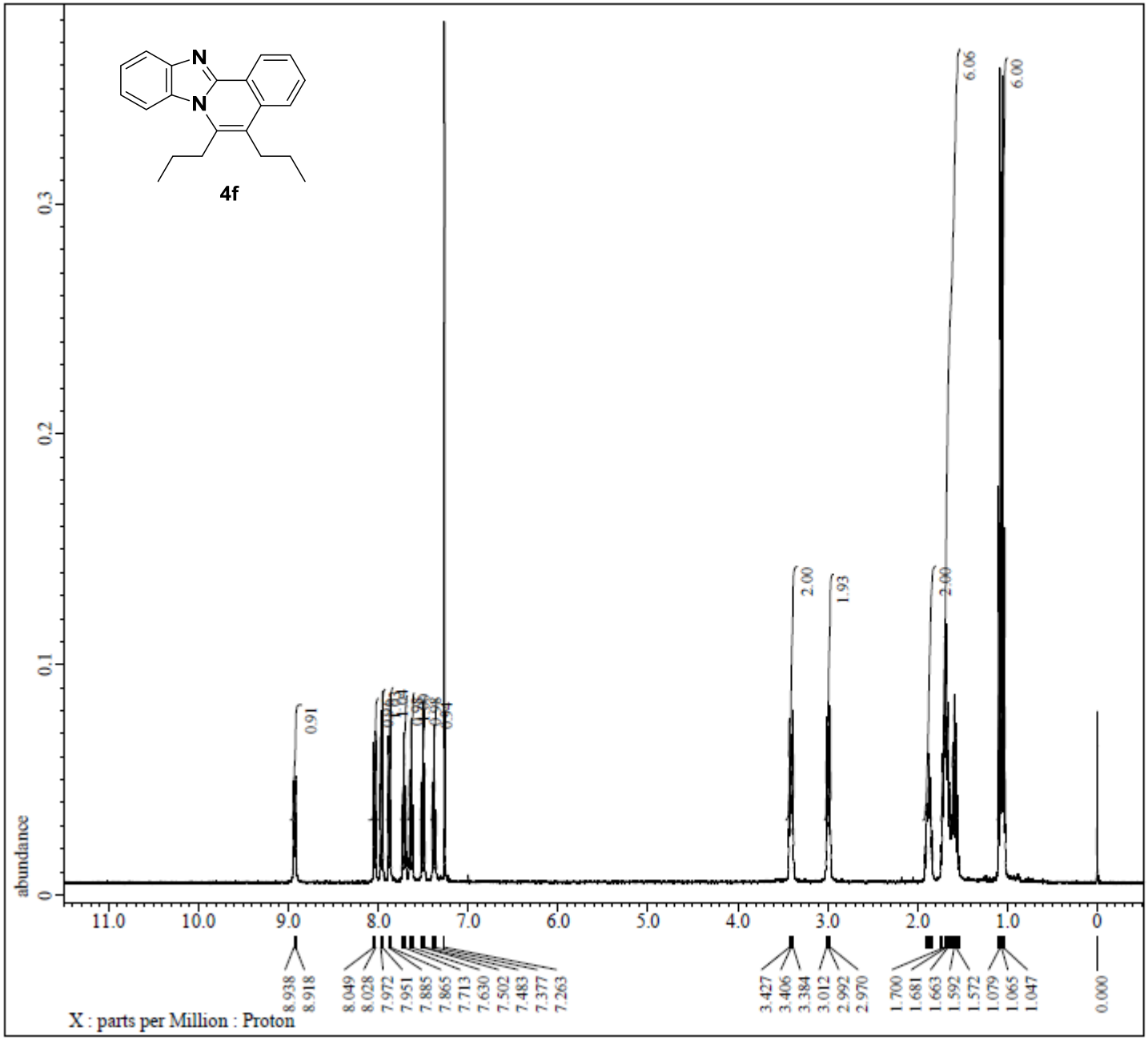
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= AS_338 column F1_Carbon-1-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= AS_338 column F1
Solvent	= CHLOROFORM-D
Creation_Time	= 17-JUL-2018 22:40:04
Revision_Time	= 25-OCT-2018 09:31:02
Current_Time	= 25-OCT-2018 09:31:36
Comment	= AS_338 column F1
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 25.1[dC]
X_90_Width	= 10.5[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 6[dB]
X_Pulse	= 3.5[us]
Irr_Atn_Dec	= 21.5[dB]
Irr_Atn_Noe	= 21.5[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE



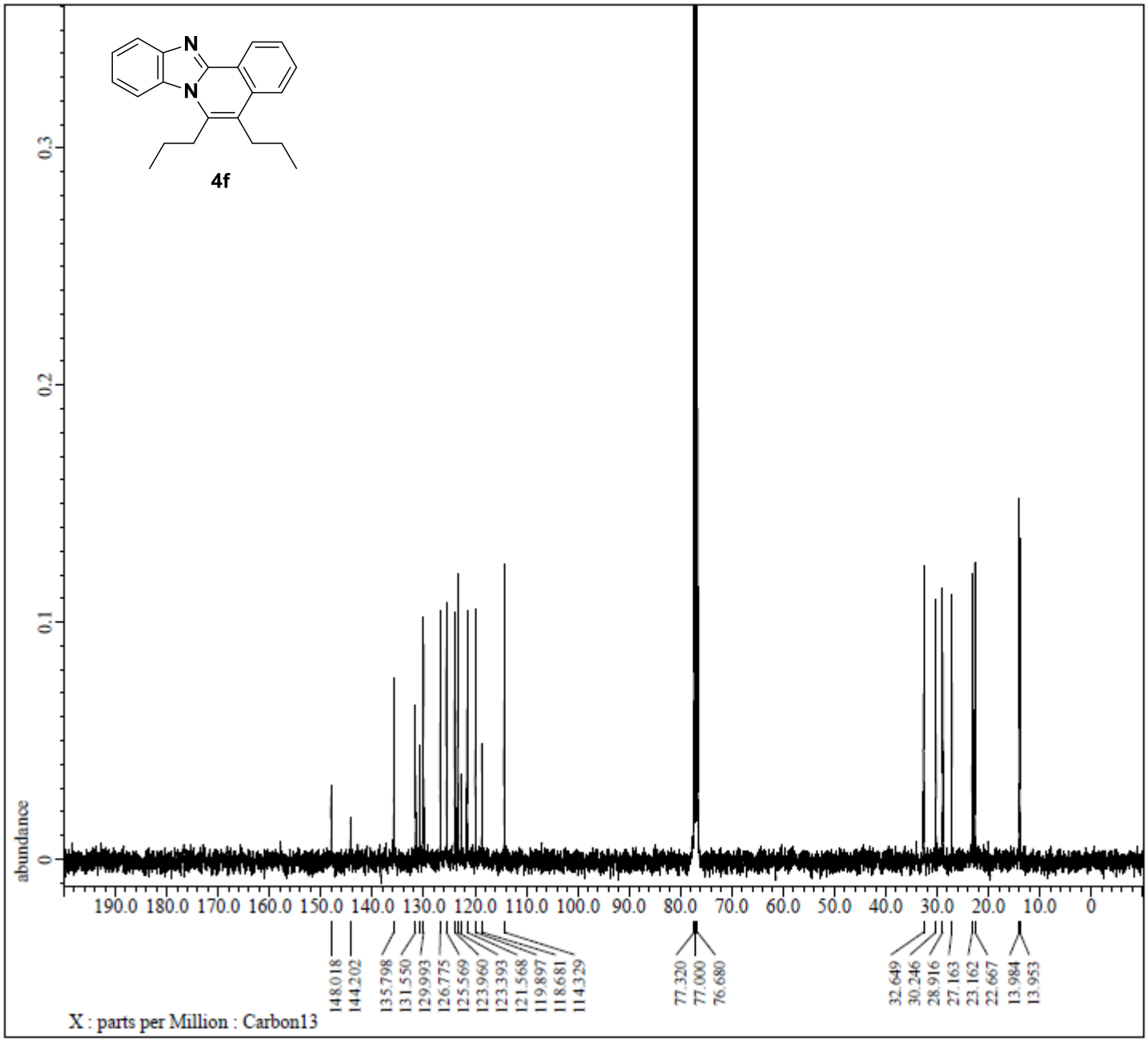

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename          = AS_311 column f29-36 HPLC
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AS_311 column f29-36 HPLC
Solvent           = CHLOROFORM-D
Creation_Time     =  1-MAR-2018 21:14:29
Revision_Time     =  7-JUN-2018 22:58:25
Current_Time      = 25-OCT-2018 09:06:19

Comment           = AS_311 column f29-36 HPLC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

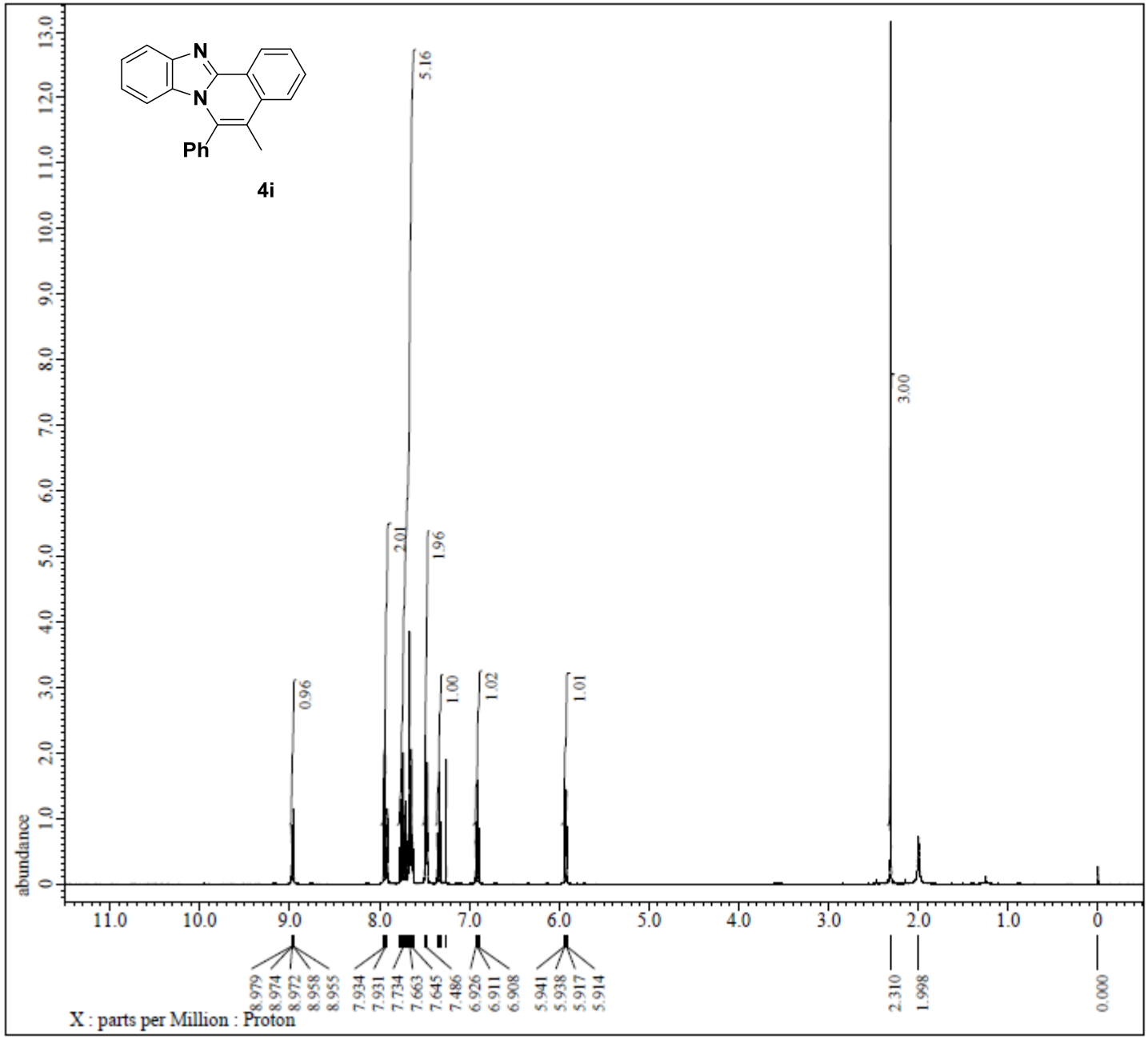
Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 32
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= AS_311 column f26-28_Carbo
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= AS_311 column f26-28
Solvent	= CHLOROFORM-D
Creation_Time	= 25-FEB-2018 04:06:06
Revision_Time	= 25-MAY-2018 22:39:18
Current_Time	= 25-OCT-2018 09:04:45
Comment	= AS_311 column f26-28
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 0.96468992[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.03660252[Hz]
X_Sweep	= 33.9673913[kHz]
X_Sweep_Clipped	= 27.17391304[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 460.0[dC]
X_90_Width	= 12.6[us]
X_Acq_Time	= 0.96468992[s]
X_Angle	= 30[deg]
X_Atn	= 6[dB]
X_Pulse	= 4.2[us]
Irr_Atn_Dec	= 20.776[dB]
Irr_Atn_Noe	= 20.776[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE



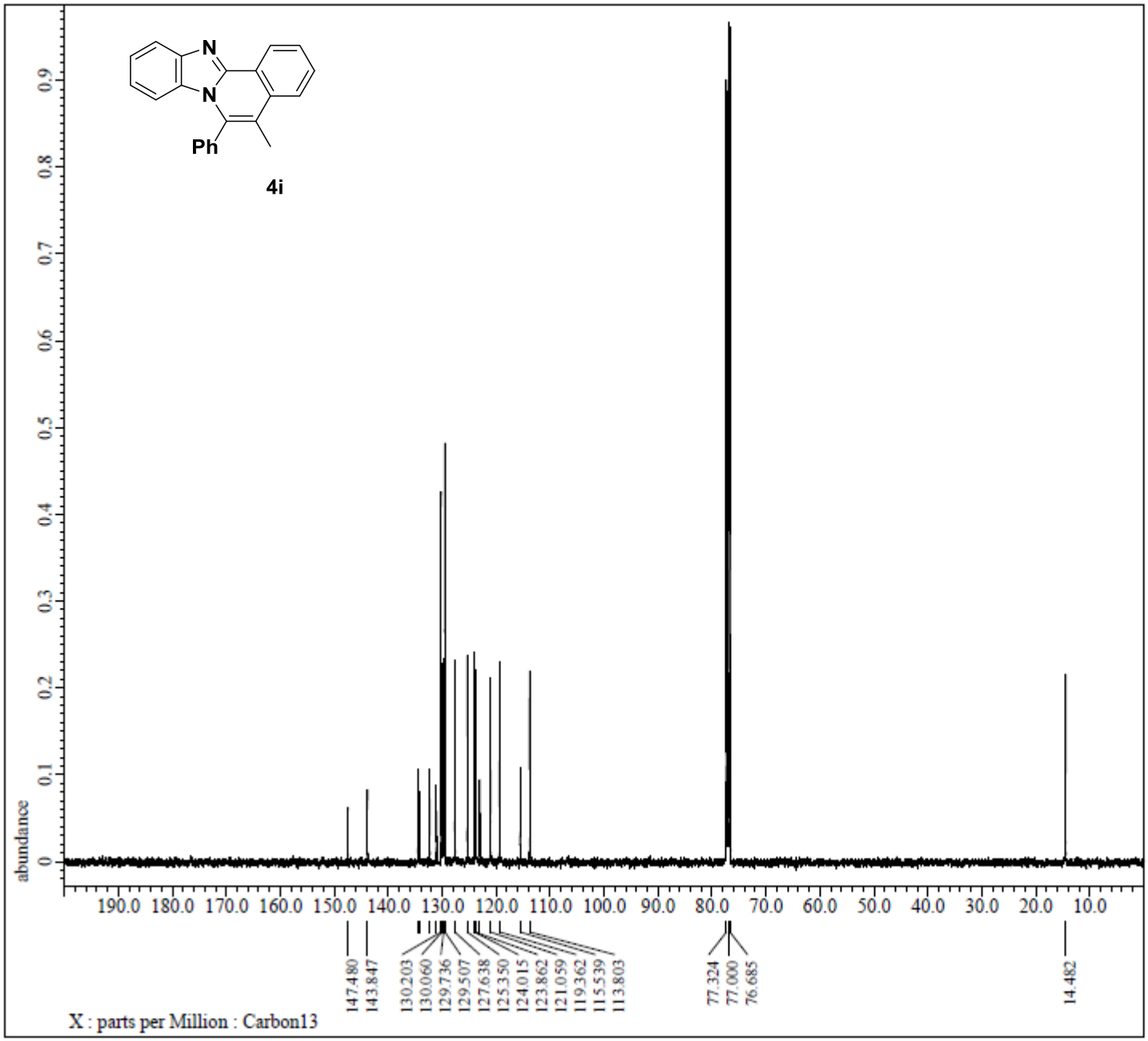

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = AS_365 rc 1_Proton-1-3.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AS_365 rc 1
Solvent           = CHLOROFORM-D
Creation_Time     = 12-SEP-2018 23:54:36
Revision_Time     = 25-OCT-2018 09:21:35
Current_Time      = 25-OCT-2018 09:21:59

Comment           = AS_365 rc 1
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-EC8400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 38
Temp_Get          = 19.8[dC]
X_90_Width        = 11.5[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.75[us]
Irr_Mode          = Off
Tri_Mode          = Off
```



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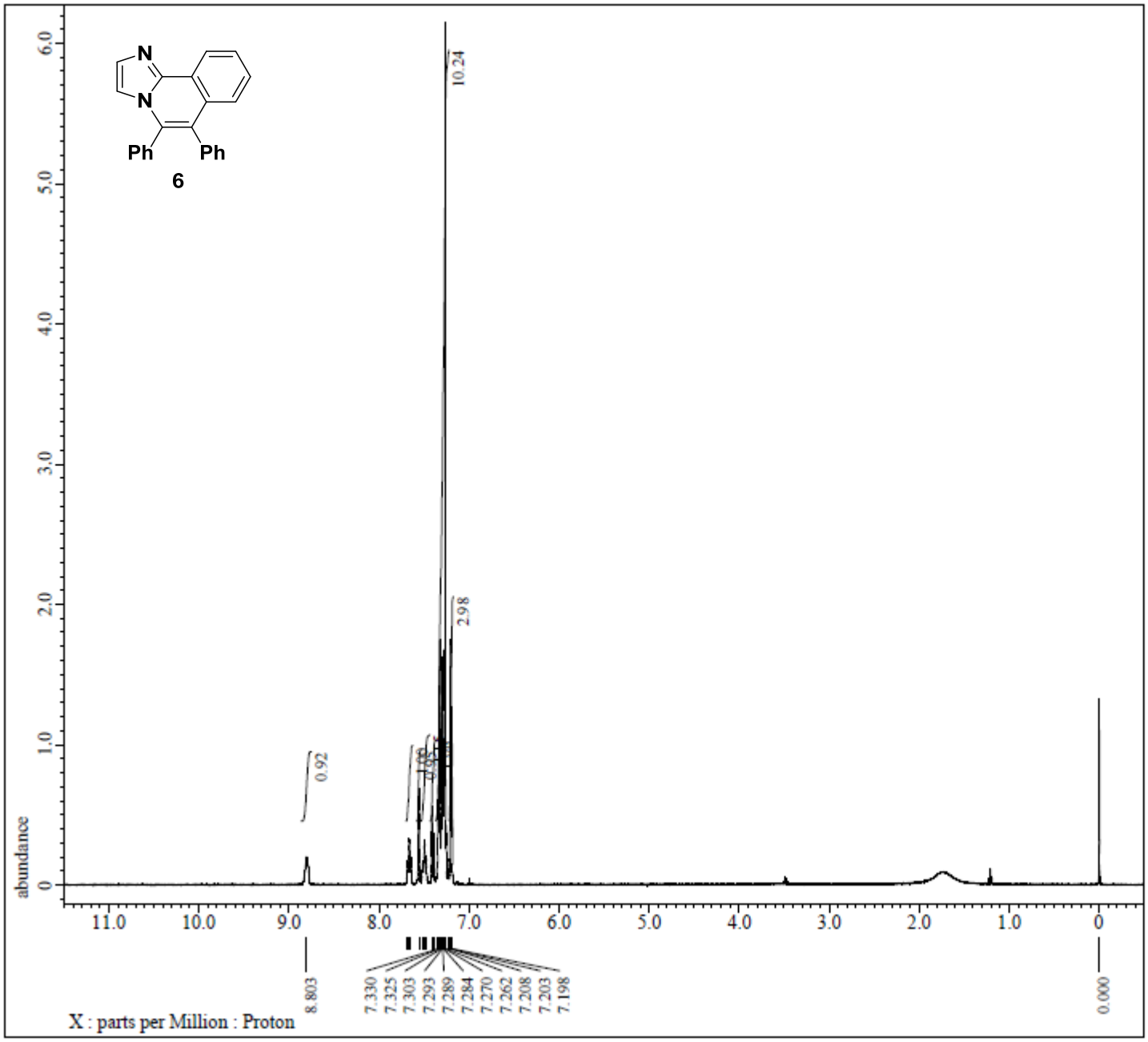
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= AS_365 rc 1_Carbon-1-2.jdf
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= AS_365 rc 1
Solvent	= CHLOROFORM-D
Creation_Time	= 13-SEP-2018 03:06:41
Revision_Time	= 13-SEP-2018 15:00:19
Current_Time	= 25-OCT-2018 09:22:40
Comment	= AS_365 rc 1
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.7[dC]
X_90_Width	= 10.5[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 6[dB]
X_Pulse	= 3.5[us]
Irr_Atn_Dec	= 21.5[dB]
Irr_Atn_Noe	= 21.5[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE



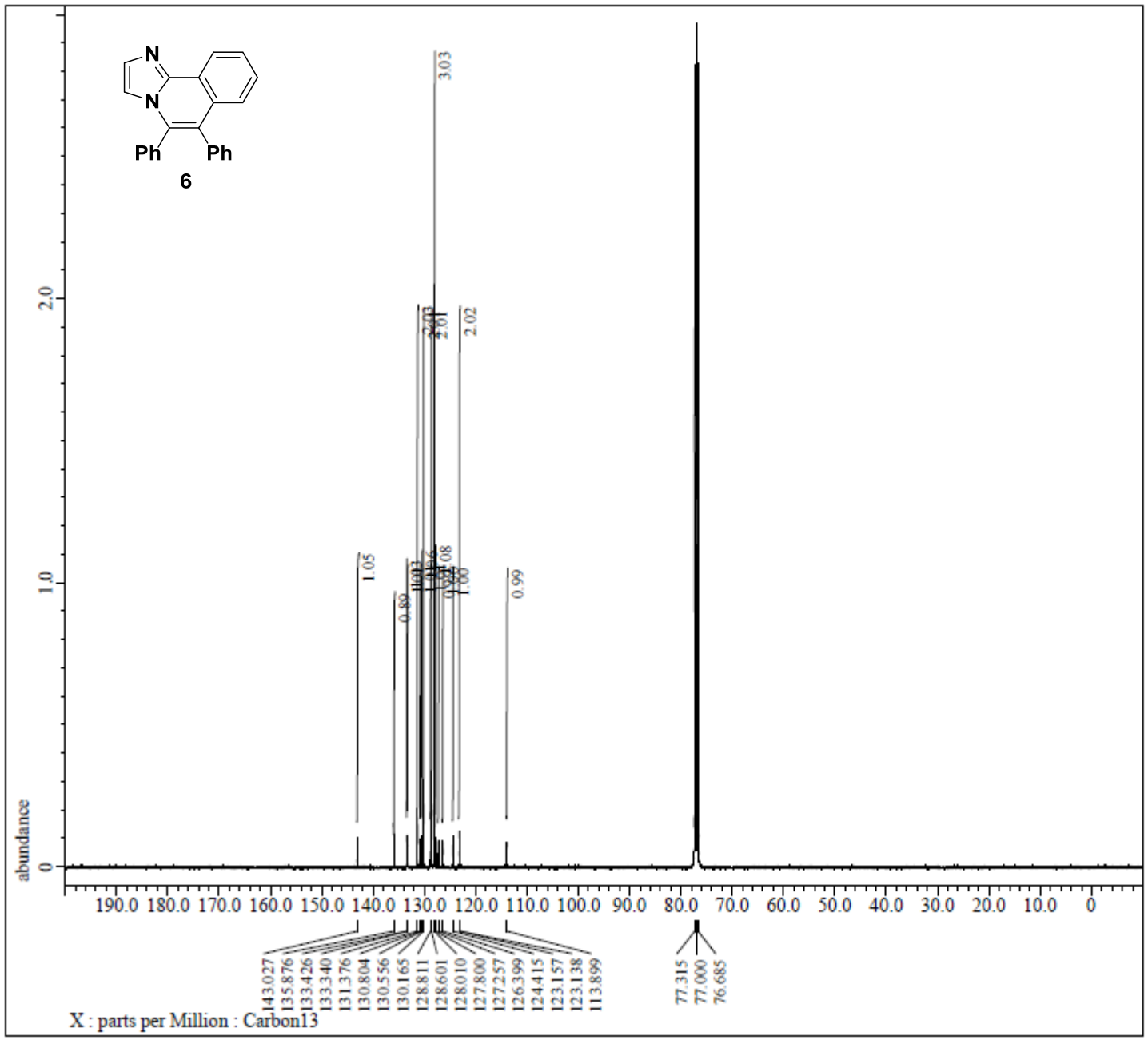

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = AS_374 rc_Proton-1-2.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = AS_374 rc
Solvent           = CHLOROFORM-D
Creation_Time     = 12-SEP-2018 23:32:06
Revision_Time     = 12-SEP-2018 23:35:54
Current_Time      = 25-OCT-2018 09:24:09

Comment           = AS_374 rc
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 50
Temp_Get          = 19.8[dC]
X_90_Width        = 11.5[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1.5[dB]
X_Pulse           = 5.75[us]
Irr_Mode          = Off
Tri_Mode          = Off
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename          = AS_374 rc_Carbon-2-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AS_374 rc
Solvent           = CHLOROFORM-D
Creation_Time     = 16-SEP-2018 01:10:00
Revision_Time     = 18-SEP-2018 10:44:40
Current_Time      = 25-OCT-2018 09:23:40

Comment           = AS_374 rc
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 1.04333312[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 0.95846665[Hz]
X_Sweep           = 31.40703518[kHz]
X_Sweep_Clipped   = 25.12562814[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 30[s]
Recvr_Gain        = 60
Temp_Get          = 20[dC]
X_90_Width        = 10.5[us]
X_Acq_Time        = 1.04333312[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 3.5[us]
Irr_Atn_Dec       = 21.5[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
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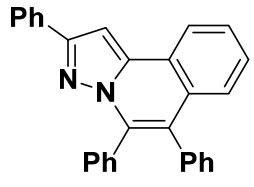

8


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Author            = delta
Experiment        = proton.jxp
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Solvent           = CHLOROFORM-D
Creation_Time     = 26-FEB-2018 21:13:16
Revision_Time     =  6-MAR-2018 12:40:13
Current_Time      = 16-MAR-2018 19:12:08

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Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 28
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
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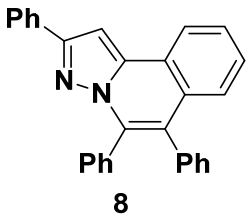

8


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Filename          = AO-1042 GPC_Carbon-1-1.jdf
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Experiment        = carbon.jxp
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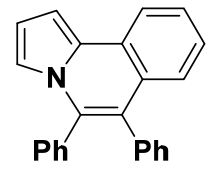
Solvent           = CHLOROFORM-D
Creation_Time     = 27-FEB-2018 01:04:29
Revision_Time     = 27-FEB-2018 13:02:06
Current_Time      = 16-MAR-2018 19:11:47

Comment           = AO-1042 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```



10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Author            = delta
Experiment        = proton.jxp
Sample_Id         = AO-1011 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 26-FEB-2018 21:07:15
Revision_Time     =  6-MAR-2018 12:39:01
Current_Time      = 16-MAR-2018 19:08:55

Comment           = AO-1011 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 2.18103808[s]
X_Domain          = 1H
X_Freq            = 399.78219838[MHz]
X_Offset          = 5[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.45849727[Hz]
X_Sweep           = 7.51201923[kHz]
X_Sweep_Clipped   = 6.00961538[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Proton
Tri_Freq          = 399.78219838[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 30
Temp_Get          = 460.0[dC]
X_90_Width        = 11.1[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 5.55[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```
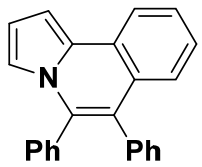
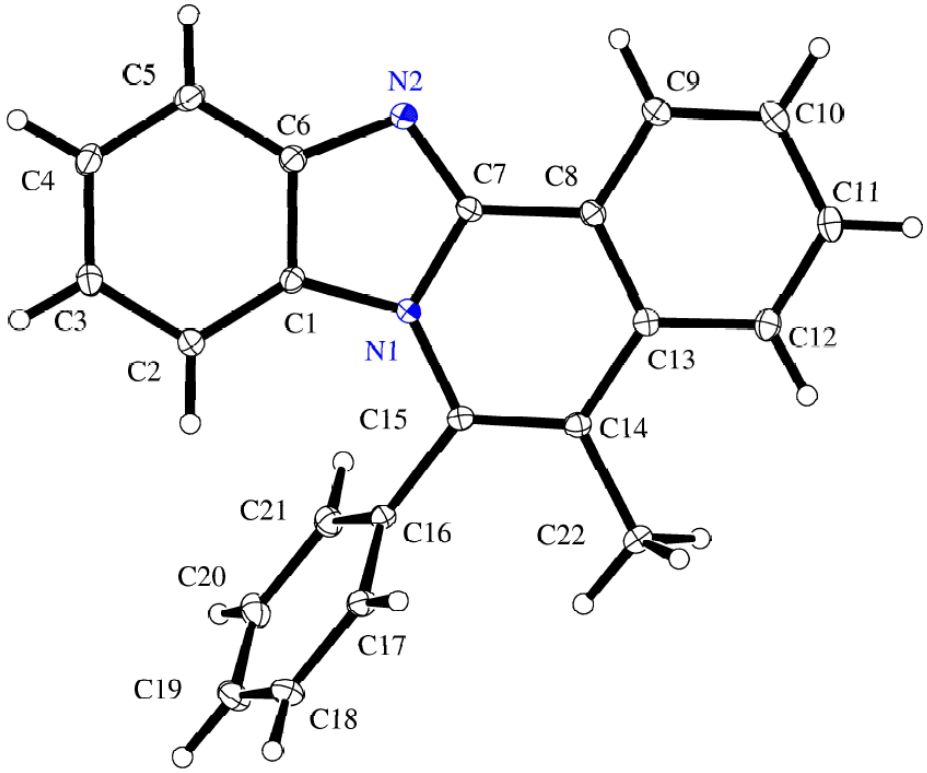



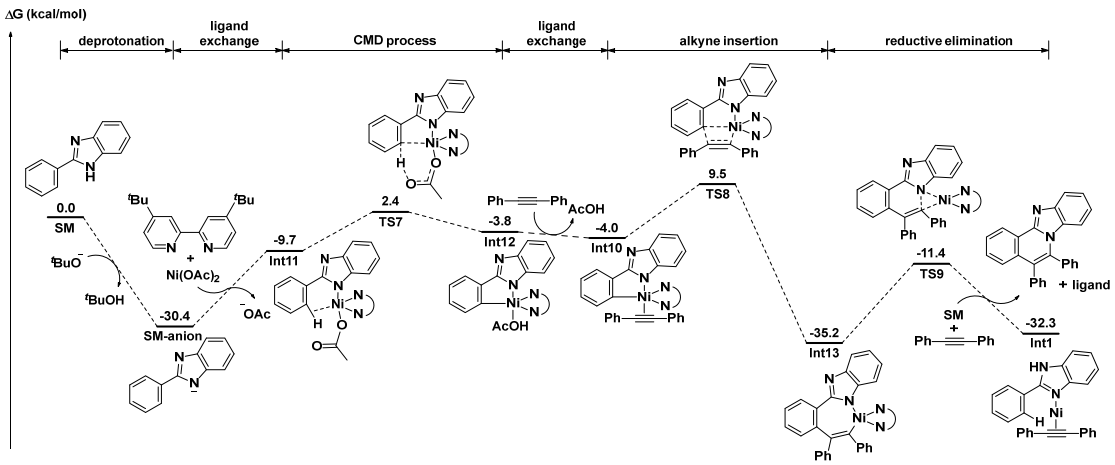
10


```
Filename          = AO-1011 GPC_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = AO-1011 GPC
Solvent           = CHLOROFORM-D
Creation_Time     = 27-FEB-2018 00:04:55
Revision_Time     = 12-MAR-2018 14:18:32
Current_Time      = 16-MAR-2018 19:11:23

Comment           = AO-1011 GPC
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECS400
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.389766[T] (400[MHz])
X_Acq_Duration    = 0.96468992[s]
X_Domain          = 13C
X_Freq            = 100.52530333[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.03660252[Hz]
X_Sweep           = 33.9673913[kHz]
X_Sweep_Clipped   = 27.17391304[kHz]
Irr_Domain        = Proton
Irr_Freq          = 399.78219838[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 460.0[dC]
X_90_Width        = 12.6[us]
X_Acq_Time        = 0.96468992[s]
X_Angle           = 30[deg]
X_Atn             = 6[dB]
X_Pulse           = 4.2[us]
Irr_Atn_Dec       = 20.776[dB]
Irr_Atn_Noe       = 20.776[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 0.115[ms]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.96468992[s]
```

ORTEP of 4i



6. Gibbs Free Energy Profile of the Initial Path



Scheme S1 Gibbs free energy profile of the initial path calculated at the B3PW91/6-311+G(2d,p)-SDD(Ni)/PCM//B3LYP/6-31+G(d)-Lanl2dz(Ni) level of theory. Gibbs free energies are given based on **SM**.

The energy profile of the initial path is shown in Scheme S1. Deprotonation of the amide **SM** by a *tert*-butoxide anion proceeds with a dramatic energy drop to give the **SM-anion**. After ligand exchange of the nickel catalyst by the **SM-anion**, the acetate ligand promotes a concerted-metalation-deprotonation (CMD) process. Coordination of the *ortho* C-H bond would facilitate the formation of the nickelacycle **Int12**. Following acetic acid-alkyne exchange, an alkyne is inserted into the Ni-C bond, which proceeds through **TS8** with an activation energy of 13.5 kcal/mol. This step is highly exothermic due to the stability of the seven-membered metalacycle **Int13**. The free energy barrier associated with the final reductive elimination step through **TS9** is 23.8 kcal/mol. The Ni(0) species generated in the reductive elimination step from **Int13** participates in the main catalytic cycle after ligand exchange to give **Int1**.

7. Computational Details

Calculations were performed with the Gaussian 09 (G09) program.[1] Geometry optimizations and frequency calculations for all reported structures were performed using B3LYP with the 6-31+G(d) basis set for C, H, O, N and the Lanl2dz effective core potential (ECP) for Ni.[2-4] Single point energy calculations were performed using B3PW91 with the 6-311+G(2d,p) basis set for C, H, O, N and the SDD ECP for Ni.[5-7] PCM[8-10] solvent effects were incorporated for all calculations with toluene as the solvent. Each reported minimum has zero imaginary frequency and each transition state (TS) structure has only one imaginary frequency. From TSs, reaction paths were traced by the intrinsic reaction coordinate (IRC) method[11,12] to obtain the energy-minimum geometries. Energy changes were shown by the use of Gibbs free energies (T = 298.15 K and P = 1 atm).

8. Energies for Calculated Structures

Electronic energies, as well as zero point energy (ZPE), enthalpy (H), Gibbs free energy (G), and imaginary frequency (Im. Freq.) for all structures calculated at B3LYP/6-31+G(d)-Lanl2dz level of theory are provided. PCM solvent effects were incoorporated for all calculations with toluene as the solvent.

Table S1 Energies for the main catalytic cycle in Scheme 4 (in hartrees)

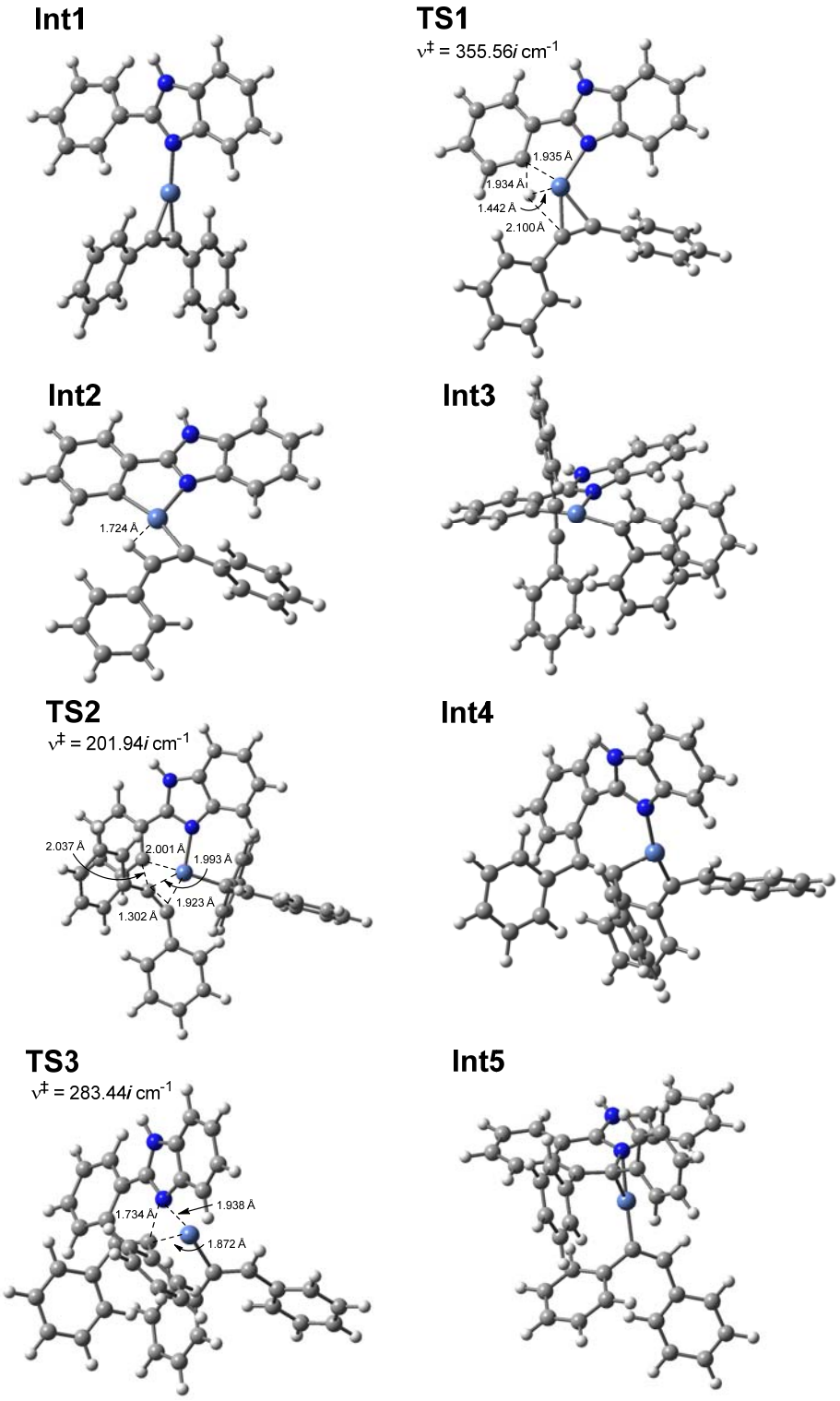
structure	E	ZPE	H	G°	Im. Freq.
Int1	-1319.78416694	0.393029	0.419206	0.331712	-
TS1	-1319.73903463	0.387709	0.413361	0.329652	355.56i
Int2	-1319.76955183	0.392925	0.418292	0.335016	-
PhCCPh	-539.4839997	0.191624	0.203658	0.150820	-
Int3	-1859.25666236	0.585769	0.623985	0.510726	-
TS2	-1859.23906214	0.585791	0.622978	0.512065	201.94i
Int4	-1859.30363181	0.587933	0.625071	0.514791	-
TS3	-1859.25466071	0.586704	0.623231	0.515122	283.44i
Int5	-1859.25918432	0.587932	0.624983	0.516133	-
SM	-610.957845118	0.199299	0.211013	0.161744	-
product	-1149.29395473	0.373014	0.395000	0.321484	-
cis-alkene	-540.724309507	0.215114	0.227151	0.176472	-
Int6	-1319.75782531	0.392566	0.418765	0.331364	-
TS4	-1319.72655622	0.386119	0.412222	0.326188	989.12i
Int7	-1319.74745542	0.387976	0.414341	0.327871	-
TS5	-1319.73827565	0.387175	0.412750	0.329358	452.59i
Int8	-1319.76530499	0.391632	0.417377	0.332398	-
TS6	-1319.72530152	0.387851	0.412922	0.330977	1316.21i
Int9	-1319.78847160	0.393917	0.418918	0.337973	-
Int10	-2128.50832792	0.755585	0.801652	0.673988	-

Table S2 Energies for the initial path in Scheme S1 (in hartrees)

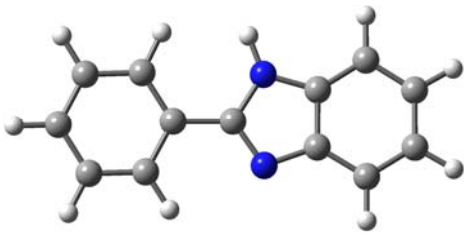
structure	E	ZPE	H	G°	Im. Freq.
^{t}BuO^{-}	-233.1362105	0.121180	0.128439	0.092531	-
^{t}BuOH	-233.6864178	0.135623	0.143314	0.106597	-
SM-anion	-610.452441027	0.185441	0.196838	0.148437	-
Ni(OAc)$_2$	-626.3663171	0.103704	0.115232	0.065672	-
ligand	-809.920035806	0.382981	0.403823	0.334045	-
OAc^{-}	-228.5986816	0.048238	0.052749	0.022342	-
Int11	-1818.13908944	0.625061	0.665008	0.550052	-
TS7	-1818.11101568	0.620775	0.659683	0.549213	1372.72i
Int12	-1818.12646347	0.625876	0.665365	0.553345	-
AcOH	-229.0999814	0.061617	0.067160	0.034208	-
TS8	-2128.48254772	0.754242	0.799788	0.672527	274.17i
Int13	-2128.56492263	0.758002	0.803088	0.678794	-
TS9	-2128.52589970	0.756150	0.800680	0.678127	230.20i

9. B3LYP/6-31+G(d)-Lanl2dz-optimized structures of the model compounds

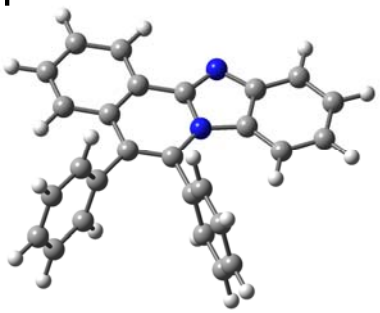
Figure S1 B3LYP/6-31+G(d)-Lanl2dz-optimized structures of the model compounds of the red line in Scheme 4.



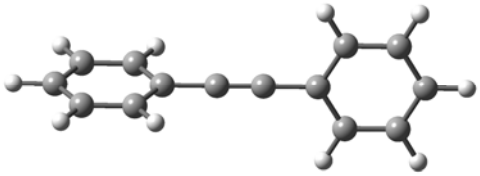
SM



product



PhCCPh



***cis*-alkene**

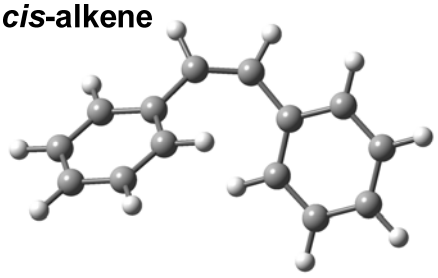


Figure S2 B3LYP/6-31+G(d)-Lanl2dz-optimized structures of the model compounds of the blue line in Scheme 4.

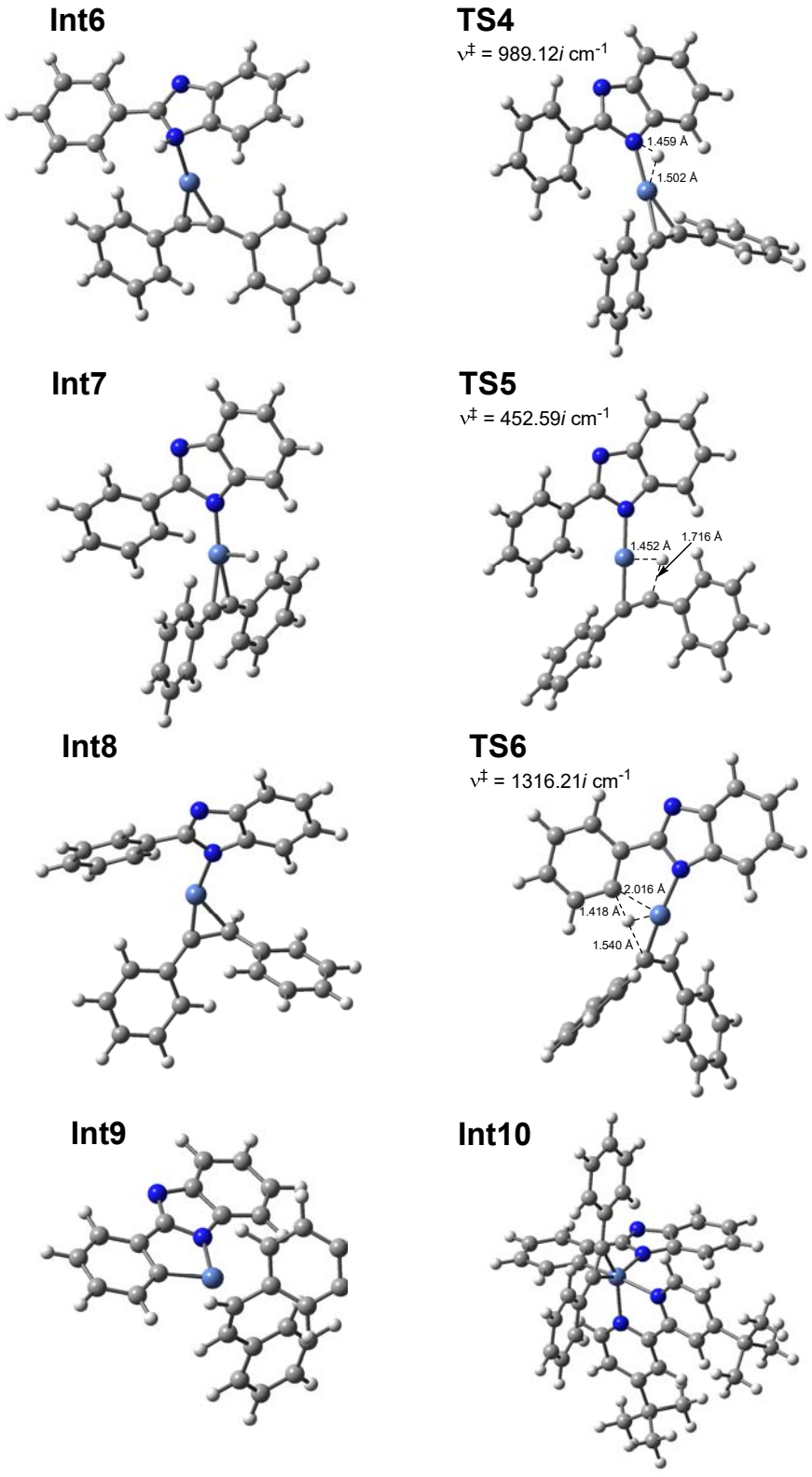
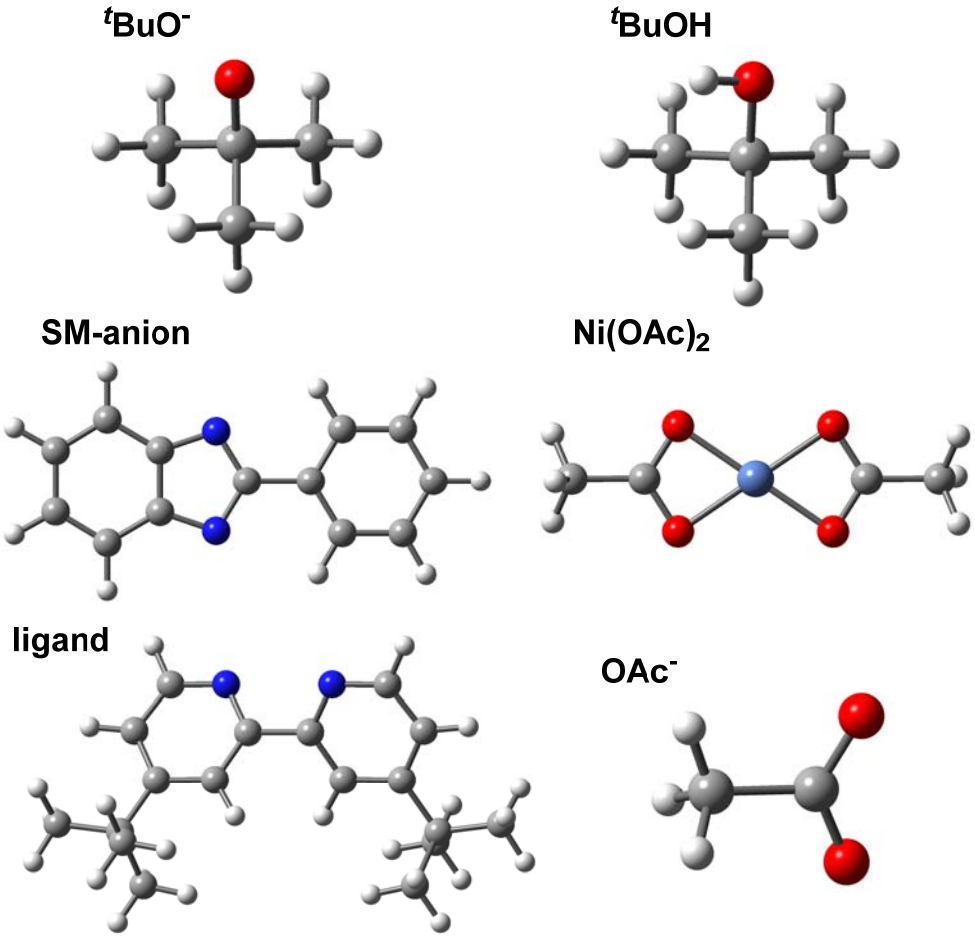
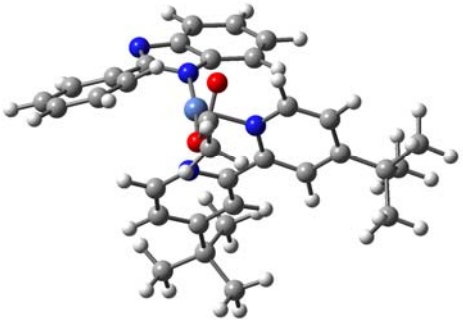


Figure S3 B3LYP/6-31+G(d)-Lanl2dz-optimized structures of the model compounds in Scheme S1.

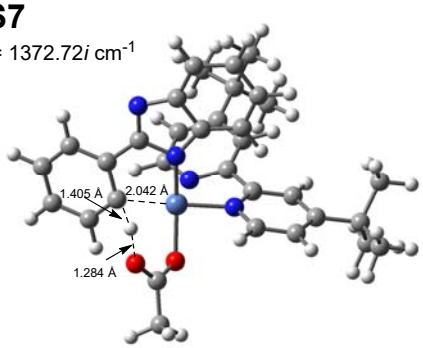


Int11

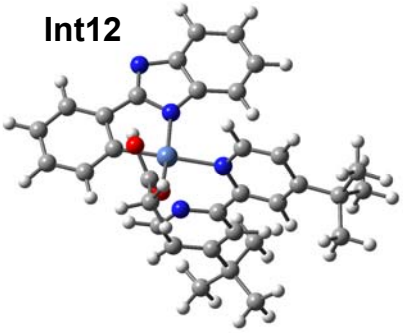


TS7

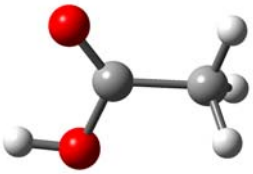
$\nu^{\ddagger}$ = 1372.72*i* cm^{-1}



Int12

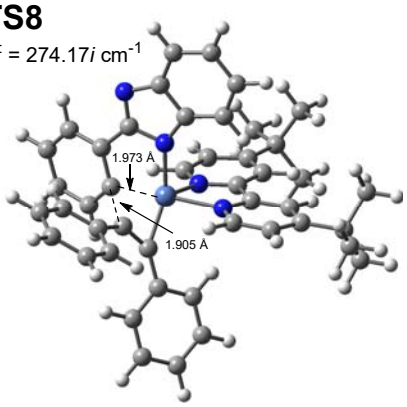


AcOH

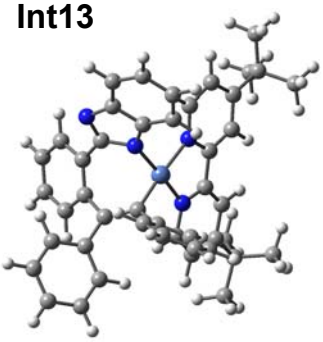


TS8

$\nu^{\ddagger}$ = 274.17*i* cm^{-1}

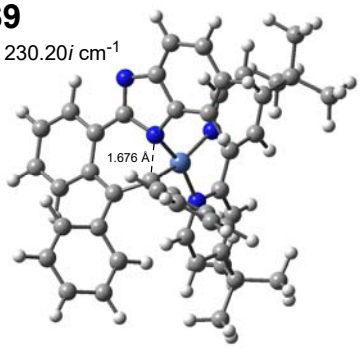


Int13



TS9

$\nu^{\ddagger}$ = 230.20*i* cm^{-1}



10. Cartesian coordinates of the optimized geometries and energies

Scheme 4

Int1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.988275	0.646478	0.162508
2	6	0	-1.776212	-0.385683	-0.582430
3	28	0	-0.155406	0.395704	-0.102765
4	1	0	0.672630	-1.894568	0.821466
5	6	0	1.396724	-1.952016	1.628467
6	6	0	1.208134	-2.847427	2.680910
7	6	0	2.522752	-1.111022	1.609409
8	6	0	2.137690	-2.919176	3.723348
9	6	0	3.452813	-1.185882	2.662817
10	6	0	3.259871	-2.084906	3.712181
11	1	0	0.333413	-3.491803	2.683386
12	1	0	1.986717	-3.617667	4.542064
13	1	0	3.979356	-2.124243	4.525483
14	1	0	4.309868	-0.517273	2.687812
15	6	0	-2.900459	1.578851	0.790795
16	6	0	-4.284873	1.553596	0.508373
17	6	0	-2.429903	2.547524	1.701908
18	6	0	-5.156940	2.457856	1.114012
19	1	0	-4.667070	0.823273	-0.199350
20	6	0	-3.304294	3.448542	2.309796
21	1	0	-1.367116	2.579615	1.927125
22	6	0	-4.672877	3.409548	2.019838
23	1	0	-6.218170	2.421029	0.878547
24	1	0	-2.917634	4.184194	3.011334
25	1	0	-5.354225	4.112414	2.492628
26	6	0	-2.231983	-1.550595	-1.310236
27	6	0	-1.375114	-2.234968	-2.197628

28	6	0	-3.547620	-2.041058	-1.148538
29	6	0	-1.815378	-3.357425	-2.899441
30	1	0	-0.361267	-1.867188	-2.332056
31	6	0	-3.983683	-3.165810	-1.848421
32	1	0	-4.219821	-1.536156	-0.460362
33	6	0	-3.121611	-3.830140	-2.729346
34	1	0	-1.137851	-3.864987	-3.582232
35	1	0	-4.999940	-3.526259	-1.706032
36	1	0	-3.464246	-4.705158	-3.275843
37	6	0	2.738694	-0.178805	0.496018
38	6	0	3.882388	1.053566	-0.981358
39	6	0	2.494183	1.193122	-1.187913
40	6	0	4.830187	1.708563	-1.771747
41	6	0	2.013134	2.019561	-2.211619
42	6	0	4.337617	2.523555	-2.789689
43	1	0	5.896977	1.591362	-1.603981
44	6	0	2.950498	2.676823	-3.004723
45	1	0	0.945384	2.133220	-2.371515
46	1	0	5.036886	3.053370	-3.430522
47	1	0	2.608426	3.322812	-3.808423
48	7	0	3.995759	0.186696	0.093330
49	7	0	1.807331	0.415844	-0.252744
50	1	0	4.854651	-0.209505	0.450050

SCF Done: E(RB3LYP) = -1319.78416694 A.U. after 1 cycles

Zero-point correction= 0.393029

(Hartree/Particle)

Thermal correction to Energy= 0.418262

Thermal correction to Enthalpy= 0.419206

Thermal correction to Gibbs Free Energy= 0.331712

Sum of electronic and zero-point Energies= -1319.391138

Sum of electronic and thermal Energies= -1319.365905

Sum of electronic and thermal Enthalpies= -1319.364961

Sum of electronic and thermal Free Energies= -1319.452455

SCF Done: E(RB3PW91) = -1321.28629331 A.U. after 16 cycles

TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.012258	1.184268	0.080833
2	6	0	-1.966952	0.373681	-0.153975
3	28	0	-0.310170	-0.653360	-0.180418
4	1	0	-1.255345	-1.441995	-0.931783
5	6	0	-0.058614	-2.550790	0.106454
6	6	0	-0.985170	-3.568266	0.377832
7	6	0	1.314981	-2.888222	0.237817
8	6	0	-0.573400	-4.856569	0.745677
9	6	0	1.735585	-4.175685	0.604424
10	6	0	0.786554	-5.167240	0.852392
11	1	0	-2.050239	-3.364481	0.301947
12	1	0	-1.319084	-5.623487	0.943747
13	1	0	1.103413	-6.167625	1.134550
14	1	0	2.793782	-4.404958	0.719241
15	6	0	-0.560876	2.535498	0.347682
16	6	0	-0.858267	3.580371	-0.551678
17	6	0	0.164502	2.839537	1.516222
18	6	0	-0.442451	4.886194	-0.285750
19	1	0	-1.412730	3.357181	-1.459101
20	6	0	0.564186	4.149336	1.784578
21	1	0	0.409194	2.040060	2.209818
22	6	0	0.266842	5.178291	0.884421
23	1	0	-0.678245	5.678143	-0.992551
24	1	0	1.116898	4.365161	2.695617
25	1	0	0.586363	6.196424	1.091205
26	6	0	-3.398165	0.145896	-0.265438
27	6	0	-3.948235	-0.970054	-0.918233
28	6	0	-4.277681	1.097397	0.294265
29	6	0	-5.331610	-1.133135	-1.012009
30	1	0	-3.283067	-1.706895	-1.359819

31	6	0	-5.658863	0.929171	0.204711
32	1	0	-3.865463	1.964166	0.803199
33	6	0	-6.193362	-0.186720	-0.449741
34	1	0	-5.735909	-2.001889	-1.525518
35	1	0	-6.319575	1.670897	0.646688
36	1	0	-7.270222	-0.316510	-0.519756
37	6	0	2.213006	-1.769475	0.021081
38	6	0	3.982649	-0.461053	-0.314903
39	6	0	2.787722	0.297795	-0.372962
40	6	0	5.243815	0.104609	-0.507247
41	6	0	2.847595	1.670638	-0.644922
42	6	0	5.285018	1.474193	-0.769746
43	1	0	6.151166	-0.490861	-0.460833
44	6	0	4.104051	2.241847	-0.839573
45	1	0	1.943351	2.264852	-0.700947
46	1	0	6.245662	1.956619	-0.927524
47	1	0	4.175507	3.305076	-1.051703
48	7	0	3.575810	-1.763521	-0.056943
49	7	0	1.708597	-0.547906	-0.143916
50	1	0	4.174849	-2.574908	0.007951

SCF Done: E(RB3LYP) = -1319.73903463 A.U. after 2 cycles

Zero-point correction= 0.387709

(Hartree/Particle)

Thermal correction to Energy= 0.412417

Thermal correction to Enthalpy= 0.413361

Thermal correction to Gibbs Free Energy= 0.329652

Sum of electronic and zero-point Energies= -1319.351326

Sum of electronic and thermal Energies= -1319.326618

Sum of electronic and thermal Enthalpies= -1319.325674

Sum of electronic and thermal Free Energies= -1319.409382

SCF Done: E(RB3PW91) = -1321.25474350 A.U. after 16 cycles

Int2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.210217	0.478788	-0.036320
2	6	0	-1.905231	-0.651542	-0.123083
3	28	0	0.227020	-0.792650	-0.043127
4	1	0	-1.274647	-1.617388	-0.237176
5	6	0	1.242449	-2.474833	0.022059
6	6	0	0.854262	-3.823530	0.055162
7	6	0	2.639820	-2.233181	0.067177
8	6	0	1.795371	-4.862192	0.124540
9	6	0	3.596948	-3.255804	0.138167
10	6	0	3.166868	-4.583077	0.166100
11	1	0	-0.201227	-4.090452	0.027456
12	1	0	1.457946	-5.896683	0.146449
13	1	0	3.891567	-5.391165	0.220088
14	1	0	4.662959	-3.034511	0.172346
15	6	0	-1.607832	1.878470	0.054782
16	6	0	-2.016899	2.592406	-1.090634
17	6	0	-1.559945	2.563684	1.286043
18	6	0	-2.373881	3.939480	-1.003106
19	1	0	-2.048999	2.082574	-2.050031
20	6	0	-1.928410	3.907656	1.370554
21	1	0	-1.231490	2.032486	2.175564
22	6	0	-2.335334	4.604422	0.227400
23	1	0	-2.686295	4.469789	-1.899654
24	1	0	-1.892013	4.413151	2.332670
25	1	0	-2.615853	5.652411	0.294017
26	6	0	-3.321331	-1.055532	-0.085236
27	6	0	-3.674770	-2.409378	-0.233937
28	6	0	-4.350478	-0.110992	0.099500
29	6	0	-5.011048	-2.811097	-0.201247
30	1	0	-2.894086	-3.153551	-0.377298
31	6	0	-5.684763	-0.515076	0.131382
32	1	0	-4.101957	0.937990	0.219943
33	6	0	-6.023692	-1.864997	-0.018774

34	1	0	-5.259941	-3.862825	-0.318509
35	1	0	-6.464557	0.228649	0.275990
36	1	0	-7.065197	-2.174621	0.007419
37	6	0	2.941479	-0.814833	0.025583
38	6	0	3.908585	1.192486	-0.047255
39	6	0	2.500017	1.331223	-0.090118
40	6	0	4.773295	2.286376	-0.087520
41	6	0	1.927123	2.604867	-0.183242
42	6	0	4.186706	3.549201	-0.176066
43	1	0	5.852219	2.162768	-0.055490
44	6	0	2.786124	3.702211	-0.224309
45	1	0	0.852083	2.728305	-0.222062
46	1	0	4.822274	4.429630	-0.210957
47	1	0	2.364411	4.700914	-0.296556
48	7	0	4.143066	-0.175228	0.027483
49	7	0	1.933771	0.062460	-0.037288
50	1	0	5.047091	-0.625123	0.066377

SCF Done: E(RB3LYP) = -1319.76955183 A.U. after 2 cycles

Zero-point correction= 0.392925

(Hartree/Particle)

Thermal correction to Energy= 0.417348

Thermal correction to Enthalpy= 0.418292

Thermal correction to Gibbs Free Energy= 0.335016

Sum of electronic and zero-point Energies= -1319.376627

Sum of electronic and thermal Energies= -1319.352204

Sum of electronic and thermal Enthalpies= -1319.351260

Sum of electronic and thermal Free Energies= -1319.434536

SCF Done: E(RB3PW91) = -1321.28026713 A.U. after 16 cycles

PhCCPh

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.608811	-0.000222	-0.000227
2	6	0	0.608811	0.000180	-0.000018
3	6	0	2.040270	0.000089	0.000009
4	6	0	2.756823	-0.858737	-0.858373
5	6	0	2.756895	0.858843	0.858404
6	6	0	4.151744	-0.855729	-0.855285
7	1	0	2.210918	-1.522834	-1.522199
8	6	0	4.151816	0.855690	0.855336
9	1	0	2.211046	1.523003	1.522212
10	6	0	4.854048	-0.000057	0.000033
11	1	0	4.691364	-1.523083	-1.522299
12	1	0	4.691493	1.522993	1.522355
13	1	0	5.940859	-0.000112	0.000041
14	6	0	-2.040270	-0.000100	-0.000091
15	6	0	-2.756851	-0.858799	0.858395
16	6	0	-2.756867	0.858698	-0.858465
17	6	0	-4.151772	-0.855637	0.855412
18	1	0	-2.210968	-1.522931	1.522203
19	6	0	-4.151788	0.855699	-0.855293
20	1	0	-2.210997	1.522752	-1.522361
21	6	0	-4.854048	0.000075	0.000110
22	1	0	-4.691414	-1.522901	1.522497
23	1	0	-4.691443	1.523021	-1.522310
24	1	0	-5.940859	0.000140	0.000185

SCF Done: E(RB3LYP) = -539.483999693 A.U. after 1 cycles

Zero-point correction= 0.191624

(Hartree/Particle)

Thermal correction to Energy= 0.202713

Thermal correction to Enthalpy= 0.203658

Thermal correction to Gibbs Free Energy= 0.150820

Sum of electronic and zero-point Energies= -539.292376

Sum of electronic and thermal Energies= -539.281286

Sum of electronic and thermal Enthalpies= -539.280342

Sum of electronic and thermal Free Energies= -539.333179

SCF Done: E(RB3PW91) = -539.397622379 A.U. after 13 cycles

Int3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.455313	2.257449	1.473007
2	6	0	-3.181520	2.112617	0.901045
3	6	0	-2.623919	0.852667	0.643014
4	6	0	-3.432073	-0.262561	0.983308
5	6	0	-4.701949	-0.141667	1.566855
6	6	0	-5.214759	1.132729	1.815635
7	1	0	-4.859281	3.252586	1.650225
8	1	0	-2.626797	3.013458	0.642741
9	1	0	-5.290675	-1.019241	1.831210
10	1	0	-6.197164	1.247639	2.266143
11	6	0	-0.506745	2.039534	-1.023834
12	6	0	0.761382	2.927434	1.137187
13	6	0	0.122170	3.254111	2.350016
14	6	0	2.130046	3.225810	0.978333
15	6	0	0.836412	3.878064	3.372197
16	1	0	-0.928213	3.014119	2.480972
17	6	0	2.835812	3.848826	2.007260
18	1	0	2.628250	2.957609	0.051991
19	6	0	2.192995	4.177720	3.205309
20	1	0	0.333083	4.128889	4.302284
21	1	0	3.890736	4.073574	1.874115
22	1	0	2.746482	4.661670	4.005694
23	6	0	-0.969044	2.126005	-2.385255
24	6	0	-0.248314	2.936760	-3.288389
25	6	0	-2.111290	1.441782	-2.841031
26	6	0	-0.671393	3.063656	-4.610641
27	1	0	0.638539	3.460306	-2.943419
28	6	0	-2.527054	1.576076	-4.165700
29	1	0	-2.663303	0.815928	-2.148318

30	6	0	-1.811373	2.384345	-5.054799
31	1	0	-0.108121	3.691916	-5.295741
32	1	0	-3.412231	1.044302	-4.504831
33	1	0	-2.137179	2.482528	-6.086974
34	6	0	0.040762	2.322835	0.051461
35	28	0	-0.777785	0.296191	0.087227
36	6	0	1.095612	-0.363364	0.012394
37	6	0	1.903124	-0.207598	-1.061579
38	1	0	1.447418	0.202165	-1.966520
39	6	0	1.470030	-1.033014	1.280889
40	6	0	1.188701	-0.433807	2.528167
41	6	0	2.035343	-2.327931	1.306234
42	6	0	1.476108	-1.080486	3.733022
43	1	0	0.757024	0.561601	2.553954
44	6	0	2.313194	-2.980120	2.507372
45	1	0	2.264134	-2.824399	0.368813
46	6	0	2.038090	-2.360170	3.731935
47	1	0	1.256266	-0.581230	4.674247
48	1	0	2.747075	-3.977613	2.487120
49	1	0	2.256195	-2.868233	4.668164
50	6	0	3.349217	-0.481268	-1.240989
51	6	0	3.830594	-0.742234	-2.540856
52	6	0	4.294864	-0.432759	-0.196164
53	6	0	5.184571	-0.981754	-2.785027
54	1	0	3.124392	-0.760796	-3.369274
55	6	0	5.649412	-0.665969	-0.438468
56	1	0	3.965217	-0.200044	0.810917
57	6	0	6.104071	-0.948946	-1.731962
58	1	0	5.521632	-1.189156	-3.798267
59	1	0	6.355823	-0.619146	0.387470
60	1	0	7.160015	-1.130224	-1.916765
61	6	0	-2.812969	-1.519353	0.602985
62	6	0	-2.414470	-3.629155	0.009764
63	6	0	-1.316732	-2.807665	-0.341873
64	6	0	-2.458070	-4.993637	-0.277696
65	6	0	-0.234959	-3.356448	-1.041027

66	6	0	-1.363670	-5.527904	-0.958098
67	1	0	-3.308239	-5.608810	0.003399
68	6	0	-0.274966	-4.717221	-1.339834
69	1	0	0.594525	-2.728890	-1.344130
70	1	0	-1.356021	-6.585419	-1.207126
71	1	0	0.552876	-5.164840	-1.883201
72	7	0	-3.332151	-2.778321	0.614155
73	7	0	-1.589721	-1.506156	0.067775
74	1	0	-4.252932	-3.032595	0.944246

SCF Done: E(RB3LYP) = -1859.25666236 A.U. after 3 cycles

Zero-point correction= 0.585769

(Hartree/Particle)

Thermal correction to Energy= 0.623041

Thermal correction to Enthalpy= 0.623985

Thermal correction to Gibbs Free Energy= 0.510726

Sum of electronic and zero-point Energies= -1858.670894

Sum of electronic and thermal Energies= -1858.633622

Sum of electronic and thermal Enthalpies= -1858.632677

Sum of electronic and thermal Free Energies= -1858.745936

SCF Done: E(RB3PW91) = -1860.67877022 A.U. after 10 cycles

TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.646617	0.122008	3.066817
2	6	0	-2.723392	0.604050	2.130530
3	6	0	-2.142895	-0.243356	1.177817
4	6	0	-2.475366	-1.624321	1.241653
5	6	0	-3.413652	-2.102352	2.166623
6	6	0	-4.017550	-1.224825	3.068242
7	1	0	-4.084679	0.807452	3.787996
8	1	0	-2.477063	1.660981	2.127801

9	1	0	-3.636040	-3.166019	2.222200
10	1	0	-4.745708	-1.595747	3.783983
11	6	0	-1.939790	1.051816	-0.380785
12	6	0	-0.416489	3.150952	-0.334247
13	6	0	-1.217910	4.217550	0.132165
14	6	0	0.822524	3.465651	-0.929021
15	6	0	-0.802607	5.542670	-0.002803
16	1	0	-2.162024	3.998245	0.623424
17	6	0	1.226607	4.792658	-1.074993
18	1	0	1.462530	2.661024	-1.269763
19	6	0	0.420102	5.838949	-0.613451
20	1	0	-1.436116	6.343898	0.370296
21	1	0	2.182251	5.009374	-1.546140
22	1	0	0.743562	6.870948	-0.722149
23	6	0	-3.182744	0.986982	-1.146390
24	6	0	-3.922118	2.163035	-1.382896
25	6	0	-3.635737	-0.214719	-1.721666
26	6	0	-5.075596	2.133239	-2.168126
27	1	0	-3.587318	3.100785	-0.952756
28	6	0	-4.789347	-0.241074	-2.505140
29	1	0	-3.068619	-1.126663	-1.565212
30	6	0	-5.517353	0.931943	-2.730881
31	1	0	-5.630976	3.052343	-2.337577
32	1	0	-5.117722	-1.179446	-2.945326
33	1	0	-6.417256	0.910012	-3.339927
34	6	0	-0.884970	1.786702	-0.171539
35	28	0	-0.382812	-0.020283	0.251870
36	6	0	1.553314	0.183694	0.194827
37	6	0	2.304140	0.263248	-0.923457
38	1	0	1.763416	0.273935	-1.873311
39	6	0	2.027476	0.113221	1.592421
40	6	0	2.039080	1.258252	2.417642
41	6	0	2.413969	-1.115947	2.168446
42	6	0	2.447559	1.181603	3.749965
43	1	0	1.731086	2.212372	1.997814
44	6	0	2.818280	-1.190920	3.502981

45	1	0	2.405202	-2.012991	1.554478
46	6	0	2.840516	-0.043112	4.302770
47	1	0	2.458268	2.082406	4.359907
48	1	0	3.120027	-2.150031	3.918712
49	1	0	3.156464	-0.101958	5.341351
50	6	0	3.768972	0.335673	-1.124471
51	6	0	4.249645	0.278813	-2.450948
52	6	0	4.727571	0.471117	-0.096906
53	6	0	5.613159	0.340777	-2.743205
54	1	0	3.533002	0.183985	-3.265109
55	6	0	6.091133	0.535227	-0.388275
56	1	0	4.406443	0.532054	0.935870
57	6	0	6.546306	0.468236	-1.710043
58	1	0	5.945490	0.292139	-3.777830
59	1	0	6.804176	0.641232	0.426387
60	1	0	7.609853	0.518534	-1.929842
61	6	0	-1.636980	-2.497734	0.440739
62	6	0	-0.720085	-4.221049	-0.624237
63	6	0	0.114945	-3.080124	-0.718488
64	6	0	-0.386462	-5.446878	-1.203295
65	6	0	1.334122	-3.160410	-1.406084
66	6	0	0.826811	-5.507551	-1.887747
67	1	0	-1.037597	-6.312836	-1.124076
68	6	0	1.671971	-4.381646	-1.984746
69	1	0	1.985066	-2.296863	-1.474329
70	1	0	1.127934	-6.441910	-2.353192
71	1	0	2.611635	-4.470862	-2.522831
72	7	0	-1.819281	-3.811729	0.119418
73	7	0	-0.489696	-2.029363	-0.038619
74	1	0	-2.626996	-4.373123	0.352409

SCF Done: E(RB3LYP) = -1859.23906214 A.U. after 5 cycles

Zero-point correction= 0.585791

(Hartree/Particle)

Thermal correction to Energy= 0.622034

Thermal correction to Enthalpy= 0.622978

Thermal correction to Gibbs Free Energy= 0.512065

Sum of electronic and zero-point Energies= -1858.653271

Sum of electronic and thermal Energies= -1858.617028

Sum of electronic and thermal Enthalpies= -1858.616084

Sum of electronic and thermal Free Energies= -1858.726997

SCF Done: E(RB3PW91) = -1860.66698109 A.U. after 30 cycles

Int4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.080938	-1.231536	-4.115450
2	6	0	-2.019661	-1.501551	-2.750121
3	6	0	-1.840062	-0.489277	-1.786289
4	6	0	-1.747458	0.845651	-2.264600
5	6	0	-1.827055	1.113061	-3.645966
6	6	0	-1.985927	0.086703	-4.572265
7	1	0	-2.202365	-2.048823	-4.821836
8	1	0	-2.112685	-2.527465	-2.405730
9	1	0	-1.732536	2.138999	-3.993818
10	1	0	-2.027483	0.311551	-5.634315
11	6	0	-1.836270	-0.872908	-0.339072
12	6	0	-0.941932	-0.676292	1.996881
13	6	0	-2.001801	-0.114147	2.737386
14	6	0	0.050647	-1.381901	2.704370
15	6	0	-2.074468	-0.262937	4.124387
16	1	0	-2.774409	0.442354	2.213614
17	6	0	-0.030412	-1.545493	4.087655
18	1	0	0.884766	-1.810316	2.158633
19	6	0	-1.091391	-0.984133	4.808152
20	1	0	-2.903534	0.182678	4.669627
21	1	0	0.741950	-2.108953	4.606515
22	1	0	-1.147963	-1.104787	5.887197
23	6	0	-2.954714	-1.793097	0.062514

24	6	0	-2.705913	-3.000344	0.738483
25	6	0	-4.290096	-1.476909	-0.249911
26	6	0	-3.752730	-3.849368	1.106775
27	1	0	-1.681570	-3.274850	0.971962
28	6	0	-5.339363	-2.321444	0.119135
29	1	0	-4.508603	-0.554089	-0.782679
30	6	0	-5.075300	-3.513265	0.802286
31	1	0	-3.532354	-4.777481	1.628946
32	1	0	-6.363245	-2.048130	-0.125901
33	1	0	-5.889985	-4.173561	1.089126
34	6	0	-0.875186	-0.463651	0.529590
35	28	0	0.515893	0.670089	0.005308
36	6	0	2.017136	-0.431772	0.042679
37	6	0	2.932081	0.542759	0.291189
38	1	0	2.541013	1.477604	0.728090
39	6	0	4.389227	0.627349	0.045914
40	6	0	5.143017	1.584548	0.754689
41	6	0	5.065449	-0.174140	-0.895935
42	6	0	6.518352	1.719155	0.556184
43	1	0	4.639635	2.225510	1.476204
44	6	0	6.439208	-0.037670	-1.097584
45	1	0	4.509106	-0.900419	-1.479013
46	6	0	7.176158	0.904999	-0.370763
47	1	0	7.074844	2.461738	1.123286
48	1	0	6.936338	-0.666572	-1.832536
49	1	0	8.246254	1.008302	-0.531777
50	6	0	2.277488	-1.836622	-0.296294
51	6	0	1.602445	-2.464105	-1.362175
52	6	0	3.165497	-2.618868	0.472649
53	6	0	1.831160	-3.806709	-1.668801
54	1	0	0.895948	-1.885560	-1.950329
55	6	0	3.377721	-3.966893	0.180254
56	1	0	3.687989	-2.157117	1.306521
57	6	0	2.717038	-4.567222	-0.897557
58	1	0	1.307026	-4.264273	-2.504905
59	1	0	4.063112	-4.548946	0.792220

60	1	0	2.884548	-5.616333	-1.128476
61	6	0	-1.605383	2.003805	-1.369618
62	6	0	-0.926700	3.399566	0.170357
63	6	0	-1.960333	4.049987	-0.538928
64	6	0	-0.284194	4.042356	1.235727
65	6	0	-2.388687	5.340314	-0.217551
66	6	0	-0.705484	5.329375	1.560634
67	1	0	0.507389	3.547013	1.790033
68	6	0	-1.741506	5.968584	0.845466
69	1	0	-3.185751	5.832403	-0.767408
70	1	0	-0.229361	5.854249	2.383996
71	1	0	-2.041880	6.973059	1.129998
72	7	0	-0.730366	2.136996	-0.379200
73	7	0	-2.357855	3.141167	-1.506961
74	1	0	-3.131599	3.246857	-2.149609

SCF Done: E(RB3LYP) = -1859.30363181 A.U. after 4 cycles

Zero-point correction= 0.587933

(Hartree/Particle)

Thermal correction to Energy= 0.624127

Thermal correction to Enthalpy= 0.625071

Thermal correction to Gibbs Free Energy= 0.514791

Sum of electronic and zero-point Energies= -1858.715699

Sum of electronic and thermal Energies= -1858.679505

Sum of electronic and thermal Enthalpies= -1858.678560

Sum of electronic and thermal Free Energies= -1858.788841

SCF Done: E(RB3PW91) = -1860.72463574 A.U. after 21 cycles

TS3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.541163	-2.475829	-3.662201
2	6	0	-2.183242	-2.420556	-2.334409

3	6	0	-1.986968	-1.179488	-1.647100
4	6	0	-2.190789	0.018150	-2.431245
5	6	0	-2.579974	-0.067642	-3.798415
6	6	0	-2.749425	-1.286988	-4.411171
7	1	0	-2.649309	-3.442284	-4.147958
8	1	0	-2.012529	-3.342605	-1.789925
9	1	0	-2.703951	0.846105	-4.375573
10	1	0	-3.019556	-1.341212	-5.461834
11	6	0	-1.684827	-1.132380	-0.255021
12	6	0	-1.332987	0.246581	1.850156
13	6	0	-2.627420	0.313096	2.395040
14	6	0	-0.233407	0.412349	2.707222
15	6	0	-2.818568	0.541409	3.758976
16	1	0	-3.487254	0.185712	1.742166
17	6	0	-0.422595	0.624942	4.075028
18	1	0	0.767778	0.372138	2.287802
19	6	0	-1.715201	0.695639	4.604585
20	1	0	-3.827116	0.594766	4.161530
21	1	0	0.440766	0.739142	4.725901
22	1	0	-1.862048	0.869186	5.667720
23	6	0	-1.898146	-2.355725	0.581068
24	6	0	-0.834381	-2.948276	1.282681
25	6	0	-3.172848	-2.943061	0.685670
26	6	0	-1.040289	-4.084194	2.070374
27	1	0	0.162760	-2.527253	1.193859
28	6	0	-3.380809	-4.076867	1.473538
29	1	0	-4.008548	-2.498925	0.150084
30	6	0	-2.313352	-4.651920	2.171683
31	1	0	-0.200556	-4.527879	2.599631
32	1	0	-4.376454	-4.508511	1.545307
33	1	0	-2.472878	-5.534984	2.785505
34	6	0	-1.148443	0.026181	0.379199
35	28	0	0.308208	0.875520	-0.433130
36	6	0	2.101240	0.247504	-0.229933
37	6	0	3.022878	1.242516	-0.090757
38	1	0	2.640392	2.250307	0.096823

39	6	0	4.503127	1.229001	-0.161890
40	6	0	5.209464	2.305700	0.415084
41	6	0	5.259713	0.234652	-0.816755
42	6	0	6.603057	2.374541	0.373572
43	1	0	4.648593	3.097620	0.908739
44	6	0	6.652810	0.304139	-0.864089
45	1	0	4.752098	-0.592815	-1.299569
46	6	0	7.335783	1.369223	-0.265254
47	1	0	7.116132	3.214984	0.835905
48	1	0	7.208903	-0.476562	-1.378422
49	1	0	8.421169	1.418869	-0.304682
50	6	0	2.437665	-1.189566	-0.314188
51	6	0	2.037714	-1.972521	-1.416742
52	6	0	3.096377	-1.849521	0.745707
53	6	0	2.317872	-3.339216	-1.477179
54	1	0	1.503748	-1.493451	-2.234046
55	6	0	3.360293	-3.219987	0.695503
56	1	0	3.407634	-1.271586	1.612724
57	6	0	2.979520	-3.974341	-0.420078
58	1	0	2.007395	-3.912722	-2.348069
59	1	0	3.870411	-3.699439	1.528593
60	1	0	3.187026	-5.040832	-0.461123
61	6	0	-2.128021	1.264071	-1.776140
62	6	0	-1.842899	2.758533	-0.112134
63	6	0	-2.580025	3.379434	-1.138138
64	6	0	-1.499255	3.456402	1.046316
65	6	0	-3.015784	4.701224	-1.037297
66	6	0	-1.935910	4.779204	1.153255
67	1	0	-0.924596	2.989287	1.836780
68	6	0	-2.683874	5.389857	0.130847
69	1	0	-3.587197	5.173023	-1.831130
70	1	0	-1.688484	5.346551	2.045565
71	1	0	-3.007351	6.420179	0.248433
72	7	0	-1.542162	1.440376	-0.544568
73	7	0	-2.721082	2.441810	-2.153835
74	1	0	-3.355549	2.525710	-2.936467

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SCF Done:  E(RB3LYP) =  -1859.25466071     A.U. after    5 cycles
Zero-point correction=                           0.586704
(Hartree/Particle)
 Thermal correction to Energy=                    0.622286
 Thermal correction to Enthalpy=                  0.623231
 Thermal correction to Gibbs Free Energy=         0.515122
 Sum of electronic and zero-point Energies=          -1858.667956
 Sum of electronic and thermal Energies=             -1858.632374
 Sum of electronic and thermal Enthalpies=           -1858.631430
 Sum of electronic and thermal Free Energies=        -1858.739538
SCF Done:  E(RB3PW91) =  -1860.67630050     A.U. after   18 cycles

Int5
                         Standard orientation:
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 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -3.415414   -2.590651   -3.132862
      2          6           0       -2.863805   -2.465798   -1.883966
      3          6           0       -2.440917   -1.192698   -1.363781
      4          6           0       -2.612658   -0.050683   -2.244572
      5          6           0       -3.198994   -0.214543   -3.538334
      6          6           0       -3.594722   -1.451132   -3.976342
      7          1           0       -3.709433   -3.572650   -3.494372
      8          1           0       -2.720771   -3.347546   -1.269337
      9          1           0       -3.314412    0.647312   -4.191714
     10          1           0       -4.029237   -1.569739   -4.964749
     11          6           0       -1.909311   -1.041162   -0.071484
     12          6           0       -1.439511    0.521987    1.873330
     13          6           0       -2.678169    0.885416    2.425797
     14          6           0       -0.322499    0.436328    2.713952
     15          6           0       -2.795512    1.171955    3.787656
     16          1           0       -3.555144    0.943990    1.784671
     17          6           0       -0.441356    0.706850    4.080314
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18	1	0	0.637617	0.164851	2.285187
19	6	0	-1.675419	1.081577	4.620292
20	1	0	-3.760622	1.458683	4.198053
21	1	0	0.433464	0.629250	4.721065
22	1	0	-1.764728	1.299617	5.681551
23	6	0	-1.899782	-2.196347	0.878617
24	6	0	-0.696443	-2.801070	1.275700
25	6	0	-3.105741	-2.700720	1.396447
26	6	0	-0.699562	-3.878169	2.166536
27	1	0	0.242933	-2.435541	0.872851
28	6	0	-3.109882	-3.774739	2.289391
29	1	0	-4.045685	-2.241694	1.099592
30	6	0	-1.904394	-4.367540	2.678648
31	1	0	0.243302	-4.336037	2.455290
32	1	0	-4.053549	-4.145767	2.682308
33	1	0	-1.905331	-5.204457	3.372657
34	6	0	-1.348839	0.211904	0.396724
35	28	0	0.255439	0.721814	-0.523064
36	6	0	2.041475	0.076403	-0.347122
37	6	0	2.976705	1.022166	-0.042958
38	1	0	2.608902	1.997246	0.285772
39	6	0	4.457897	0.983111	-0.085794
40	6	0	5.174932	1.904277	0.706778
41	6	0	5.205866	0.123598	-0.917070
42	6	0	6.570321	1.944307	0.702229
43	1	0	4.621172	2.594996	1.340545
44	6	0	6.600775	0.166814	-0.929142
45	1	0	4.689815	-0.574697	-1.566811
46	6	0	7.294029	1.070995	-0.115962
47	1	0	7.091990	2.660660	1.333148
48	1	0	7.150225	-0.506270	-1.583623
49	1	0	8.380786	1.100739	-0.128136
50	6	0	2.374329	-1.336923	-0.633584
51	6	0	1.964916	-1.958628	-1.831775
52	6	0	3.042192	-2.139547	0.316686
53	6	0	2.241342	-3.303628	-2.085174

54	1	0	1.424332	-1.369595	-2.569610
55	6	0	3.303206	-3.489706	0.073235
56	1	0	3.360372	-1.689433	1.254110
57	6	0	2.910477	-4.081007	-1.132645
58	1	0	1.922494	-3.749761	-3.024892
59	1	0	3.819799	-4.081109	0.826612
60	1	0	3.114824	-5.131693	-1.323593
61	6	0	-2.245563	1.198015	-1.752920
62	6	0	-1.556097	2.771188	-0.241564
63	6	0	-2.081267	3.424454	-1.371259
64	6	0	-1.051429	3.498772	0.836133
65	6	0	-2.131073	4.815354	-1.459393
66	6	0	-1.102627	4.894123	0.751711
67	1	0	-0.638861	3.009564	1.708313
68	6	0	-1.634261	5.541455	-0.374852
69	1	0	-2.541867	5.309831	-2.334235
70	1	0	-0.718007	5.484302	1.577957
71	1	0	-1.658959	6.626892	-0.407271
72	7	0	-1.626063	1.368292	-0.510316
73	7	0	-2.476936	2.446307	-2.270990
74	1	0	-2.976009	2.616917	-3.132133

SCF Done: E(RB3LYP) = -1859.25918432 A.U. after 4 cycles

Zero-point correction= 0.587932

(Hartree/Particle)

Thermal correction to Energy= 0.624039

Thermal correction to Enthalpy= 0.624983

Thermal correction to Gibbs Free Energy= 0.516133

Sum of electronic and zero-point Energies= -1858.671252

Sum of electronic and thermal Energies= -1858.635145

Sum of electronic and thermal Enthalpies= -1858.634201

Sum of electronic and thermal Free Energies= -1858.743051

SCF Done: E(RB3PW91) = -1860.68132577 A.U. after 25 cycles

SM

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.534699	-0.028168	0.005292
2	6	0	3.843086	1.185367	-0.042108
3	6	0	2.447035	1.198933	-0.047198
4	6	0	1.719524	-0.003357	-0.003664
5	6	0	2.424941	-1.220117	0.042641
6	6	0	3.818380	-1.230070	0.046901
7	1	0	5.621411	-0.037708	0.008955
8	1	0	4.388814	2.124512	-0.077492
9	1	0	1.937497	2.157977	-0.092191
10	1	0	1.862976	-2.147551	0.075729
11	1	0	4.348038	-2.178460	0.083721
12	6	0	0.250980	-0.032166	-0.005167
13	6	0	-1.797595	-0.707152	-0.020449
14	6	0	-1.854107	0.708738	0.017020
15	6	0	-2.986336	-1.452491	-0.038637
16	6	0	-3.060687	1.413595	0.039276
17	6	0	-4.193716	-0.757894	-0.016991
18	1	0	-2.954687	-2.537953	-0.068123
19	6	0	-4.230606	0.653840	0.021741
20	1	0	-3.092359	2.499443	0.068479
21	1	0	-5.129608	-1.310200	-0.029967
22	1	0	-5.192046	1.160193	0.038056
23	7	0	-0.480959	-1.132211	-0.033234
24	7	0	-0.530699	1.108394	0.023650
25	1	0	-0.202007	2.062112	0.067977

SCF Done: E(RB3LYP) = -610.957845118 A.U. after 1 cycles

Zero-point correction= 0.199299

(Hartree/Particle)

Thermal correction to Energy= 0.210069

Thermal correction to Enthalpy= 0.211013

Thermal correction to Gibbs Free Energy= 0.161744

Sum of electronic and zero-point Energies= -610.758546

Sum of electronic and thermal Energies= -610.747776

Sum of electronic and thermal Enthalpies= -610.746832

Sum of electronic and thermal Free Energies= -610.796101

SCF Done: E(RB3PW91) = -610.871079190 A.U. after 12 cycles

product

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.475792	0.915602	0.012683
2	6	0	2.596796	-0.200047	0.028593
3	6	0	3.086646	-1.512997	0.075438
4	6	0	4.470465	-1.679886	0.097578
5	6	0	5.351594	-0.577805	0.075071
6	6	0	4.866886	0.724060	0.033575
7	6	0	1.504221	1.754528	-0.018672
8	1	0	2.434994	-2.375724	0.096155
9	1	0	4.875906	-2.687458	0.134032
10	1	0	6.424097	-0.753391	0.092899
11	1	0	5.532357	1.582553	0.020060
12	6	0	0.355948	2.622411	-0.029159
13	6	0	-0.938379	2.039536	-0.011470
14	6	0	0.511416	4.022587	-0.053406
15	6	0	-2.057232	2.904818	-0.024395
16	6	0	-0.602956	4.847255	-0.062362
17	1	0	1.515546	4.434074	-0.065139
18	6	0	-1.892096	4.282533	-0.048624
19	1	0	-3.056166	2.482009	-0.016903
20	1	0	-0.480878	5.926814	-0.081043
21	1	0	-2.766519	4.928043	-0.058258
22	6	0	-1.073173	0.588004	0.004769
23	6	0	0.033590	-0.217838	0.002315
24	6	0	-0.048259	-1.708704	-0.013598

25	6	0	-0.196737	-2.428514	1.180290
26	6	0	0.021916	-2.405382	-1.229231
27	6	0	-0.268930	-3.823948	1.159589
28	1	0	-0.252522	-1.895455	2.125617
29	6	0	-0.051070	-3.799908	-1.249870
30	1	0	0.138768	-1.853582	-2.158433
31	6	0	-0.194328	-4.512358	-0.054893
32	1	0	-0.383973	-4.371207	2.091503
33	1	0	0.003737	-4.328688	-2.197850
34	1	0	-0.249940	-5.597690	-0.070770
35	6	0	-2.445398	-0.015269	0.013074
36	6	0	-3.148027	-0.168997	1.218430
37	6	0	-3.067982	-0.402301	-1.183099
38	6	0	-4.436772	-0.709351	1.229856
39	1	0	-2.679827	0.135668	2.151419
40	6	0	-4.357022	-0.942855	-1.174419
41	1	0	-2.538925	-0.279891	-2.124857
42	6	0	-5.044614	-1.099235	0.032563
43	1	0	-4.964228	-0.825792	2.173349
44	1	0	-4.822275	-1.241624	-2.110447
45	1	0	-6.046932	-1.519820	0.040194
46	7	0	2.776579	2.102845	-0.015903
47	7	0	1.309565	0.363659	0.000864

SCF Done: E(RB3LYP) = -1149.29395473 A.U. after 2 cycles

Zero-point correction= 0.373014

(Hartree/Particle)

Thermal correction to Energy= 0.394056

Thermal correction to Enthalpy= 0.395000

Thermal correction to Gibbs Free Energy= 0.321484

Sum of electronic and zero-point Energies= -1148.920941

Sum of electronic and thermal Energies= -1148.899899

Sum of electronic and thermal Enthalpies= -1148.898955

Sum of electronic and thermal Free Energies= -1148.972470

SCF Done: E(RB3PW91) = -1149.12017708 A.U. after 14 cycles

cis-alkene

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.675974	1.837035	0.001384
2	1	0	-1.144590	2.820922	-0.038592
3	6	0	0.675904	1.836826	-0.001150
4	1	0	1.144788	2.820575	0.039008
5	6	0	-1.643448	0.723167	0.070771
6	6	0	-2.886508	0.862053	-0.576430
7	6	0	-1.415300	-0.446865	0.820577
8	6	0	-3.851208	-0.145650	-0.513132
9	1	0	-3.092303	1.769105	-1.141073
10	6	0	-2.382545	-1.449546	0.893917
11	1	0	-0.480045	-0.563893	1.358966
12	6	0	-3.602109	-1.308709	0.221410
13	1	0	-4.798795	-0.018609	-1.030756
14	1	0	-2.186881	-2.341132	1.484665
15	1	0	-4.353539	-2.091938	0.279718
16	6	0	1.643259	0.722919	-0.070882
17	6	0	2.886621	0.862270	0.575742
18	6	0	1.415041	-0.447488	-0.820049
19	6	0	3.851460	-0.145274	0.512533
20	1	0	3.092511	1.769621	1.139867
21	6	0	2.382454	-1.450035	-0.893319
22	1	0	0.479684	-0.564995	-1.358132
23	6	0	3.602261	-1.308719	-0.221388
24	1	0	4.799243	-0.017808	1.029692
25	1	0	2.186676	-2.341905	-1.483598
26	1	0	4.353801	-2.091844	-0.279674

SCF Done: E(RB3LYP) = -540.724309507 A.U. after 1 cycles

Zero-point correction= 0.215114

(Hartree/Particle)

Thermal correction to Energy= 0.226206

Thermal correction to Enthalpy= 0.227151

Thermal correction to Gibbs Free Energy= 0.176472

Sum of electronic and zero-point Energies= -540.509195

Sum of electronic and thermal Energies= -540.498103

Sum of electronic and thermal Enthalpies= -540.497159

Sum of electronic and thermal Free Energies= -540.547838

SCF Done: E(RB3PW91) = -540.641809612 A.U. after 13 cycles

Int6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.818357	-0.831379	-0.117712
2	6	0	-0.793821	-1.604427	-0.025603
3	28	0	-0.250923	0.155993	-0.359690
4	1	0	1.193445	1.595675	-1.861871
5	6	0	4.435451	1.035478	0.601049
6	6	0	5.576581	0.264110	0.390224
7	6	0	3.282316	0.825777	-0.178003
8	6	0	5.590754	-0.719629	-0.605461
9	6	0	3.300819	-0.170485	-1.170612
10	6	0	4.449704	-0.933090	-1.384517
11	1	0	6.459541	0.434395	1.000388
12	1	0	6.483158	-1.317473	-0.770232
13	1	0	4.447327	-1.701760	-2.152512
14	1	0	2.411701	-0.377262	-1.760762
15	6	0	-3.243840	-0.582584	-0.129561
16	6	0	-4.152108	-1.608063	-0.473630
17	6	0	-3.765264	0.685526	0.200221
18	6	0	-5.526803	-1.372373	-0.480076
19	1	0	-3.768797	-2.587287	-0.745838
20	6	0	-5.141063	0.915437	0.198666
21	1	0	-3.077697	1.483699	0.465369

22	6	0	-6.029571	-0.110778	-0.141613
23	1	0	-6.207999	-2.175975	-0.749724
24	1	0	-5.521830	1.898576	0.465059
25	1	0	-7.101356	0.070250	-0.144150
26	6	0	-0.216253	-2.903131	0.253103
27	6	0	1.176924	-3.074670	0.377980
28	6	0	-1.043843	-4.035981	0.418740
29	6	0	1.722719	-4.328280	0.654968
30	1	0	1.826166	-2.212121	0.261306
31	6	0	-0.495490	-5.287859	0.695294
32	1	0	-2.120733	-3.923130	0.335026
33	6	0	0.890896	-5.442034	0.813525
34	1	0	2.800619	-4.435622	0.749982
35	1	0	-1.151936	-6.145659	0.821061
36	1	0	1.316793	-6.418584	1.029239
37	6	0	2.112466	1.681968	0.042672
38	6	0	0.794603	3.236865	0.766723
39	6	0	0.187965	2.769612	-0.418240
40	6	0	0.209301	4.286319	1.484804
41	6	0	-0.964823	3.341264	-0.953327
42	6	0	-0.953171	4.858426	0.967638
43	1	0	0.660489	4.644406	2.405223
44	6	0	-1.525702	4.401877	-0.236600
45	1	0	-1.413042	2.980619	-1.874283
46	1	0	-1.425421	5.680370	1.498701
47	1	0	-2.424656	4.880044	-0.615257
48	7	0	1.974887	2.546846	1.014724
49	7	0	1.004542	1.690823	-0.865023
50	1	0	4.421743	1.807965	1.362780

SCF Done: E(RB3LYP) = -1319.75782531 A.U. after 2 cycles

Zero-point correction= 0.392566

(Hartree/Particle)

Thermal correction to Energy= 0.417820

Thermal correction to Enthalpy= 0.418765

Thermal correction to Gibbs Free Energy= 0.331364

Sum of electronic and zero-point Energies= -1319.365260

Sum of electronic and thermal Energies= -1319.340005

Sum of electronic and thermal Enthalpies= -1319.339061

Sum of electronic and thermal Free Energies= -1319.426462

SCF Done: E(RB3PW91) = -1321.25755221 A.U. after 15 cycles

TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.593237	2.093141	0.107430
2	6	0	-0.651182	2.002415	-0.073225
3	28	0	0.115159	0.203721	0.032097
4	1	0	0.281141	-0.716205	-1.143384
5	6	0	-2.438555	-3.882011	-0.146666
6	6	0	-3.826544	-3.879777	-0.020547
7	6	0	-1.685745	-2.744951	0.203623
8	6	0	-4.491366	-2.744989	0.459961
9	6	0	-2.362493	-1.615766	0.692786
10	6	0	-3.753492	-1.613590	0.817400
11	1	0	-4.392500	-4.764817	-0.299920
12	1	0	-5.573803	-2.745350	0.559008
13	1	0	-4.256150	-0.730548	1.202616
14	1	0	-1.799936	-0.738560	1.010054
15	6	0	1.924836	2.649244	0.154792
16	6	0	2.287353	3.672128	-0.746030
17	6	0	2.868949	2.199902	1.098205
18	6	0	3.563828	4.230950	-0.696020
19	1	0	1.563853	4.017227	-1.478864
20	6	0	4.143593	2.765081	1.142374
21	1	0	2.593671	1.415283	1.797086
22	6	0	4.495035	3.780053	0.246539
23	1	0	3.832717	5.018725	-1.394760
24	1	0	4.862446	2.412626	1.877149

25	1	0	5.489123	4.217619	0.281956
26	6	0	-2.015053	2.474075	-0.170381
27	6	0	-2.965245	1.803817	-0.962544
28	6	0	-2.399531	3.641568	0.521294
29	6	0	-4.267281	2.294493	-1.066827
30	1	0	-2.673727	0.904470	-1.496231
31	6	0	-3.703719	4.123336	0.416150
32	1	0	-1.670628	4.159784	1.137821
33	6	0	-4.641119	3.452898	-0.378237
34	1	0	-4.990305	1.770637	-1.686374
35	1	0	-3.988885	5.023507	0.954396
36	1	0	-5.656502	3.831753	-0.459258
37	6	0	-0.222142	-2.788611	0.069036
38	6	0	1.789388	-3.539896	-0.090401
39	6	0	1.879263	-2.130942	-0.183966
40	6	0	2.944928	-4.330743	-0.162614
41	6	0	3.101350	-1.480689	-0.378037
42	6	0	4.166331	-3.685922	-0.349959
43	1	0	2.879219	-5.412078	-0.078685
44	6	0	4.242329	-2.280759	-0.461391
45	1	0	3.167144	-0.399428	-0.460060
46	1	0	5.079046	-4.272819	-0.414079
47	1	0	5.210325	-1.810129	-0.613099
48	7	0	0.467011	-3.916367	0.064956
49	7	0	0.572386	-1.642754	-0.055292
50	1	0	-1.918215	-4.758749	-0.518209

SCF Done: E(RB3LYP) = -1319.72655622 A.U. after 2 cycles

Zero-point correction= 0.386119

(Hartree/Particle)

Thermal correction to Energy= 0.411278

Thermal correction to Enthalpy= 0.412222

Thermal correction to Gibbs Free Energy= 0.326188

Sum of electronic and zero-point Energies= -1319.340437

Sum of electronic and thermal Energies= -1319.315279

Sum of electronic and thermal Enthalpies= -1319.314334

Sum of electronic and thermal Free Energies= -1319.400368

SCF Done: E(RB3PW91) = -1321.23246617 A.U. after 16 cycles

Int7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.968908	0.560445	-0.606015
2	6	0	-1.800740	-0.673130	-0.727736
3	28	0	0.014525	0.162247	-0.441357
4	1	0	0.256787	0.144872	-1.851119
5	6	0	1.890828	-1.016094	3.290106
6	6	0	1.021088	-1.277668	4.348006
7	6	0	1.495736	-0.172698	2.237216
8	6	0	-0.259935	-0.709628	4.374893
9	6	0	0.219340	0.418216	2.289948
10	6	0	-0.658282	0.142333	3.343049
11	1	0	1.338377	-1.935576	5.153109
12	1	0	-0.934831	-0.921732	5.199793
13	1	0	-1.637359	0.613490	3.366759
14	1	0	-0.058627	1.181428	1.558256
15	6	0	-2.542028	1.874198	-0.484703
16	6	0	-1.802749	3.037919	-0.774074
17	6	0	-3.886317	1.995911	-0.071346
18	6	0	-2.398914	4.292954	-0.656731
19	1	0	-0.769247	2.952419	-1.096098
20	6	0	-4.472195	3.255265	0.041615
21	1	0	-4.458833	1.101959	0.158409
22	6	0	-3.731884	4.406810	-0.249016
23	1	0	-1.820135	5.183604	-0.885110
24	1	0	-5.508135	3.337837	0.359178
25	1	0	-4.191993	5.386920	-0.158264
26	6	0	-2.049595	-2.072276	-0.958422
27	6	0	-1.005860	-2.988379	-1.186423

28	6	0	-3.384236	-2.530814	-0.963790
29	6	0	-1.292860	-4.333638	-1.415055
30	1	0	0.022739	-2.641442	-1.185894
31	6	0	-3.660208	-3.877855	-1.189893
32	1	0	-4.193298	-1.827135	-0.791028
33	6	0	-2.617182	-4.783070	-1.416559
34	1	0	-0.479253	-5.031672	-1.591604
35	1	0	-4.691251	-4.221139	-1.191279
36	1	0	-2.836187	-5.832647	-1.592918
37	6	0	2.376705	0.059806	1.084355
38	6	0	4.088920	0.290283	-0.174398
39	6	0	2.937845	0.469376	-0.991020
40	6	0	5.376169	0.394279	-0.724892
41	6	0	3.054468	0.740446	-2.360976
42	6	0	5.486711	0.669317	-2.085711
43	1	0	6.255035	0.260716	-0.099277
44	6	0	4.338914	0.839302	-2.893581
45	1	0	2.175901	0.870886	-2.987802
46	1	0	6.471266	0.753913	-2.539272
47	1	0	4.461373	1.050410	-3.953152
48	7	0	3.701917	0.025776	1.126782
49	7	0	1.838703	0.321022	-0.161736
50	1	0	2.877627	-1.467262	3.256917

SCF Done: E(RB3LYP) = -1319.74745542 A.U. after 2 cycles

Zero-point correction= 0.387976

(Hartree/Particle)

Thermal correction to Energy= 0.413396

Thermal correction to Enthalpy= 0.414341

Thermal correction to Gibbs Free Energy= 0.327871

Sum of electronic and zero-point Energies= -1319.359480

Sum of electronic and thermal Energies= -1319.334059

Sum of electronic and thermal Enthalpies= -1319.333115

Sum of electronic and thermal Free Energies= -1319.419585

SCF Done: E(RB3PW91) = -1321.25360949 A.U. after 16 cycles

TS5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.838351	0.437544	-0.476337
2	6	0	1.241322	1.471216	-0.053876
3	28	0	-0.091421	-0.019509	-0.378871
4	1	0	-0.381728	1.385503	-0.604997
5	6	0	-1.406308	-3.233848	2.004363
6	6	0	-0.332210	-3.948007	2.533386
7	6	0	-1.228294	-2.432327	0.865208
8	6	0	0.939005	-3.872841	1.945134
9	6	0	0.046017	-2.390395	0.259529
10	6	0	1.127056	-3.094509	0.802816
11	1	0	-0.480943	-4.561050	3.418676
12	1	0	1.770519	-4.429449	2.368475
13	1	0	2.097060	-3.055697	0.316437
14	1	0	0.152348	-1.970765	-0.755296
15	6	0	2.967955	-0.394103	-0.818624
16	6	0	2.952189	-1.203127	-1.971640
17	6	0	4.113468	-0.396191	0.004246
18	6	0	4.059273	-1.986696	-2.297496
19	1	0	2.075346	-1.204408	-2.613059
20	6	0	5.213846	-1.186716	-0.326009
21	1	0	4.128339	0.215447	0.901580
22	6	0	5.191666	-1.983149	-1.476344
23	1	0	4.036603	-2.601457	-3.193200
24	1	0	6.089916	-1.181327	0.317055
25	1	0	6.051279	-2.597167	-1.730710
26	6	0	1.227108	2.831716	0.450259
27	6	0	0.049294	3.473375	0.868337
28	6	0	2.454228	3.521685	0.536184
29	6	0	0.095414	4.779531	1.357063
30	1	0	-0.898490	2.945132	0.816488

31	6	0	2.491981	4.826142	1.024416
32	1	0	3.368255	3.033198	0.211181
33	6	0	1.313873	5.459829	1.437118
34	1	0	-0.822857	5.263654	1.677807
35	1	0	3.442458	5.349940	1.081003
36	1	0	1.346974	6.476857	1.818176
37	6	0	-2.291320	-1.581284	0.331075
38	6	0	-4.150150	-0.686304	-0.199437
39	6	0	-3.110905	0.137631	-0.724608
40	6	0	-5.497184	-0.344817	-0.405198
41	6	0	-3.400383	1.305220	-1.445399
42	6	0	-5.777769	0.814743	-1.123181
43	1	0	-6.291426	-0.973270	-0.010333
44	6	0	-4.741654	1.630620	-1.636186
45	1	0	-2.607061	1.931328	-1.846971
46	1	0	-6.812057	1.103079	-1.294831
47	1	0	-4.999255	2.528539	-2.192749
48	7	0	-3.600434	-1.763701	0.469286
49	7	0	-1.918969	-0.460856	-0.374698
50	1	0	-2.384863	-3.269554	2.472752

SCF Done: E(RB3LYP) = -1319.73827565 A.U. after 2 cycles

Zero-point correction= 0.387175

(Hartree/Particle)

Thermal correction to Energy= 0.411806

Thermal correction to Enthalpy= 0.412750

Thermal correction to Gibbs Free Energy= 0.329358

Sum of electronic and zero-point Energies= -1319.351101

Sum of electronic and thermal Energies= -1319.326470

Sum of electronic and thermal Enthalpies= -1319.325525

Sum of electronic and thermal Free Energies= -1319.408917

SCF Done: E(RB3PW91) = -1321.24792403 A.U. after 11 cycles

Int8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.755176	0.232877	0.696609
2	6	0	-1.048782	1.389703	1.058597
3	28	0	-0.083257	-0.335619	0.733592
4	1	0	-0.821625	1.504586	2.125173
5	6	0	1.469852	-3.851064	-1.036872
6	6	0	0.547807	-4.895449	-1.076033
7	6	0	1.352845	-2.833686	-0.073036
8	6	0	-0.511579	-4.949070	-0.157951
9	6	0	0.301291	-2.910651	0.864236
10	6	0	-0.630120	-3.955790	0.814978
11	1	0	0.649041	-5.672464	-1.829629
12	1	0	-1.224549	-5.768594	-0.193333
13	1	0	-1.422670	-4.005992	1.557312
14	1	0	0.282791	-2.228988	1.720767
15	6	0	-3.078769	-0.071950	0.254716
16	6	0	-4.115500	0.892147	0.348723
17	6	0	-3.386193	-1.355077	-0.262303
18	6	0	-5.407042	0.580462	-0.060993
19	1	0	-3.885408	1.876823	0.744133
20	6	0	-4.678302	-1.657992	-0.676568
21	1	0	-2.595554	-2.096123	-0.330663
22	6	0	-5.689514	-0.692599	-0.575235
23	1	0	-6.195711	1.323683	0.015450
24	1	0	-4.904413	-2.642493	-1.076270
25	1	0	-6.699563	-0.932700	-0.896678
26	6	0	-0.896605	2.628346	0.265900
27	6	0	-0.587130	3.832083	0.926070
28	6	0	-1.063143	2.652324	-1.132179
29	6	0	-0.464170	5.027065	0.214868
30	1	0	-0.446543	3.828785	2.004963
31	6	0	-0.941862	3.846192	-1.840857
32	1	0	-1.268707	1.727463	-1.664608
33	6	0	-0.643055	5.039312	-1.171428

34	1	0	-0.225088	5.946423	0.743236
35	1	0	-1.067184	3.844914	-2.920519
36	1	0	-0.540636	5.967017	-1.728025
37	6	0	2.265256	-1.684156	-0.058636
38	6	0	3.938155	-0.389490	-0.313171
39	6	0	2.882464	0.371447	0.271215
40	6	0	5.177709	0.208980	-0.589055
41	6	0	3.046785	1.732224	0.569397
42	6	0	5.335074	1.560170	-0.285904
43	1	0	5.985792	-0.370639	-1.028359
44	6	0	4.281831	2.312354	0.284055
45	1	0	2.239254	2.316856	1.001908
46	1	0	6.284144	2.049542	-0.491828
47	1	0	4.439902	3.365777	0.502994
48	7	0	3.512958	-1.688936	-0.518510
49	7	0	1.808943	-0.481064	0.433347
50	1	0	2.281860	-3.798820	-1.755313

SCF Done: E(RB3LYP) = -1319.76530499 A.U. after 2 cycles

Zero-point correction= 0.391632

(Hartree/Particle)

Thermal correction to Energy= 0.416433

Thermal correction to Enthalpy= 0.417377

Thermal correction to Gibbs Free Energy= 0.332398

Sum of electronic and zero-point Energies= -1319.373673

Sum of electronic and thermal Energies= -1319.348872

Sum of electronic and thermal Enthalpies= -1319.347928

Sum of electronic and thermal Free Energies= -1319.432907

SCF Done: E(RB3PW91) = -1321.26654207 A.U. after 11 cycles

TS6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.409549	-0.136022	0.029481
2	6	0	-1.676306	0.974853	0.767835
3	28	0	0.481919	-0.042226	-0.330678
4	1	0	-0.870705	1.324875	1.418721
5	6	0	2.861454	-2.824447	1.535592
6	6	0	2.135152	-3.993722	1.770655
7	6	0	2.245501	-1.701705	0.968050
8	6	0	0.788365	-4.068576	1.408389
9	6	0	0.857643	-1.756426	0.661148
10	6	0	0.153315	-2.953712	0.846569
11	1	0	2.629373	-4.855258	2.211964
12	1	0	0.224213	-4.983880	1.565698
13	1	0	-0.899320	-3.017798	0.586803
14	1	0	-0.279562	-0.911571	0.731725
15	6	0	-2.334316	-1.019262	-0.703048
16	6	0	-3.454913	-1.578073	-0.054688
17	6	0	-2.088051	-1.375613	-2.042974
18	6	0	-4.306761	-2.451657	-0.730697
19	1	0	-3.649590	-1.323714	0.983735
20	6	0	-2.945410	-2.243545	-2.720727
21	1	0	-1.223367	-0.960471	-2.554835
22	6	0	-4.056860	-2.785411	-2.066718
23	1	0	-5.164755	-2.874122	-0.214148
24	1	0	-2.743688	-2.499436	-3.757504
25	1	0	-4.721492	-3.465613	-2.592635
26	6	0	-2.871882	1.831027	0.822435
27	6	0	-2.973324	2.749279	1.887284
28	6	0	-3.895349	1.815141	-0.146960
29	6	0	-4.072943	3.599879	2.001382
30	1	0	-2.182189	2.788494	2.632709
31	6	0	-4.987838	2.673515	-0.037581
32	1	0	-3.829729	1.139767	-0.992647
33	6	0	-5.085818	3.563816	1.038656
34	1	0	-4.134758	4.293848	2.835347
35	1	0	-5.764499	2.651853	-0.797555
36	1	0	-5.940857	4.229684	1.119697

37	6	0	3.004976	-0.538787	0.516432
38	6	0	4.488694	0.904975	0.027476
39	6	0	3.285613	1.270830	-0.654204
40	6	0	5.645144	1.690663	-0.109813
41	6	0	3.229169	2.409779	-1.471867
42	6	0	5.581183	2.819495	-0.922901
43	1	0	6.560881	1.417086	0.408311
44	6	0	4.387923	3.173966	-1.595768
45	1	0	2.316187	2.688939	-1.993273
46	1	0	6.463095	3.443459	-1.046084
47	1	0	4.376447	4.062559	-2.222490
48	7	0	4.280209	-0.247143	0.759781
49	7	0	2.346394	0.319754	-0.324562
50	1	0	3.925510	-2.776188	1.748282

SCF Done: E(RB3LYP) = -1319.72530152 A.U. after 2 cycles

Zero-point correction= 0.387851

(Hartree/Particle)

Thermal correction to Energy= 0.411978

Thermal correction to Enthalpy= 0.412922

Thermal correction to Gibbs Free Energy= 0.330977

Sum of electronic and zero-point Energies= -1319.337451

Sum of electronic and thermal Energies= -1319.313323

Sum of electronic and thermal Enthalpies= -1319.312379

Sum of electronic and thermal Free Energies= -1319.394325

SCF Done: E(RB3PW91) = -1321.23549976 A.U. after 11 cycles

Int9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.726988	-1.638850	-0.322563
2	6	0	-1.689511	-1.355452	1.040447
3	28	0	0.038573	-0.575997	0.156929

4	1	0	-1.362788	-2.173362	1.678656
5	6	0	3.654589	-2.523862	0.109637
6	6	0	3.374637	-3.873486	0.343832
7	6	0	2.607940	-1.596653	0.064043
8	6	0	2.056282	-4.292836	0.536125
9	6	0	1.273941	-2.022836	0.248088
10	6	0	0.999196	-3.365790	0.488831
11	1	0	4.185539	-4.596320	0.380115
12	1	0	1.836968	-5.341431	0.723049
13	1	0	-0.012649	-3.729491	0.645741
14	1	0	-1.373382	-2.629447	-0.598828
15	6	0	-2.416064	-0.928352	-1.432707
16	6	0	-3.736504	-0.460601	-1.302632
17	6	0	-1.781676	-0.819420	-2.684798
18	6	0	-4.393890	0.119876	-2.388334
19	1	0	-4.253850	-0.567742	-0.353621
20	6	0	-2.435137	-0.224670	-3.765183
21	1	0	-0.768373	-1.194283	-2.804736
22	6	0	-3.742759	0.248671	-3.619816
23	1	0	-5.417112	0.467734	-2.273198
24	1	0	-1.924127	-0.135763	-4.719942
25	1	0	-4.254491	0.706212	-4.462245
26	6	0	-2.106883	-0.160236	1.801909
27	6	0	-2.111551	-0.266733	3.210195
28	6	0	-2.421797	1.093274	1.231049
29	6	0	-2.436054	0.822052	4.014958
30	1	0	-1.854890	-1.217905	3.670201
31	6	0	-2.728074	2.187252	2.041986
32	1	0	-2.441032	1.219494	0.154512
33	6	0	-2.743540	2.056974	3.433012
34	1	0	-2.439934	0.711184	5.095787
35	1	0	-2.960798	3.143444	1.581397
36	1	0	-2.988855	2.910448	4.058956
37	6	0	2.743011	-0.160722	-0.144194
38	6	0	3.300191	1.869789	-0.449356
39	6	0	1.877426	1.835588	-0.310721

40	6	0	3.957981	3.090303	-0.661199
41	6	0	1.110122	3.005650	-0.383556
42	6	0	3.189409	4.251745	-0.731631
43	1	0	5.039706	3.119991	-0.765662
44	6	0	1.784264	4.209156	-0.594371
45	1	0	0.028155	2.983894	-0.277320
46	1	0	3.677512	5.209578	-0.894486
47	1	0	1.216171	5.134505	-0.654003
48	7	0	3.818363	0.589025	-0.338710
49	7	0	1.547572	0.509186	-0.116055
50	1	0	4.675273	-2.179291	-0.033329

SCF Done: E(RB3LYP) = -1319.78847160 A.U. after 2 cycles

Zero-point correction= 0.393917

(Hartree/Particle)

Thermal correction to Energy= 0.417974

Thermal correction to Enthalpy= 0.418918

Thermal correction to Gibbs Free Energy= 0.337973

Sum of electronic and zero-point Energies= -1319.394554

Sum of electronic and thermal Energies= -1319.370498

Sum of electronic and thermal Enthalpies= -1319.369554

Sum of electronic and thermal Free Energies= -1319.450498

SCF Done: E(RB3PW91) = -1321.29330788 A.U. after 11 cycles

Int10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.214921	-2.752998	-2.905985
2	6	0	2.572977	-1.605388	-2.411734
3	6	0	2.035746	-1.603478	-1.124330
4	6	0	2.154899	-2.757110	-0.320749
5	6	0	2.802207	-3.899536	-0.815118
6	6	0	3.331317	-3.896003	-2.107406

7	1	0	3.629833	-2.744797	-3.911808
8	1	0	2.505728	-0.724526	-3.044114
9	1	0	2.878122	-4.778252	-0.179658
10	1	0	3.835530	-4.780176	-2.490290
11	6	0	2.584906	1.001279	-0.451392
12	6	0	1.397456	2.020822	-2.581801
13	6	0	2.135875	3.154362	-2.991777
14	6	0	0.263286	1.652369	-3.331595
15	6	0	1.747989	3.889212	-4.110219
16	1	0	3.012299	3.452558	-2.423939
17	6	0	-0.118126	2.390219	-4.452859
18	1	0	-0.307966	0.781995	-3.027150
19	6	0	0.619566	3.510649	-4.847476
20	1	0	2.328685	4.758199	-4.409309
21	1	0	-0.994248	2.087442	-5.020881
22	1	0	0.320242	4.083367	-5.721281
23	6	0	3.763305	1.096180	0.374154
24	6	0	4.805202	1.971136	-0.006653
25	6	0	3.903496	0.347006	1.557927
26	6	0	5.948935	2.092011	0.780000
27	1	0	4.713054	2.545036	-0.924266
28	6	0	5.052274	0.473368	2.339525
29	1	0	3.108066	-0.331975	1.846801
30	6	0	6.077075	1.344363	1.956925
31	1	0	6.743841	2.766794	0.472290
32	1	0	5.146660	-0.115301	3.248187
33	1	0	6.971498	1.438181	2.567338
34	6	0	1.825145	1.277769	-1.424192
35	28	0	0.994700	-0.204556	-0.325163
36	6	0	1.544370	-2.660389	0.998809
37	6	0	0.782690	-2.953289	2.961276
38	6	0	0.440677	-1.623346	2.546790
39	6	0	0.405474	-3.422224	4.230065
40	6	0	-0.270617	-0.768826	3.406023
41	6	0	-0.304837	-2.566143	5.070242
42	1	0	0.667193	-4.430604	4.542288

43	6	0	-0.637059	-1.254594	4.661680
44	1	0	-0.527203	0.243927	3.110890
45	1	0	-0.606959	-2.908522	6.057548
46	1	0	-1.187911	-0.609097	5.342706
47	7	0	1.482848	-3.587992	1.956832
48	7	0	0.949740	-1.461691	1.276628
49	7	0	-0.887278	-0.900903	-1.071816
50	6	0	-1.097392	-1.989424	-1.818550
51	6	0	-1.959749	-0.290807	-0.515879
52	6	0	-2.364347	-2.522565	-2.052558
53	1	0	-0.211670	-2.453097	-2.240965
54	6	0	-3.254693	-0.778939	-0.700698
55	6	0	-1.649640	0.914564	0.293965
56	6	0	-3.492260	-1.920795	-1.482029
57	1	0	-2.442911	-3.408806	-2.670481
58	1	0	-4.085293	-0.276700	-0.219414
59	6	0	-2.625886	1.769565	0.810840
60	7	0	-0.333493	1.153942	0.497442
61	6	0	-2.276865	2.900822	1.563677
62	1	0	-3.670281	1.556950	0.618120
63	6	0	0.018281	2.233033	1.203638
64	6	0	-0.905810	3.118966	1.752371
65	1	0	1.084215	2.389113	1.335305
66	1	0	-0.536056	3.963912	2.320282
67	6	0	-3.364522	3.827417	2.126970
68	6	0	-2.767708	5.007358	2.918163
69	1	0	-2.125550	5.638204	2.292187
70	1	0	-3.579016	5.638688	3.297076
71	1	0	-2.184197	4.667921	3.781805
72	6	0	-4.282191	3.016527	3.074767
73	1	0	-5.059169	3.670049	3.488799
74	1	0	-4.782987	2.191201	2.556962
75	1	0	-3.711882	2.594413	3.910096
76	6	0	-4.203763	4.397620	0.957020
77	1	0	-4.982100	5.063526	1.348130
78	1	0	-3.577782	4.974630	0.266387

79	1	0	-4.700207	3.607363	0.383374
80	6	0	-4.920765	-2.452861	-1.670111
81	6	0	-5.786970	-1.359654	-2.342770
82	1	0	-6.811297	-1.726588	-2.478540
83	1	0	-5.838261	-0.446953	-1.739027
84	1	0	-5.388984	-1.091394	-3.328577
85	6	0	-4.958261	-3.715062	-2.552901
86	1	0	-4.384638	-4.539282	-2.113436
87	1	0	-5.994558	-4.054697	-2.658049
88	1	0	-4.571474	-3.522566	-3.560609
89	6	0	-5.518078	-2.806879	-0.285738
90	1	0	-4.921320	-3.576907	0.216179
91	1	0	-5.568822	-1.935687	0.376346
92	1	0	-6.537708	-3.191305	-0.408183

SCF Done: E(RB3LYP) = -2128.50832792 A.U. after 4 cycles

Zero-point correction= 0.755585

(Hartree/Particle)

Thermal correction to Energy= 0.800708

Thermal correction to Enthalpy= 0.801652

Thermal correction to Gibbs Free Energy= 0.673988

Sum of electronic and zero-point Energies= -2127.752743

Sum of electronic and thermal Energies= -2127.707620

Sum of electronic and thermal Enthalpies= -2127.706676

Sum of electronic and thermal Free Energies= -2127.834340

SCF Done: E(RB3PW91) = -2129.90653582 A.U. after 24 cycles

Scheme S1

$^{t}BuO^{-}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000125	-0.000009	0.140135
2	6	0	0.490186	-1.369580	-0.434321

3	1	0	1.505495	-1.574156	-0.067535
4	1	0	-0.164051	-2.172626	-0.068036
5	1	0	0.504284	-1.407887	-1.537222
6	6	0	-1.430013	0.261112	-0.437189
7	1	0	-2.116188	-0.515711	-0.072344
8	1	0	-1.798261	1.229678	-0.071300
9	1	0	-1.467684	0.268400	-1.540157
10	6	0	0.942330	1.108557	-0.433453
11	1	0	0.612458	2.090798	-0.068425
12	1	0	1.964529	0.943056	-0.065686
13	1	0	0.970171	1.138776	-1.536238
14	8	0	-0.003128	-0.000101	1.501989

SCF Done: E(RB3LYP) = -233.136210459 A.U. after 1 cycles
Zero-point correction= 0.121180
(Hartree/Particle)
Thermal correction to Energy= 0.127494
Thermal correction to Enthalpy= 0.128439
Thermal correction to Gibbs Free Energy= 0.092531
Sum of electronic and zero-point Energies= -233.015031
Sum of electronic and thermal Energies= -233.008716
Sum of electronic and thermal Enthalpies= -233.007772
Sum of electronic and thermal Free Energies= -233.043680
SCF Done: E(RB3PW91) = -233.111838928 A.U. after 14 cycles

^{t}BuOH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.006313	-0.000001	0.011156
2	6	0	1.496874	-0.000080	-0.336110
3	1	0	1.986760	0.887852	0.078785
4	1	0	1.986669	-0.888067	0.078773
5	1	0	1.639805	-0.000081	-1.422421

6	6	0	-0.682703	-1.265131	-0.521427
7	1	0	-0.204309	-2.161831	-0.112120
8	1	0	-1.743538	-1.281557	-0.237895
9	1	0	-0.630163	-1.312123	-1.615862
10	6	0	-0.682564	1.265204	-0.521428
11	1	0	-1.743398	1.281747	-0.237901
12	1	0	-0.204072	2.161851	-0.112121
13	1	0	-0.630013	1.312189	-1.615863
14	8	0	-0.039425	-0.000001	1.458231
15	1	0	-0.969866	0.000078	1.737623

SCF Done: E(RB3LYP) = -233.686417788 A.U. after 1 cycles

Zero-point correction= 0.135623

(Hartree/Particle)

Thermal correction to Energy= 0.142370

Thermal correction to Enthalpy= 0.143314

Thermal correction to Gibbs Free Energy= 0.106597

Sum of electronic and zero-point Energies= -233.550795

Sum of electronic and thermal Energies= -233.544048

Sum of electronic and thermal Enthalpies= -233.543104

Sum of electronic and thermal Free Energies= -233.579821

SCF Done: E(RB3PW91) = -233.671451408 A.U. after 11 cycles

SM-anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.518835	-0.000000	0.000000
2	6	0	3.809511	1.207423	0.000033
3	6	0	2.413510	1.207905	0.000032
4	6	0	1.689261	-0.000000	0.000009
5	6	0	2.413510	-1.207905	-0.000022
6	6	0	3.809511	-1.207423	-0.000031
7	1	0	5.606838	0.000000	-0.000002

8	1	0	4.347617	2.153692	0.000057
9	1	0	1.857862	2.140263	0.000043
10	1	0	1.857862	-2.140264	-0.000032
11	1	0	4.347617	-2.153693	-0.000058
12	6	0	0.214937	0.000000	0.000008
13	6	0	-1.792679	-0.718886	-0.000010
14	6	0	-1.792679	0.718886	-0.000001
15	6	0	-3.006297	-1.431581	-0.000000
16	6	0	-3.006297	1.431581	0.000006
17	6	0	-4.199596	-0.708811	0.000009
18	1	0	-3.008317	-2.520494	0.000019
19	6	0	-4.199597	0.708811	0.000006
20	1	0	-3.008318	2.520494	-0.000020
21	1	0	-5.150437	-1.239713	0.000018
22	1	0	-5.150437	1.239713	0.000001
23	7	0	-0.495134	-1.157558	0.000057
24	7	0	-0.495134	1.157558	-0.000095

SCF Done: E(RB3LYP) = -610.452441027 A.U. after 2 cycles

Zero-point correction= 0.185441

(Hartree/Particle)

Thermal correction to Energy= 0.195893

Thermal correction to Enthalpy= 0.196838

Thermal correction to Gibbs Free Energy= 0.148437

Sum of electronic and zero-point Energies= -610.267000

Sum of electronic and thermal Energies= -610.256548

Sum of electronic and thermal Enthalpies= -610.255603

Sum of electronic and thermal Free Energies= -610.304004

SCF Done: E(RB3PW91) = -610.360658584 A.U. after 12 cycles

$Ni(OAc)_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-1.590295	1.079659	-0.015992
2	8	0	-1.589918	-1.079466	-0.016026
3	8	0	1.590199	-1.079634	0.015987
4	8	0	1.590049	1.079515	0.015958
5	28	0	-0.000009	0.000053	-0.000073
6	6	0	-2.280389	-0.000016	-0.016635
7	6	0	2.280383	-0.000008	0.016692
8	6	0	-3.773709	-0.000272	0.010879
9	1	0	-4.107824	0.003960	1.055701
10	1	0	-4.161729	0.896857	-0.477317
11	1	0	-4.161393	-0.901261	-0.470349
12	6	0	3.773709	0.000068	-0.010642
13	1	0	4.161559	-0.897166	0.477495
14	1	0	4.107947	-0.004058	-1.055423
15	1	0	4.161442	0.900951	0.470750

SCF Done: E(RB3LYP) = -626.366317115 A.U. after 1 cycles

Zero-point correction= 0.103704

(Hartree/Particle)

Thermal correction to Energy= 0.114288

Thermal correction to Enthalpy= 0.115232

Thermal correction to Gibbs Free Energy= 0.065672

Sum of electronic and zero-point Energies= -626.262614

Sum of electronic and thermal Energies= -626.252029

Sum of electronic and thermal Enthalpies= -626.251085

Sum of electronic and thermal Free Energies= -626.300645

SCF Done: E(RB3PW91) = -628.000795156 A.U. after 15 cycles

ligand

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.559438	2.330146	0.958074
2	6	0	3.412764	1.254656	0.691429

3	6	0	2.894952	0.090878	0.110450
4	6	0	1.516344	0.098793	-0.156846
5	6	0	0.733883	1.220452	0.144661
6	7	0	1.250389	2.334951	0.696272
7	1	0	2.957609	3.237473	1.410224
8	1	0	4.464205	1.348240	0.938493
9	1	0	1.043557	-0.758233	-0.626300
10	6	0	-0.733914	1.220464	-0.144625
11	6	0	-1.516387	0.098803	0.156851
12	7	0	-1.250401	2.334965	-0.696243
13	6	0	-2.894987	0.090899	-0.110463
14	1	0	-1.043613	-0.758239	0.626296
15	6	0	-2.559440	2.330159	-0.958100
16	6	0	-3.412776	1.254672	-0.691485
17	1	0	-2.957594	3.237490	-1.410258
18	1	0	-4.464198	1.348253	-0.938614
19	6	0	3.753341	-1.134097	-0.244034
20	6	0	5.229360	-0.946525	0.157223
21	1	0	5.797517	-1.845430	-0.108323
22	1	0	5.690849	-0.099577	-0.363922
23	1	0	5.343847	-0.790871	1.236578
24	6	0	3.203613	-2.379446	0.493195
25	1	0	2.167943	-2.598090	0.211385
26	1	0	3.808976	-3.259988	0.245494
27	1	0	3.235342	-2.239952	1.580324
28	6	0	3.690238	-1.372816	-1.772715
29	1	0	4.077116	-0.506376	-2.321978
30	1	0	4.297320	-2.245853	-2.042250
31	1	0	2.666490	-1.558260	-2.115394
32	6	0	-3.753349	-1.134098	0.244017
33	6	0	-3.690665	-1.372405	1.772782
34	1	0	-4.297611	-2.245524	2.042356
35	1	0	-2.666971	-1.557497	2.115816
36	1	0	-4.077927	-0.505917	2.321696
37	6	0	-3.203176	-2.379548	-0.492687
38	1	0	-3.808391	-3.260148	-0.244835

39	1	0	-3.234699	-2.240410	-1.579868
40	1	0	-2.167516	-2.597870	-0.210580
41	6	0	-5.229281	-0.946886	-0.157762
42	1	0	-5.691114	-0.099924	0.363054
43	1	0	-5.343449	-0.791481	-1.237187
44	1	0	-5.797357	-1.845841	0.107788

SCF Done: E(RB3LYP) = -809.920035806 A.U. after 1 cycles
Zero-point correction= 0.382981
(Hartree/Particle)
Thermal correction to Energy= 0.402879
Thermal correction to Enthalpy= 0.403823
Thermal correction to Gibbs Free Energy= 0.334045
Sum of electronic and zero-point Energies= -809.537055
Sum of electronic and thermal Energies= -809.517157
Sum of electronic and thermal Enthalpies= -809.516213
Sum of electronic and thermal Free Energies= -809.585991
SCF Done: E(RB3PW91) = -809.814485830 A.U. after 12 cycles

OAc^-

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.197378	0.000135	-0.001163
2	8	0	0.817547	-1.101383	0.000273
3	8	0	0.701026	1.161117	0.000158
4	6	0	-1.353181	-0.055841	-0.000403
5	1	0	-1.738008	0.434347	0.903559
6	1	0	-1.745080	0.505353	-0.858609
7	1	0	-1.730684	-1.083333	-0.038997

SCF Done: E(RB3LYP) = -228.598681617 A.U. after 1 cycles
Zero-point correction= 0.048238
(Hartree/Particle)

Thermal correction to Energy= 0.051805

Thermal correction to Enthalpy= 0.052749

Thermal correction to Gibbs Free Energy= 0.022342

Sum of electronic and zero-point Energies= -228.550444

Sum of electronic and thermal Energies= -228.546876

Sum of electronic and thermal Enthalpies= -228.545932

Sum of electronic and thermal Free Energies= -228.576340

SCF Done: E(RB3PW91) = -228.572710861 A.U. after 10 cycles

Int11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.795210	0.109577	0.430613
2	6	0	-3.685978	-1.143475	-0.209147
3	6	0	-4.501505	-1.459712	-1.305624
4	6	0	-5.456874	-0.545957	-1.743820
5	6	0	-4.770061	1.019779	-0.013332
6	6	0	-5.594998	0.687783	-1.085289
7	1	0	-4.403304	-2.428673	-1.785820
8	1	0	-6.102869	-0.790356	-2.582624
9	1	0	-4.854609	1.982401	0.481497
10	1	0	-6.346512	1.397047	-1.423372
11	1	0	-3.116815	-1.959901	0.265869
12	28	0	-1.298538	-1.207796	-0.142818
13	8	0	-1.207695	-2.217180	-1.731190
14	6	0	-1.403191	-3.495995	-1.582454
15	8	0	-1.635444	-4.039451	-0.489752
16	6	0	-1.298148	-4.305161	-2.865832
17	1	0	-0.241813	-4.533581	-3.056464
18	1	0	-1.840805	-5.248049	-2.763512
19	1	0	-1.674918	-3.739509	-3.722877
20	6	0	-1.001805	1.843195	-1.688995
21	6	0	-0.330637	3.055132	-1.866147

22	6	0	1.019458	3.157545	-1.509934
23	6	0	1.618010	1.992128	-1.004293
24	6	0	0.881570	0.810453	-0.875835
25	7	0	-0.420594	0.744858	-1.206597
26	1	0	-2.055250	1.753877	-1.944044
27	1	0	-0.878700	3.899830	-2.266477
28	1	0	2.652966	2.016584	-0.684330
29	6	0	1.488992	-0.450063	-0.354974
30	6	0	2.870578	-0.658206	-0.330104
31	7	0	0.648350	-1.413775	0.085387
32	6	0	3.426497	-1.848732	0.161075
33	1	0	3.519860	0.113444	-0.724670
34	6	0	1.151195	-2.566525	0.549283
35	6	0	2.519131	-2.815522	0.613459
36	1	0	0.426519	-3.307808	0.868429
37	1	0	2.848446	-3.768714	1.008231
38	6	0	-2.830810	0.437911	1.476850
39	6	0	-1.789540	1.279028	3.128868
40	6	0	-0.929340	0.308228	2.527221
41	6	0	-1.378504	1.992045	4.267360
42	6	0	0.341767	0.046894	3.066068
43	6	0	-0.114037	1.731178	4.786654
44	1	0	-2.040466	2.723295	4.724558
45	6	0	0.733540	0.767906	4.192082
46	1	0	0.999290	-0.700038	2.635034
47	1	0	0.228760	2.269036	5.667352
48	1	0	1.711490	0.579576	4.629215
49	7	0	-1.628198	-0.227695	1.463606
50	7	0	-2.981680	1.343395	2.438087
51	6	0	4.948922	-2.050684	0.170179
52	6	0	5.348948	-3.413379	0.767845
53	1	0	4.942201	-4.250662	0.188899
54	1	0	6.440441	-3.508137	0.759266
55	1	0	5.017565	-3.518540	1.807567
56	6	0	5.607876	-0.933001	1.015621
57	1	0	6.695066	-1.073202	1.033082

58	1	0	5.408350	0.064145	0.608367
59	1	0	5.245852	-0.954371	2.050029
60	6	0	5.477206	-1.978412	-1.283993
61	1	0	6.563834	-2.124171	-1.291698
62	1	0	5.024766	-2.758287	-1.907399
63	1	0	5.267759	-1.009321	-1.749876
64	6	0	1.830961	4.456458	-1.635916
65	6	0	3.043826	4.214125	-2.567501
66	1	0	3.631427	5.135141	-2.662846
67	1	0	3.710029	3.434546	-2.181978
68	1	0	2.717570	3.914028	-3.570296
69	6	0	0.993673	5.609468	-2.221832
70	1	0	0.136407	5.858150	-1.585519
71	1	0	1.616174	6.507742	-2.300840
72	1	0	0.622430	5.376407	-3.226843
73	6	0	2.332591	4.880340	-0.233351
74	1	0	1.492764	5.061886	0.446984
75	1	0	2.974409	4.118288	0.221823
76	1	0	2.916082	5.805673	-0.310504

SCF Done: E(RB3LYP) = -1818.13908944 A.U. after 4 cycles

Zero-point correction= 0.625061

(Hartree/Particle)

Thermal correction to Energy= 0.664063

Thermal correction to Enthalpy= 0.665008

Thermal correction to Gibbs Free Energy= 0.550052

Sum of electronic and zero-point Energies= -1817.514029

Sum of electronic and thermal Energies= -1817.475026

Sum of electronic and thermal Enthalpies= -1817.474082

Sum of electronic and thermal Free Energies= -1817.589037

SCF Done: E(RB3PW91) = -1819.59446199 A.U. after 29 cycles

TS7

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.688705	0.328855	0.463939
2	6	0	-3.287265	-0.479440	-0.630272
3	6	0	-3.975591	-0.317571	-1.849366
4	6	0	-5.072283	0.540986	-1.955406
5	6	0	-4.799826	1.178560	0.369132
6	6	0	-5.495195	1.272929	-0.836342
7	1	0	-3.679787	-0.905089	-2.716000
8	1	0	-5.604507	0.631572	-2.899383
9	1	0	-5.084244	1.781472	1.226976
10	1	0	-6.356856	1.931904	-0.913333
11	1	0	-3.130637	-1.871623	-0.528000
12	28	0	-1.330893	-1.005315	-0.375075
13	8	0	-1.339903	-2.278953	-1.886924
14	6	0	-2.223088	-3.180114	-1.758589
15	8	0	-3.159898	-3.103793	-0.886864
16	6	0	-2.197735	-4.383939	-2.666606
17	1	0	-1.308477	-4.375022	-3.298888
18	1	0	-2.224022	-5.298951	-2.066133
19	1	0	-3.095812	-4.381009	-3.294430
20	6	0	-0.703724	2.080669	-1.841607
21	6	0	0.004326	3.282626	-1.759515
22	6	0	1.297526	3.292055	-1.222557
23	6	0	1.806735	2.049170	-0.810708
24	6	0	1.038371	0.889593	-0.944871
25	7	0	-0.210153	0.906198	-1.447685
26	1	0	-1.717366	2.063061	-2.236335
27	1	0	-0.473941	4.192275	-2.103255
28	1	0	2.789667	1.990076	-0.356154
29	6	0	1.538670	-0.448772	-0.527380
30	6	0	2.900407	-0.758817	-0.495095
31	7	0	0.609892	-1.377836	-0.198315
32	6	0	3.354696	-2.031686	-0.119275
33	1	0	3.610695	0.002556	-0.795428
34	6	0	1.023049	-2.601853	0.157581

35	6	0	2.364990	-2.965748	0.214507
36	1	0	0.245546	-3.312176	0.418723
37	1	0	2.611412	-3.975601	0.518553
38	6	0	-2.785032	0.316542	1.603091
39	6	0	-1.761378	0.612340	3.441692
40	6	0	-0.870525	-0.080431	2.558696
41	6	0	-1.362666	0.943846	4.747236
42	6	0	0.419251	-0.436866	2.988952
43	6	0	-0.081802	0.586989	5.158882
44	1	0	-2.047364	1.466761	5.410566
45	6	0	0.796580	-0.095740	4.286986
46	1	0	1.110576	-0.964633	2.342161
47	1	0	0.250971	0.833197	6.164523
48	1	0	1.790735	-0.364080	4.637780
49	7	0	-1.561581	-0.261388	1.376626
50	7	0	-2.960483	0.853940	2.807695
51	6	0	4.857011	-2.347708	-0.097762
52	6	0	5.138506	-3.799088	0.336349
53	1	0	4.688031	-4.526979	-0.348621
54	1	0	6.219848	-3.975137	0.337920
55	1	0	4.770951	-4.002592	1.348913
56	6	0	5.561038	-1.393180	0.897974
57	1	0	6.635860	-1.608350	0.923141
58	1	0	5.437946	-0.342000	0.615754
59	1	0	5.165246	-1.519590	1.912304
60	6	0	5.441226	-2.137321	-1.516654
61	1	0	6.513508	-2.365927	-1.513816
62	1	0	4.954735	-2.795745	-2.245720
63	1	0	5.322156	-1.104630	-1.861699
64	6	0	2.134900	4.569565	-1.055238
65	6	0	3.468859	4.414751	-1.826117
66	1	0	4.073510	5.322246	-1.710999
67	1	0	4.062591	3.571771	-1.455596
68	1	0	3.290472	4.258789	-2.896697
69	6	0	1.406921	5.816265	-1.593656
70	1	0	0.469942	6.007667	-1.057963

71	1	0	2.046175	6.696477	-1.461843
72	1	0	1.181788	5.729213	-2.663294
73	6	0	2.431080	4.786949	0.449197
74	1	0	1.503451	4.902328	1.021260
75	1	0	2.990097	3.950382	0.882078
76	1	0	3.030826	5.695286	0.583896

SCF Done: E(RB3LYP) = -1818.11101568 A.U. after 3 cycles
Zero-point correction= 0.620775
(Hartree/Particle)
Thermal correction to Energy= 0.658739
Thermal correction to Enthalpy= 0.659683
Thermal correction to Gibbs Free Energy= 0.549213
Sum of electronic and zero-point Energies= -1817.490240
Sum of electronic and thermal Energies= -1817.452277
Sum of electronic and thermal Enthalpies= -1817.451332
Sum of electronic and thermal Free Energies= -1817.561803
SCF Done: E(RB3PW91) = -1819.57437024 A.U. after 26 cycles

Int12

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.915008	0.446573	0.300585
2	6	0	-3.161360	0.236078	-0.877714
3	6	0	-3.718815	0.644839	-2.096012
4	6	0	-5.003664	1.211674	-2.144783
5	6	0	-5.198061	1.005264	0.260599
6	6	0	-5.744421	1.382014	-0.970053
7	1	0	-3.161978	0.531437	-3.024742
8	1	0	-5.422560	1.519346	-3.101004
9	1	0	-5.749253	1.154151	1.185737
10	1	0	-6.740441	1.816735	-1.011868
11	1	0	-3.088937	-1.959900	-1.448634

12	28	0	-1.397541	-0.464387	-0.557851
13	8	0	-1.189560	-1.166005	-2.479601
14	6	0	-1.891614	-2.093224	-2.897599
15	8	0	-2.938059	-2.558674	-2.226488
16	6	0	-1.645241	-2.785412	-4.204527
17	1	0	-0.704234	-2.444669	-4.636956
18	1	0	-1.626846	-3.869880	-4.057361
19	1	0	-2.469328	-2.562169	-4.891687
20	6	0	-0.180839	2.636081	-1.232745
21	6	0	0.739773	3.662012	-1.004649
22	6	0	2.021622	3.352379	-0.533725
23	6	0	2.296663	1.989313	-0.333794
24	6	0	1.324892	1.021259	-0.602758
25	7	0	0.093528	1.345204	-1.042108
26	1	0	-1.186984	2.862131	-1.578852
27	1	0	0.433272	4.685513	-1.185862
28	1	0	3.260266	1.685893	0.060157
29	6	0	1.566985	-0.434414	-0.399723
30	6	0	2.851171	-0.984147	-0.358616
31	7	0	0.470309	-1.216881	-0.259784
32	6	0	3.053313	-2.358542	-0.161210
33	1	0	3.702552	-0.329730	-0.504881
34	6	0	0.645739	-2.530159	-0.064238
35	6	0	1.898214	-3.136128	-0.006889
36	1	0	-0.258324	-3.117447	0.066375
37	1	0	1.947179	-4.205302	0.159542
38	6	0	-3.182624	0.094757	1.509372
39	6	0	-2.430256	-0.226817	3.472044
40	6	0	-1.376997	-0.537520	2.550561
41	6	0	-2.226214	-0.340138	4.855818
42	6	0	-0.118665	-0.944540	3.024118
43	6	0	-0.975431	-0.752824	5.311918
44	1	0	-3.031802	-0.104132	5.547255
45	6	0	0.065015	-1.047382	4.403909
46	1	0	0.698209	-1.167553	2.346993
47	1	0	-0.793548	-0.845379	6.380230

48	1	0	1.034046	-1.359338	4.787906
49	7	0	-1.896111	-0.329336	1.287403
50	7	0	-3.557824	0.171948	2.782663
51	6	0	4.474350	-2.940054	-0.129739
52	6	0	4.473825	-4.462411	0.108466
53	1	0	3.947790	-5.002490	-0.687509
54	1	0	5.506334	-4.828270	0.126621
55	1	0	4.014653	-4.727194	1.068083
56	6	0	5.275414	-2.266974	1.011880
57	1	0	6.293501	-2.672868	1.041530
58	1	0	5.353290	-1.182927	0.875882
59	1	0	4.806783	-2.452842	1.985174
60	6	0	5.167922	-2.655700	-1.485128
61	1	0	6.184938	-3.065111	-1.475653
62	1	0	4.621502	-3.121698	-2.313472
63	1	0	5.242858	-1.582624	-1.691521
64	6	0	3.088057	4.413853	-0.221406
65	6	0	4.348344	4.143002	-1.079150
66	1	0	5.117190	4.893756	-0.860674
67	1	0	4.779751	3.156861	-0.875107
68	1	0	4.116151	4.195526	-2.149466
69	6	0	2.593454	5.841507	-0.523964
70	1	0	1.719574	6.109468	0.080988
71	1	0	3.387861	6.559120	-0.289874
72	1	0	2.334343	5.969919	-1.581598
73	6	0	3.458921	4.333339	1.279964
74	1	0	2.584343	4.523073	1.912722
75	1	0	3.862590	3.351731	1.550732
76	1	0	4.221270	5.085240	1.517245

SCF Done: E(RB3LYP) = -1818.12646347 A.U. after 4 cycles

Zero-point correction= 0.625876

(Hartree/Particle)

Thermal correction to Energy= 0.664421

Thermal correction to Enthalpy= 0.665365

Thermal correction to Gibbs Free Energy= 0.553345

```
 Sum of electronic and zero-point Energies=          -1817.500588
 Sum of electronic and thermal Energies=             -1817.462042
 Sum of electronic and thermal Enthalpies=           -1817.461098
 Sum of electronic and thermal Free Energies=        -1817.573119
SCF Done:  E(RB3PW91) =  -1819.58840142     A.U. after   21 cycles
```

AcOH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.088187	0.123460	-0.000263
2	8	0	-0.635038	1.208946	0.000033
3	8	0	-0.789807	-1.038368	-0.000060
4	1	0	-1.739616	-0.810955	0.000732
5	6	0	1.397018	-0.120048	-0.000088
6	1	0	1.679955	-0.696083	0.887579
7	1	0	1.678842	-0.711201	-0.877978
8	1	0	1.926599	0.833147	-0.008017

```
SCF Done:  E(RB3LYP) =  -229.099981446     A.U. after    1 cycles
Zero-point correction=                           0.061617
(Hartree/Particle)
 Thermal correction to Energy=                    0.066216
 Thermal correction to Enthalpy=                  0.067160
 Thermal correction to Gibbs Free Energy=         0.034208
 Sum of electronic and zero-point Energies=           -229.038364
 Sum of electronic and thermal Energies=              -229.033766
 Sum of electronic and thermal Enthalpies=            -229.032821
 Sum of electronic and thermal Free Energies=         -229.065774
SCF Done:  E(RB3PW91) =  -229.083814680     A.U. after   10 cycles
```

TS8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.346748	-2.548804	-2.819050
2	6	0	2.687268	-1.407327	-2.358247
3	6	0	2.333623	-1.267120	-0.999670
4	6	0	2.610418	-2.354298	-0.117379
5	6	0	3.305589	-3.479334	-0.585797
6	6	0	3.683897	-3.574402	-1.925109
7	1	0	3.623391	-2.622224	-3.868077
8	1	0	2.491927	-0.590482	-3.046442
9	1	0	3.502360	-4.291088	0.109337
10	1	0	4.223243	-4.450488	-2.276516
11	6	0	2.616660	0.580555	-0.632068
12	6	0	1.356482	2.285478	-2.170338
13	6	0	2.399807	3.059600	-2.735989
14	6	0	0.027670	2.606352	-2.523860
15	6	0	2.118392	4.114164	-3.600974
16	1	0	3.430019	2.820884	-2.487038
17	6	0	-0.248308	3.664147	-3.389983
18	1	0	-0.781461	2.009447	-2.116563
19	6	0	0.792799	4.425740	-3.931470
20	1	0	2.935427	4.694757	-4.022491
21	1	0	-1.279824	3.891862	-3.648128
22	1	0	0.576121	5.248248	-4.608086
23	6	0	3.893068	0.902585	0.019567
24	6	0	4.057645	2.203012	0.541873
25	6	0	4.968081	0.002721	0.119906
26	6	0	5.256789	2.589171	1.138553
27	1	0	3.232445	2.906878	0.478121
28	6	0	6.167959	0.392567	0.719022
29	1	0	4.869686	-1.001957	-0.273713
30	6	0	6.319662	1.683651	1.231073
31	1	0	5.359175	3.595613	1.536941
32	1	0	6.985802	-0.320310	0.786371
33	1	0	7.253583	1.981068	1.700929

34	6	0	1.658224	1.197985	-1.279633
35	28	0	0.849177	-0.207181	-0.246416
36	6	0	2.001832	-2.309018	1.203603
37	6	0	1.325417	-2.686545	3.180236
38	6	0	0.544514	-1.611420	2.638457
39	6	0	1.089214	-3.150086	4.486335
40	6	0	-0.475153	-1.013357	3.399844
41	6	0	0.079150	-2.545676	5.230154
42	1	0	1.684293	-3.962897	4.896225
43	6	0	-0.694885	-1.490887	4.690533
44	1	0	-1.078327	-0.204448	2.999417
45	1	0	-0.122996	-2.888132	6.242597
46	1	0	-1.478188	-1.043140	5.298620
47	7	0	2.240354	-3.113373	2.245049
48	7	0	1.006858	-1.388679	1.363156
49	7	0	-0.972051	-1.011578	-1.116183
50	6	0	-1.047898	-2.071029	-1.923508
51	6	0	-2.118154	-0.491584	-0.629263
52	6	0	-2.254562	-2.668210	-2.289151
53	1	0	-0.100365	-2.458234	-2.289859
54	6	0	-3.362184	-1.041665	-0.947487
55	6	0	-1.946150	0.693145	0.258086
56	6	0	-3.460951	-2.157660	-1.793897
57	1	0	-2.228256	-3.527388	-2.948512
58	1	0	-4.261942	-0.609312	-0.526154
59	6	0	-3.012657	1.442230	0.762529
60	7	0	-0.667395	1.019372	0.546878
61	6	0	-2.790521	2.554018	1.590673
62	1	0	-4.027118	1.161436	0.505518
63	6	0	-0.435968	2.079014	1.325960
64	6	0	-1.452492	2.864236	1.866379
65	1	0	0.607629	2.301920	1.528433
66	1	0	-1.179336	3.702195	2.495837
67	6	0	-3.975150	3.363460	2.140555
68	6	0	-3.515935	4.525732	3.041807
69	1	0	-2.888939	5.242954	2.499405

70	1	0	-4.393546	5.068829	3.409720
71	1	0	-2.958333	4.169809	3.915894
72	6	0	-4.887528	2.430436	2.974212
73	1	0	-5.738310	2.998163	3.369375
74	1	0	-5.287585	1.604943	2.375910
75	1	0	-4.342313	1.999992	3.822003
76	6	0	-4.781995	3.951081	0.956488
77	1	0	-5.637897	4.521561	1.336427
78	1	0	-4.163452	4.626605	0.354028
79	1	0	-5.169922	3.168494	0.295463
80	6	0	-4.834721	-2.759469	-2.127896
81	6	0	-5.710006	-1.682656	-2.814808
82	1	0	-6.694548	-2.100376	-3.056895
83	1	0	-5.867741	-0.810953	-2.170406
84	1	0	-5.249500	-1.335386	-3.747213
85	6	0	-4.724102	-3.971320	-3.073143
86	1	0	-4.137976	-4.784729	-2.629984
87	1	0	-5.726220	-4.363171	-3.280584
88	1	0	-4.270321	-3.701948	-4.034203
89	6	0	-5.519379	-3.221996	-0.818200
90	1	0	-4.919883	-3.983954	-0.307021
91	1	0	-5.674461	-2.391917	-0.120404
92	1	0	-6.500908	-3.655547	-1.044481

SCF Done: E(RB3LYP) = -2128.48254772 A.U. after 6 cycles

Zero-point correction= 0.754242

(Hartree/Particle)

Thermal correction to Energy= 0.798844

Thermal correction to Enthalpy= 0.799788

Thermal correction to Gibbs Free Energy= 0.672527

Sum of electronic and zero-point Energies= -2127.728306

Sum of electronic and thermal Energies= -2127.683704

Sum of electronic and thermal Enthalpies= -2127.682760

Sum of electronic and thermal Free Energies= -2127.810021

SCF Done: E(RB3PW91) = -2129.88359115 A.U. after 21 cycles

Int13

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.130141	0.903198	4.391729
2	6	0	-2.392555	1.225710	3.061260
3	6	0	-2.270614	0.279854	2.025263
4	6	0	-1.879151	-1.042297	2.370941
5	6	0	-1.653100	-1.363704	3.721745
6	6	0	-1.766409	-0.405525	4.726854
7	1	0	-2.222770	1.664168	5.163112
8	1	0	-2.713877	2.233515	2.809760
9	1	0	-1.386549	-2.387453	3.967841
10	1	0	-1.576962	-0.677761	5.762328
11	6	0	-2.651832	0.674817	0.629316
12	6	0	-2.230971	0.459233	-1.850527
13	6	0	-3.396346	-0.204013	-2.292304
14	6	0	-1.428241	1.080513	-2.829946
15	6	0	-3.753559	-0.222003	-3.640573
16	1	0	-4.017101	-0.716129	-1.563269
17	6	0	-1.792651	1.076361	-4.178355
18	1	0	-0.509180	1.576864	-2.533638
19	6	0	-2.958278	0.424695	-4.592898
20	1	0	-4.654652	-0.747097	-3.948866
21	1	0	-1.158440	1.575720	-4.907718
22	1	0	-3.237131	0.411169	-5.643621
23	6	0	-3.977651	1.364517	0.498853
24	6	0	-4.135737	2.518214	-0.290040
25	6	0	-5.108677	0.877698	1.182268
26	6	0	-5.374946	3.152200	-0.406979
27	1	0	-3.277481	2.920339	-0.821279
28	6	0	-6.350366	1.505153	1.062885
29	1	0	-5.013767	-0.008816	1.803757
30	6	0	-6.490847	2.647168	0.267209

31	1	0	-5.467128	4.043036	-1.024177
32	1	0	-7.209709	1.099899	1.592085
33	1	0	-7.456454	3.138586	0.176834
34	6	0	-1.840412	0.400499	-0.423179
35	28	0	-0.116095	-0.340893	-0.121519
36	6	0	-1.744235	-2.124628	1.371473
37	6	0	-1.177513	-3.139230	-0.472146
38	6	0	-1.917750	-4.012362	0.379992
39	6	0	-0.722428	-3.558064	-1.732433
40	6	0	-2.200729	-5.325527	-0.031847
41	6	0	-1.014671	-4.864246	-2.122905
42	1	0	-0.177154	-2.883163	-2.388086
43	6	0	-1.743445	-5.738248	-1.282110
44	1	0	-2.767644	-5.994081	0.611866
45	1	0	-0.684809	-5.216607	-3.097648
46	1	0	-1.954689	-6.748721	-1.624658
47	7	0	-1.061637	-1.942819	0.200901
48	7	0	-2.256556	-3.348551	1.540179
49	7	0	0.894890	1.348126	-0.160004
50	6	0	0.377292	2.585190	-0.167707
51	6	0	2.248612	1.225118	-0.111684
52	6	0	1.157206	3.739083	-0.157365
53	1	0	-0.705047	2.640507	-0.179003
54	6	0	3.080534	2.343033	-0.105495
55	6	0	2.739664	-0.169313	-0.023487
56	6	0	2.553579	3.644169	-0.135093
57	1	0	0.650983	4.696554	-0.167135
58	1	0	4.153311	2.198612	-0.066099
59	6	0	4.085931	-0.528751	0.002917
60	7	0	1.755128	-1.096195	0.059222
61	6	0	4.469489	-1.874854	0.129270
62	1	0	4.844008	0.241540	-0.074281
63	6	0	2.102085	-2.381235	0.191980
64	6	0	3.429821	-2.806444	0.231616
65	1	0	1.284596	-3.089291	0.263816
66	1	0	3.624320	-3.866317	0.339220

67	6	0	5.955576	-2.261193	0.150570
68	6	0	6.157544	-3.780254	0.310159
69	1	0	5.734211	-4.153399	1.249907
70	1	0	5.711014	-4.342616	-0.518042
71	1	0	7.229721	-4.005455	0.319798
72	6	0	6.613514	-1.816157	-1.178965
73	1	0	6.547068	-0.732851	-1.328104
74	1	0	7.675836	-2.087558	-1.177256
75	1	0	6.139152	-2.305643	-2.037437
76	6	0	6.651846	-1.547810	1.335833
77	1	0	6.585842	-0.457117	1.257088
78	1	0	6.206726	-1.845518	2.292251
79	1	0	7.714888	-1.815150	1.357563
80	6	0	3.486337	4.863377	-0.126416
81	6	0	4.436497	4.788089	-1.347098
82	1	0	5.106572	5.655693	-1.349188
83	1	0	5.060587	3.887919	-1.330280
84	1	0	3.872982	4.791971	-2.287361
85	6	0	4.320141	4.853197	1.179005
86	1	0	4.935575	3.951255	1.267120
87	1	0	4.993019	5.718620	1.196159
88	1	0	3.672683	4.908148	2.061692
89	6	0	2.706451	6.190239	-0.197776
90	1	0	2.108657	6.265200	-1.113745
91	1	0	2.040350	6.322292	0.662686
92	1	0	3.413124	7.027380	-0.196406

SCF Done: E(RB3LYP) = -2128.56492263 A.U. after 7 cycles

Zero-point correction= 0.758002

(Hartree/Particle)

Thermal correction to Energy= 0.802143

Thermal correction to Enthalpy= 0.803088

Thermal correction to Gibbs Free Energy= 0.678794

Sum of electronic and zero-point Energies= -2127.806920

Sum of electronic and thermal Energies= -2127.762779

Sum of electronic and thermal Enthalpies= -2127.761835

Sum of electronic and thermal Free Energies= -2127.886129

SCF Done: E(RB3PW91) = -2129.96099446 A.U. after 18 cycles

TS9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.598309	0.644672	4.549378
2	6	0	-2.807370	0.982736	3.224660
3	6	0	-2.469314	0.103549	2.154355
4	6	0	-1.890780	-1.157838	2.523995
5	6	0	-1.712296	-1.496562	3.884681
6	6	0	-2.052282	-0.612068	4.892890
7	1	0	-2.851709	1.357919	5.330843
8	1	0	-3.225504	1.955731	2.985391
9	1	0	-1.294985	-2.471727	4.118595
10	1	0	-1.894361	-0.877880	5.934920
11	6	0	-2.740039	0.432296	0.773015
12	6	0	-2.482830	-0.195686	-1.678358
13	6	0	-3.709648	-0.810424	-1.983417
14	6	0	-1.742813	0.366058	-2.730636
15	6	0	-4.185588	-0.853917	-3.294920
16	1	0	-4.291828	-1.255927	-1.181232
17	6	0	-2.220682	0.335922	-4.043977
18	1	0	-0.783498	0.829489	-2.516272
19	6	0	-3.444198	-0.277042	-4.331369
20	1	0	-5.135599	-1.338023	-3.507812
21	1	0	-1.634369	0.785444	-4.842151
22	1	0	-3.814550	-0.308720	-5.353093
23	6	0	-3.861476	1.361603	0.462161
24	6	0	-3.763603	2.391111	-0.497328
25	6	0	-5.100923	1.233321	1.129671
26	6	0	-4.837742	3.238190	-0.780101
27	1	0	-2.833594	2.529007	-1.039690

28	6	0	-6.174459	2.080897	0.855681
29	1	0	-5.223093	0.442502	1.864589
30	6	0	-6.052022	3.092790	-0.103617
31	1	0	-4.720598	4.018503	-1.529119
32	1	0	-7.114439	1.942480	1.385598
33	1	0	-6.887996	3.753155	-0.320352
34	6	0	-1.976398	-0.185136	-0.263452
35	28	0	-0.092560	-0.338879	-0.034195
36	6	0	-1.594807	-2.129567	1.506070
37	6	0	-1.274817	-2.890932	-0.576645
38	6	0	-1.344554	-3.943169	0.373830
39	6	0	-1.062662	-3.136176	-1.935666
40	6	0	-1.220915	-5.277997	-0.049954
41	6	0	-0.941746	-4.467869	-2.338390
42	1	0	-0.999141	-2.330209	-2.658098
43	6	0	-1.021846	-5.524636	-1.406226
44	1	0	-1.283505	-6.087850	0.672220
45	1	0	-0.784605	-4.691650	-3.390367
46	1	0	-0.927044	-6.549848	-1.756379
47	7	0	-1.406133	-1.699479	0.173875
48	7	0	-1.540735	-3.450174	1.647052
49	7	0	0.862814	1.372917	-0.181233
50	6	0	0.293996	2.583681	-0.250789
51	6	0	2.218409	1.305911	-0.116762
52	6	0	1.023705	3.769731	-0.292131
53	1	0	-0.790269	2.593737	-0.264111
54	6	0	3.004002	2.457533	-0.150559
55	6	0	2.767818	-0.068195	0.018245
56	6	0	2.423011	3.732436	-0.249464
57	1	0	0.480415	4.704811	-0.353501
58	1	0	4.081679	2.362634	-0.089009
59	6	0	4.129172	-0.370924	0.001917
60	7	0	1.828351	-1.032233	0.167192
61	6	0	4.575083	-1.695347	0.149231
62	1	0	4.850146	0.427068	-0.131471
63	6	0	2.236734	-2.298284	0.307664

64	6	0	3.581302	-2.669051	0.308617
65	1	0	1.454212	-3.042685	0.421429
66	1	0	3.825914	-3.717027	0.431815
67	6	0	6.076981	-2.016924	0.128226
68	6	0	6.350791	-3.522992	0.304261
69	1	0	5.972453	-3.899482	1.261759
70	1	0	5.904945	-4.117368	-0.501751
71	1	0	7.431814	-3.700586	0.285026
72	6	0	6.675455	-1.566905	-1.227394
73	1	0	6.558880	-0.490006	-1.391215
74	1	0	7.748019	-1.793174	-1.255048
75	1	0	6.196202	-2.089781	-2.063231
76	6	0	6.777621	-1.255092	1.280098
77	1	0	6.655703	-0.170183	1.189595
78	1	0	6.378401	-1.559790	2.254479
79	1	0	7.852577	-1.471166	1.269974
80	6	0	3.304357	4.989242	-0.293570
81	6	0	4.257101	4.900815	-1.511410
82	1	0	4.890414	5.794794	-1.553992
83	1	0	4.917743	4.028630	-1.455867
84	1	0	3.693501	4.838568	-2.449704
85	6	0	4.137891	5.073335	1.009023
86	1	0	4.789933	4.202442	1.137305
87	1	0	4.774714	5.965650	0.986213
88	1	0	3.488273	5.141213	1.889276
89	6	0	2.470162	6.278434	-0.421886
90	1	0	1.871242	6.289269	-1.340107
91	1	0	1.797217	6.418307	0.432017
92	1	0	3.141049	7.143948	-0.456102

SCF Done: E(RB3LYP) = -2128.52589970 A.U. after 4 cycles

Zero-point correction= 0.756150

(Hartree/Particle)

Thermal correction to Energy= 0.799736

Thermal correction to Enthalpy= 0.800680

Thermal correction to Gibbs Free Energy= 0.678127

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 Sum of electronic and zero-point Energies=          -2127.769750
 Sum of electronic and thermal Energies=             -2127.726163
 Sum of electronic and thermal Enthalpies=           -2127.725219
 Sum of electronic and thermal Free Energies=        -2127.847773
SCF Done:  E(RB3PW91) =  -2129.92245528     A.U. after   22 cycles
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