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Supporting Information

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Regioselective Hypervalent Iodine(III)-Mediated Dearomatizing Phenylation of Arenols via Direct Ligand Coupling

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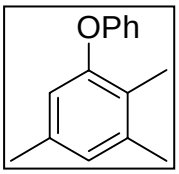
Supporting Information

Experimental Section

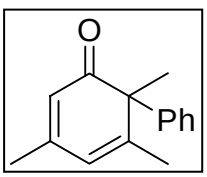
General. Chloro(diphenyl)-λ^3-iodane (Ph_2ICl, 97%) was purchased from Aldrich. Tetrafluoroboro(diphenyl)-λ^3-iodane (Ph_2IBF_4)[1] was prepared from (diacetoxy)iodobenzene (DIB). Dichloromethane (CH_2Cl_2) and *tert*-butyl alcohol (*t*BuOH) were used as received. Column chromatography was carried out under positive pressure using 40-63 μm silica gel (Merck) and the indicated solvents. Evaporations were conducted under reduced pressure at temperatures less than 30 °C. Further drying of the residues was accomplished under high vacuum. Melting points are uncorrected. NMR spectra of samples in the indicated solvent were run at 250, 300 or 400 MHz. Carbon multiplicities were determined by DEPT-135 or *J*-MOD experiments. Electron impact mass spectra were obtained at 70 eV. Low and high resolution electron impact, electrospray and liquid secondary ion mass spectrometry data (EIMS, ESIMS, LSIMS, HRMS) were obtained either from the mass spectrometry laboratory at the CESAMO, Université Bordeaux 1, or from the mass spectrometry laboratory at the Institut Européen de Chimie et Biologie, Pessac.

General Procedure for λ^3-Iodane-Mediated Phenylation of Arenols. To a stirred solution of *t*BuOK (1.4 mmol, 1.05 equiv) in *t*BuOH (4 mL, ca. 0.35 M) was added the arenol (1.3 mmol) at room temperature, and the mixture was stirred for 1 hour. The diphenyl-λ^3-iodane reagent, i.e., Ph_2IBF_4[1] or Ph_2ICl (1.5 mmol, 1.1 equiv), was added in one portion to this mixture. The resulting suspension was stirred for 20 h at room temperature, after which time water (20 mL) was added, and the mixture was extracted with CH_2Cl_2 (3 × 5 mL). The combined organic extracts were washed once with water (5 mL), dried over Na_2SO_4, filtered, evaporated, and further dried under high vacuum.

1,2,5-Trimethyl-3-phenoxybenzene (2a) and 3,5,6-trimethyl-6-phenylcyclohexa-2,4-dienone (3a). Ph_2ICl-mediated phenylation of 2,3,5-trimethyphenol **(1a**, 312 mg, 2.3 mmol) was carried out according to the general procedure to afford a crude orange oil (600 mg), which was purified by column chromatography, eluting with pentanes/EtOAc (5:1), to yield the diaryl ether **2a** as a colorless oil (309 mg, 63%), the cyclohexa-2,4-dienone **3a** as a yellow oil (40 mg, 8%) and some recovered starting phenol **1a** (50 mg, 16%).



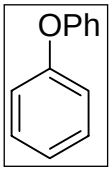
Diaryl ether **2a**: IR (NaCl, neat) 2929, 1489, 1224 cm^{-1}; ^1H NMR ($CDCl_3$, 250 MHz) δ 2.11 (s, 3H), 2.25 (s, 3H), 2.29 (s, 3H), 6.63 (s, 1H), 6.82 (s, 1H), 6.89 (d, J = 7.6 Hz, 2H), 6.99-7.06 (m, 1H), 7.26-7.33 (m, 2H); ^{13}C NMR ($CDCl_3$, 62.9 MHz) δ 158.4, 153.9, 138.4, 136.1, 129.5, 126.5, 125.5, 121.9, 118.3, 116.9, 20.8, 20.0, 11.8; EIMS *m/z* (rel intensity) 212 (M^+, 100), 197 (42), 135 (13), 119 (19), 77 (20); HRMS (EI) calcd for $C_{15}H_{16}O$ 212.1201, found 212.1199.



Cyclohexa-2,4-dienone **3a**: IR (NaCl, neat) 3024, 2978, 1666, 1636, 1580, 846 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 1.55 (s, 3H), 1.63 (s, 3H), 2.02 (s, 3H), 5.75 (s, 1H), 6.00 (s, 1H), 7.08-7.22 (m, 5H); ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 203.9, 155.5, 154.6, 140.6, 128.6, 126.9, 126.6, 122.5, 120.2, 56.7, 22.9, 22.1, 19.8; EIMS *m/z* (rel

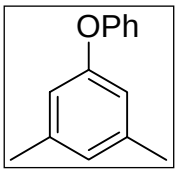
intensity) 212 (M^+, 100), 197 (42), 184 (68), 169 (88), 154 (21), 77 (25); HRMS (EI) calcd for $C_{15}H_{16}O$ 212.1201, found 212.1198.

Phenoxybenzene (2b).[2] Ph_2ICl-mediated phenylation of phenol (**1b**, 100 mg, 1.1 mmol) was



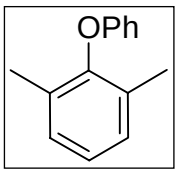
carried out according to the general procedure to afford the diaryl ether **2b** as a clean crude orange oil (140 mg, 75%), which was not further purified. IR (NaCl, neat) 3066, 3044, 1582, 1485, 1285 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 7.15-7.26 (m, 6H), 7.26-7.49 (m, 4H); ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 157.4, 129.9, 123.4, 119.0; EIMS m/z (rel intensity) 170 (M^+, 14), 51 (31), 39 (13), 18 (100).

3,5-Dimethylphenoxybenzene (2c).[3] Ph_2ICl-mediated phenylation of 3,5-dimethylphenol (**1c**, 154

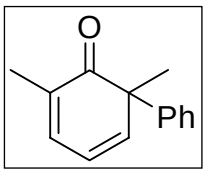


mg, 1.26 mmol) was carried out according to the general procedure to afford a crude orange oil (255 mg), which was purified by column chromatography, eluting with cyclohexane/EtOAc (9:1), to yield the diaryl ether **2c** as a colorless oil (147 mg, 59%). IR (NaCl, neat) 1585, 1490, 1220 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 2.29 (s, 6H), 6.64 (s, 2H), 6.75 (s, 1H), 7.00 (dd, J = 0.9 Hz, J = 7.8 Hz, 2H), 7.09 (t, J = 7.5 Hz, 1H), 7.33 (t, J = 8.5 Hz, 2H); ^{13}C NMR ($CDCl_3$, 62.9 MHz) δ 157.5, 157.2, 139.5, 129.6, 125.0, 122.9, 118.8, 116.6, 21.3; EIMS *m/z* (rel intensity) 198 (M^+, 100), 183 (13), 105 (24), 91 (39), 77 (94).

1,3-Dimethyl-2-phenoxybenzene (2d)[4] **and 2,6-dimethyl-6-phenylcyclohexa-2,4-dienone (3d).**[5] Ph_2ICl-mediated phenylation of 2,6-dimethylphenol (**1d**, 155 mg, 1.3 mmol) was carried out according to the general procedure to afford a crude orange oil (367 mg), which was purified by column chromatography, eluting with cyclohexane/EtOAc (9:1), to yield the diaryl ether **2d** as a colorless oil (60 mg, 24%) and the cyclohexa-2,4-dienone **3d** as a yellow oil (93 mg, 37%).

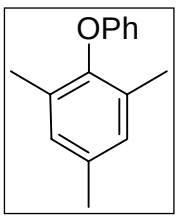


Diaryl ether **2d**:[4] IR (NaCl, neat) 3040, 2921, 1490, 1224, 750 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 2.04 (s, 6H), 6.65-6.69 (m, 2H), 6.85-6.95 (m, 1H), 6.97-7.03 (m, 3H), 7.13-7.19 (m, 2H); ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 157.8, 151.0, 131.5, 129.6, 128.9, 125.0, 121.2, 114.6, 16.3; EIMS *m/z* (rel intensity) 198 (M^+, 31), 183 (18), 77 (97), 76 (75).

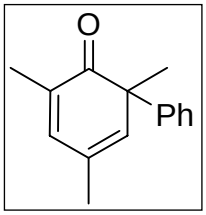


Cyclohexa-2,4-dienone **3d**:[5] IR (NaCl, neat) 3034, 2978, 1660, 742, 692 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 1.62 (s, 3H), 1.88 (s, 3H), 6.26 (dd, J = 6.0, 9.4 Hz, 1H), 6.37 (td, J = 9.4, 0.8 Hz, 1H), 6.89 (d, J = 6.0 Hz, 1H), 7.20-7.39 (m, 5H); ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 203.9, 145.3, 141.2, 138.4, 132.8, 128.9, 127.6, 127.0, 120.1, 54.6, 24.2, 16.0; EIMS *m/z* (rel intensity) 198 (M^+, 100), 183 (60), 170 (63), 155 (93).

1,3,5-Trimethyl-2-phenoxybenzene (2e),[6] **2,4,6-Trimethyl-6-phenylcyclohexa-2,4-dienone (3e),** [7] **and 2,4,6-trimethyl-4-phenylcyclohexa-2,5-dienone (4e).** Ph_2ICl-mediated phenylation of 2,4,6-trimethylphenol (**1e**, 172 mg, 1.26 mmol) was carried out according to the general procedure to afford a crude orange oil (503 mg), which was purified by column chromatography, eluting with cyclohexane/EtOAc (99:1), to yield the diaryl ether **2e** as a colorless oil (18 mg, 7%), the cyclohexa-2,4-dienone **3e** as a yellow oil (84 mg, 31%), and a 3:2 mixture of **3e**/**4e** as a yellow oil (47 mg, 18%).

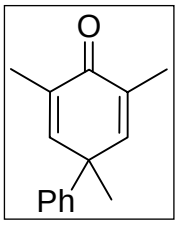


Diaryl ether **2e**:[6] IR (NaCl, neat) 3022, 2926, 1592, 1490, 1223 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 2.00 (s, 6H), 2.22 (s, 3H), 6.66-6.69 (m, 2H), 6.82 (s, 2H), 6.84-6.89 (m, 1H), 7.13-7.18 (m, 2H); ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 158.0, 148.7, 134.4, 131.0, 129.5, 129.5, 121.1, 114.6, 20.8, 16.2; EIMS *m/z* (rel intensity) 212 (M^+, 59), 197 (60), 120 (100).



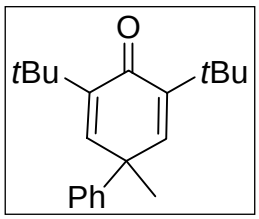
Cyclohexa-2,4-dienone **3e**:[7] IR (NaCl, neat) 3030, 2978, 1656, 1458, 710 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 1.63 (s, 3H), 1.91 (s, 3H), 2.03 (s, 3H), 6.08 (s,

1H), 6.80 (s, 1H), 7.25-7.34 (m, 5H); ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 203.6, 142.5, 141.7, 139.7, 132.1, 128.8, 127.4, 127.3, 126.9, 53.7, 24.4, 21.5, 15.9; EIMS *m/z* (rel intensity) 212 (M^+, 100), 184 (42), 169 (35), 154 (9).

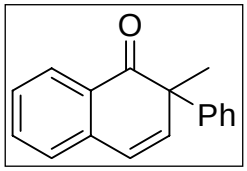


Cyclohexa-2,5-dienone **4e**: ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.66 (s, 3H), 1.96 (s, 6H), 6.73 (s, 2H), 7.23-7.35 (m, 5H); ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 187.5, 151.2, 132.9, 129.1, 127.5, 126.6, 44.3, 24.2, 16.1. These NMR data were read on the spectrum of the 3:2 mixture of the *ortho*- and the *para*-phenylated products **3e** and **4e**.

2,6-Di-*tert*-butyl-4-methyl-4-phenylcyclohexa-2,5-dienone (4f).[8] Ph_2ICl-mediated phenylation of 2,6-di-*tert*-butyl-4-methylphenol (**1f**, 277 mg, 1.3 mmol) was carried out according to the general procedure to afford **4f** (353 mg, 94%) as a clean orange oil. IR (NaCl, neat) 2958, 2869, 1658, 1639, 1370, 698 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.29 (s, 18H), 1.67 (s, 3H), 6.64 (s, 2H), 7.28-7.38 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 186.9, 147.2, 145.0, 142.8, 129.2, 127.4, 126.7, 43.9, 35.1, 30.8, 29.9; EIMS *m/z* (rel intensity) 296 (M^+, 17), 281 (47), 240 (82), 225 (100), 197 (38), 57 (83).

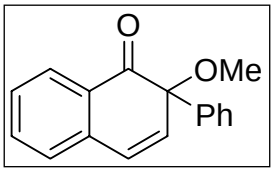


2-Methyl-2-phenyl-2*H*-naphthalen-1-one (3i). Ph_2ICl-mediated phenylation of 2-methylnaphthol (**1i**, 200 mg, 1.26 mmol) was carried out according to the general procedure to afford a crude mixture (400 mg), which was purified by column chromatography, eluting with cyclohexane/EtOAc (9:1), to furnish some recovered starting naphthol **1i** (20 mg, 10%) and **3i** as a red oil (107 mg, 36%). IR (NaCl, neat) 3060, 3027, 2978, 1680, 1597, 1286 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.72 (s, 3H), 6.28 (d, J = 9.8 Hz, 1H), 6.73 (d, J = 9.6 Hz, 1H), 7.09-7.13 (m, 1H), 7.23-7.46 (m, 5H), 7.57-7.60 (m, 1H), 7.71 (d, J = 7.1 Hz, 1H), 7.99 (d, J = 7.1 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 201.4, 141.5,

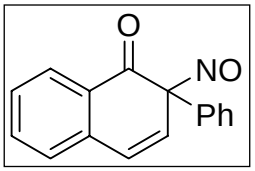


140.2, 138.8, 137.9, 135.0, 129.1, 128.6, 128.0, 127.8, 127.7, 127.2, 124.1, 53.1, 24.4; ESIMS *m/z* (rel intensity) 235 (MH^+, 100); HRMS (LSIMS) calcd for $C_{17}H_{14}O$ 235.1122, found 235.1124.

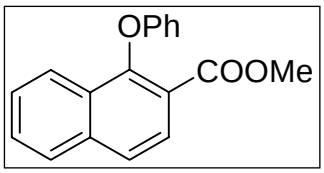
2-Methoxy-2-phenyl-2*H*-naphthalen-1-one (3j). Ph_2ICl-mediated phenylation of 2-methoxylnaphthol (**1j**, 219.3 mg, 1.26 mmol) was carried out according to the general procedure to afford a crude mixture (345 mg), which was purified by column chromatography, eluting with cyclohexane/Et_2O (5:1), to yield **3j** as a colorless oil (164 mg, 52%): IR (NaCl, neat) 3060, 2931, 1686, 1598, 1283 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 3.65 (s, 3H), 6.50 (d, J = 10.1 Hz, 1H), 7.15 (d, J = 10.1 Hz, 1H), 7.47-7.56 (m, 5H), 7.77-7.83 (m, 3H), 8.17 (dd, J = 0.75, 7.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 198.4, 137.5, 137.0, 135.6, 134.8, 129.5, 129.3, 128.4, 128.4, 128.1, 127.6, 127.4, 125.6, 83.5, 53.5; EIMS m/z (rel intensity) 250 (M^+, 100), 235 (23), 207 (31), 191 (46), 105 (61), 77 (46); HRMS (LSIMS) calcd for $C_{17}H_{14}O_2Na$ 273.0891, found 273.0887.



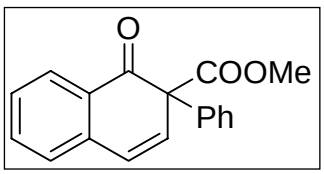
2-Nitroso-2-phenyl-2H-naphthalen-1-one (3k). Ph_2ICl-mediated phenylation of 2-nitrosonaphthol (**1k**, 218 mg, 1.26 mmol) was carried out according to the general procedure to afford a brown crude mixture (383 mg), which was purified by column chromatography, eluting with cyclohexane/Et_2O (3:1), to yield **3k** as a yellow solid (227 mg, 74%): Mp = 97–103 °C; IR (NaCl, neat) 1677, 1594, 1536, 1491, 915 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.83 (d, J = 10.0 Hz, 1H), 7.00-7.04 (m, 1H), 7.12-7.27 (m, 6H), 7.33 (dt, J = 7.58, 0.98 Hz, 1H), 7.48 (dt, J = 7.58, 1.47 Hz, 1H), 8.08 (dd, J = 7.8, 0.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 182.3, 159.4, 149.0, 136.4, 135.2; 134.0, 131.8, 130.1, 129.9, 129.3, 128.6, 124.5, 117.0, 115.9; ESIMS *m/z* (rel intensity) 250 (MH^+, 5), 272 (MNa^+, 4); HRMS (LSIMS) calcd for $C_{16}H_{11}O_2NNa$ 272.0687, found 272.0687.



Methyl-1-phenoxynaphthalene-2-carboxylate (2l), methyl-1,2-dihydro-1-oxo-2-phenylnaphthalene-2-carboxylate (3l). Ph_2ICl-mediated phenylation of methyl 1-hydroxy-naphthalene-2-carboxylate (**1l**, 255 mg, 1.3 mmol) was carried out according to the general procedure to afford a yellow oil crude mixture (423 mg), which was purified by column chromatography, eluting with cyclohexane/Et_2O (8:1), to yield **2l** as a yellow gum (73 mg, 21%), **3l** as a yellow oil (25 mg, 7%) and some recovered starting material (61 mg, 24%).

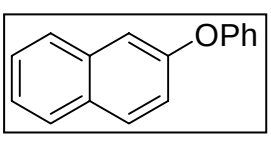


Diaryl ether **2l**: IR (NaCl, neat) 2948, 1724, 1628, 1598, 1491, 1244 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 3.74 (s, 3H), 6.81 (d, J = 8.1 Hz, 2H), 6.98 (t, J = 7.1 Hz, 1H), 7.23-7.26 (m, 2H), 7.48 (t, J = 7.3 Hz, 1H), 7.59 (t, J = 7.3 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7,90 (d, J = 8.0 Hz, 1H), 7.97 (d, J = 8.6 Hz, 1H), 8.09 (d, J = 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.6, 159.3, 151.0, 136.4, 129.1, 128.1, 127.9, 127.4, 126.5, 126.2, 124.6, 123.5, 121.3, 119.9, 114.7, 51.7; ESIMS *m/z* (rel intensity) 278 (M^+, 15); HRMS (EI) calcd for $C_{18}H_{14}O_3$ 278.0942, found 278.0943.

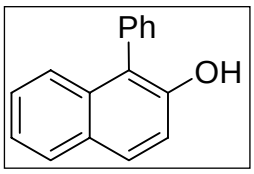


Cyclohexa-2,4-dienone **3l**: IR (NaCl, neat) 3060, 2952, 1743, 1681, 1230 cm^{-1}; ^1H NMR ($CDCl_3$, 250 MHz) δ 4.14 (s, 3H), 6.83 (d, J = 9.76 Hz, 1H), 7.29 (d, J = 9.76 Hz, 1H), 7.61-7.84 (m, 7H), 7.93 (t, J = 7.6 Hz, 1H), 8.37 (dd, J = 7.6, 0.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 194.5, 170.8, 137.4, 136.7, 135.3, 132.22, 129.9, 129.3, 128.9, 128.7, 128.6, 128.2, 128.1, 127.6, 115.5, 53.6; EIMS *m/z* (rel intensity) 301 (MNa^+, 6); HRMS (LSIMS) calcd for $C_{18}H_{14}O_3Na$ 301.0836, found 301.0840.

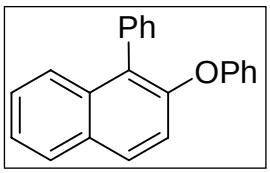
2-Phenoxy-naphthalene (2p)[9], **1-phenyl-naphthalen-2-ol (3p)**[10], **2-phenoxy-1-phenyl-naphthalene (4p).** Ph_2ICl-mediated phenylation of 2-naphthol (**1p**, 181 mg, 1.26 mmol) was carried out according to the general procedure to afford a crude orange oil (452 mg) which was purified by column chromatography, eluting with cyclohexane/Et_2O [(1:0), (9:1), (5:1)], to yield **2p** (24 mg, 9%), **3p** (49 mg, 18%) and **4p** (81 mg, 22%) as amorphous colorless solids, and some recovered starting material (50 mg, 28%).



Diaryl ether **2p**[9]: IR (NaCl, neat) 3063, 1509, 1223 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6,99 (d, *J* = 7.5 Hz, 2H), 7.05 (t, *J* = 7.5 Hz, 1H), 7.15-7.39 (m, 6H), 7.61 (d, *J* = 7.5 Hz, 1H), 7.74 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 157.1, 155.0, 134.3, 130.1, 129.8, 129.8, 127.7, 127.1, 126.5, 124.6, 123.4, 119.9, 119.1, 114.0; EIMS *m/z* (rel intensity) 220 (M^+, 100), 127 (54), 77 (39).

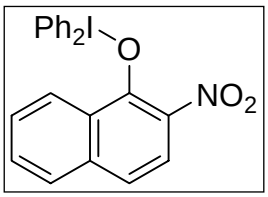


Biaryl **3p**[10]: IR (NaCl, neat) 3505, 3434, 1619, 1595, 1147, 816 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 5.07 (s, 1H), 7.12-7.50 (m, 9H), 7.70 (d, *J* = 9.0 Hz, 2H); ^{13}C NMR ($CDCl_3$,75.5 MHz) δ 150.1, 134.2, 133.3, 131.2, 129.6, 129.5, 128.9, 128.5, 128.0, 126.5, 124.6, 123.3, 121.0, 117.4; EIMS *m/z* (rel intensity) 220 (M^+, 100), 219 (45), 28 (38).

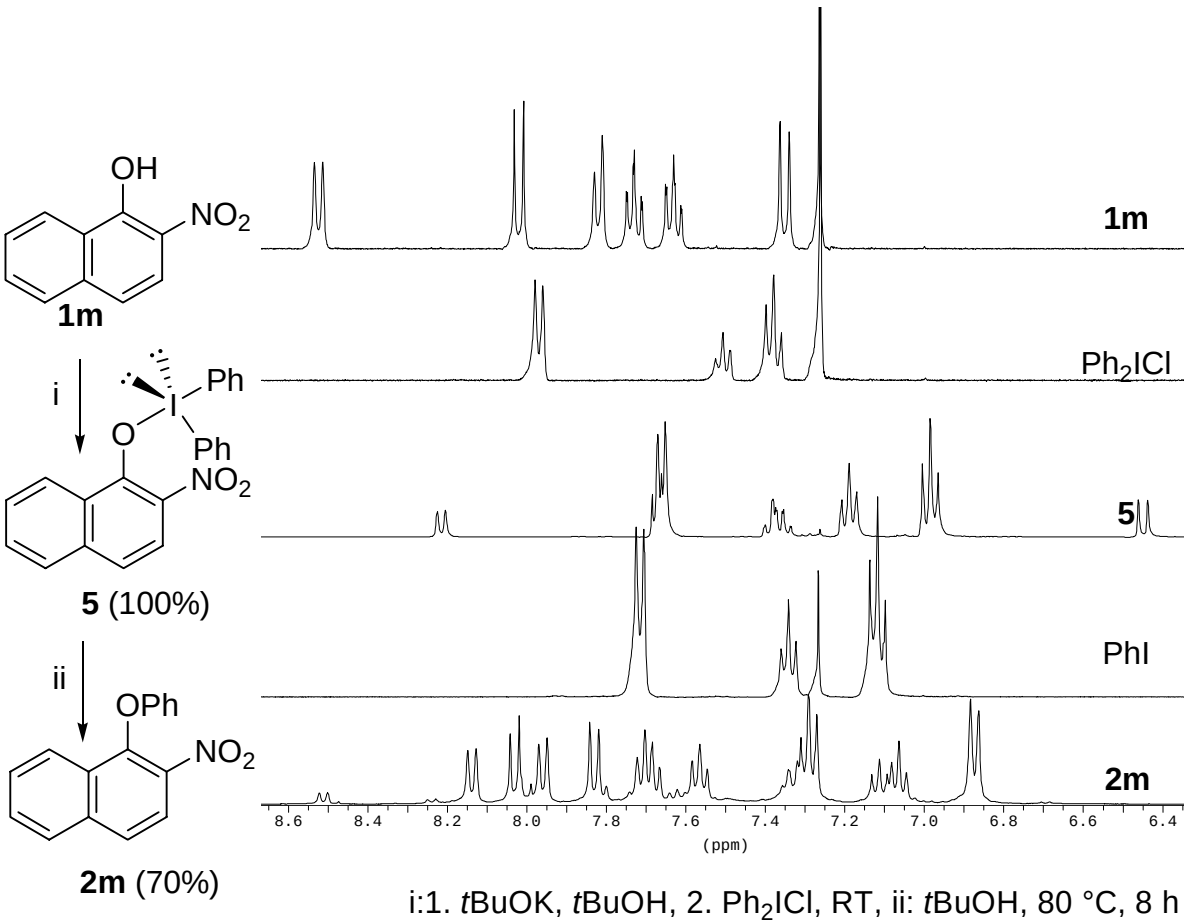


Biaryl **4p**: IR (NaCl, neat) 3057, 1589, 1490, 1234, 758 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 6.73 (d, *J* = 7.5 Hz, 2H), 6.84 (t, *J* = 7.2 Hz, 1H), 7.06-7.12 (m, 3H), 7.21-7.31 (m, 7H), 7.50 (d, *J* = 8.3 Hz, 1H), 7.71 (t, *J* = 9.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 158.5, 150.3, 135.4, 133.7, 130.8, 130.5, 129.8, 129.4, 129.3, 128.0, 127.9, 127.3, 126.4, 125.8, 124.9, 122.2, 120.6, 117.6; EIMS *m/z* (rel intensity) 296 (M^+, 100), 203 (51), 202 (62). HRMS (LSIMS) calcd for $C_{22}H_{16}O$ 296.1201, found 296.1204.

2-Nitronaphthoxy(diphenyl)-λ^3-iodane (5). Ph_2ICl-mediated phenylation of 2-nitronaphthol (**1m**, 114 mg, 0.6 mmol) was carried out according to the general procedure to afford compound **5** (282 mg, 100%) as an orange oil. IR (NaCl, neat) 3055, 1602, 1556, 1514, 1325, 1026, 765, 731 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.45 (d, *J* = 9.5 Hz, 1H), 6.99 (t, *J* = 7.8 Hz 4H),7.19 (t, *J* = 7.6 Hz 3H), 7.34-7.40 (m, 2H), 7.66-7.69 (m, 5H), 8.22 (d, *J* = 8.1, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 167.4, 137.7, 135.1, 133.6, 131.3, 131.2, 130.6, 129.6, 127.2, 127.1, 124.6, 123.8, 116.8, 112.4; ESIMS *m/z* (rel intensity) *positive mode* 281 (Ph_2I^+, 100), *negative mode* 188 ($[M\text{-}Ph_2I]^-$, 8).



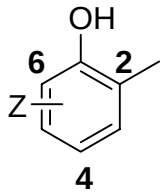
2-Nitro-1-phenoxynaphthalene (2m). 2-Nitronaphthoxy(diphenyl)-λ^3-iodane (**5**, 179 mg, 0.38 mmol) was dissolved in *t*BuOH (5 mL). The resulting solution was stirred at reflux temperature for 8 h, after which time it was worked up as described in the general procedure to give a red oil (90 mg), which was purified by column chromatography, eluting with cyclohexane/Et_2O (6:1), to furnish the diaryl ether **2m** (70 mg, 70%): mp = 81-82 °C; IR (NaCl, neat) 3062, 1625, 1583, 1531, 1264, 757, 734 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) 6.68 (d, *J* = 7.8 Hz, 2H), 6.88 (d, *J* = 6.5 Hz, 1H), 7.09 (t, *J* = 7.8 Hz, 2H), 7.38 (d, *J* = 7.3 Hz, 1H), 7.50 (d, *J* = 7.1 Hz, 1H), 7.65 (d, *J* = 9.0 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 8.8 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), ^{13}C NMR ($CDCl_3$, 100 MHz) *δ*; 158.4, 145.0, 139.1, 137.1, 136.2, 129.5, 129.4, 127.9, 127.8, 125.6, 124.3, 122.4, 120.6, 114.9. *LRMS and HRMS to come !*



i:1. *t*BuOK, *t*BuOH, 2. Ph_2ICl, RT, ii: *t*BuOH, 80 °C, 8 h

Calculations. Semi-empirical AM1 and ab-initio HF/6-31G* methods were used to calculate the relative magnitudes of HOMO atomic coefficients and the electrostatic charges distribution of **1a,d-g** (Table 3). The geometries were fully optimized by AM1 semi-empirical methods and used as the basis for optimization at the Hartree-Fock level using the 6-31G* basis set. These calculations were performed on a Silicon Graphics O_2 workstation equipped with Spartan v5.0.

Table 3. HOMO Atomic coefficients and electrostatic charge distribution of **1a,d-g** obtained from semi-empirical AM1 and ab-initio HF/6-31G* calculations



Cpds	Level	HOMO				Electrostatic Potential			
		O	C_2	C_4	C_6	O	C_2	C_4	C_6
1a	**AM1**	-0.491	0.485	-0.502	0.456	-0.72	-0.40	-0.51	-0.54
	6-31G*	-0.325	0.251	-0.279	0.228	-0.82	-0.36	-0.86	-0.83
1d	**AM1**	-0.436	0.471	-0.530	0.471	-0.67	-0.35	-0.42	-0.35
	6-31G*	-0.283	0.243	-0.299	0.243	-0.73	-0.08	-0.34	-0.08
1e	**AM1**	0.422	-0.460	0.537	-0.460	-0.67	-0.32	-0.28	-0.32
	6-31G*	0.279	-0.239	-0.305	-0.239	-0.72	0.04	0.14	0.04
1g	**AM1**	-0.442	0.471	-0.530	0.471	-0.70	-0.51	-0.44	-0.51
	6-31G*	-0.281	0.237	-0.295	0.237	-0.70	-0.54	-0.39	-0.54
1f	**AM1**	0.428	-0.460	0.537	-0.460	-0.71	-0.52	-0.29	-0.52
	6-31G*	-0.278	0.226	-0.301	0.238	-0.76	-0.52	0.12	-0.54

```
SPARTAN AB INITIO PROGRAM: SGI/R10K/32    Release 5.1.3

  2,3,5-DIMETHYLPHENOL (1a)
  Calculation started:  Tue Apr 26 08:15:59 2005

  Run type: Single point energy
  Model: RHF/6-31G*
  Number of shells:  62
    32 S shells
    20 SP shells
    10 6D shells
  Number of basis functions: 172
  Number of electrons:  74
  Use of molecular symmetry disabled
  Molecular charge:  -1
  Spin multiplicity:  1
```

Cartesian Coordinates (Angstroms)

Atom	Label	X	Y	Z
O	O1	-2.9755970	-0.1063941	0.4954270
C	C1	-1.6988176	-0.0804281	0.4310265
C	C2	1.1667542	0.0330069	0.4213140
C	C3	-0.9217533	-0.0660756	1.6094207
C	C4	-0.9540591	-0.0594451	-0.7856595
C	C5	0.4669532	0.0283996	-0.7910579
C	C6	0.4809439	-0.0292862	1.6296187
H	H3	-2.6653230	-0.5758031	-2.0391468
C	C8	-1.7022032	-0.0597900	-2.1058483
C	C7	1.2482689	0.0984948	-2.0737008
C	C9	1.2118409	0.0128374	2.9351075
H	H6	2.2507026	0.0899264	0.4226292
H	H9	-1.1426670	-0.5916802	-2.8815195
H	H10	-1.8740640	0.9703980	-2.4334939
H	H1	-1.4589418	-0.0833208	2.5587137
H	H2	2.3020747	0.3346552	-1.8898026
H	H4	0.8548349	0.8866954	-2.7236479
H	H7	1.2081853	-0.8633366	-2.5944107
H	H5	2.2161662	-0.4125488	2.8364360
H	H8	0.6862161	-0.5732124	3.6964037
H	H11	1.3004850	1.0469074	3.2821909

Point Group = C1 Order = 1 Nsymop = 1
This system has 57 degrees of freedom

SPARTAN AB INITIO PROGRAM: SGI/R10K/32 Release 5.1.3
(Job run on Swing)

2,6-DIMETHYLPHENOL (**1d**)
Calculation started: Wed Apr 27 01:13:27 2005

Run type: Single point energy
Model: RHF/6-31G*
Number of shells: 54
27 S shells
18 SP shells
9 6D shells
Number of basis functions: 153
Number of electrons: 66
Use of molecular symmetry enabled
Molecular charge: -1
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom	Label	X	Y	Z
O	O1	0.0000000	0.0009226	-2.1519797
C	C1	0.0000000	0.0011759	-0.8949285
C	C2	0.0000000	0.0006081	1.9973106
C	C3	-1.2309338	0.0009927	-0.0897388
C	C4	1.2309338	0.0009927	-0.0897388
C	C5	1.1938073	0.0006382	1.2754832
C	C6	-1.1938073	0.0006382	1.2754832
C	C7	-2.5509221	-0.0003734	-0.8503751
C	C8	2.5509221	-0.0003734	-0.8503751
H	H4	2.1327240	0.0001836	1.8223448
H	H5	-2.1327240	0.0001836	1.8223448

```
    H  H6           0.0000000    -0.0001288     3.0742927
    H  H2          -2.6347307    -0.8661804    -1.5070495
    H  H7          -2.6494633     0.8779113    -1.4885733
    H  H8          -3.4027886    -0.0144608    -0.1744389
    H  H3           2.6347307    -0.8661804    -1.5070495
    H  H9           3.4027886    -0.0144608    -0.1744389
    H  H10          2.6494633     0.8779113    -1.4885733

  Point Group = CS  Order =  1 Nsymop =  2
  This system has  26 degrees of freedom

 SPARTAN AB INITIO PROGRAM: SGI/R10K/32    Release 5.1.3
  (Job run on Swing)

  2,4,6-TRIMETHYLPHENOL (1e)
  Calculation started:  Wed Apr 27 01:32:21 2005

  Run type: Single point energy
  Model: RHF/6-31G*
  Number of shells:  62
    32 S shells
    20 SP shells
    10 6D shells
  Number of basis functions: 172
  Number of electrons:  74
  Use of molecular symmetry enabled
  Molecular charge:  -1
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------
    O  O1           0.0000000    -0.0100454     2.7382152
    C  C1           0.0000000    -0.0044248     1.4812924
    C  C2           0.0000000     0.0136760    -1.4236352
    C  C3           1.2287760     0.0008959     0.6744940
    C  C4          -1.2287760     0.0008959     0.6744940
    C  C5          -1.1915392     0.0074730    -0.6901512
    C  C6           1.1915392     0.0074730    -0.6901512
    C  C7           2.5491496     0.0025173     1.4344046
    C  C8          -2.5491496     0.0025173     1.4344046
    H  H4          -2.1307443     0.0116507    -1.2355918
    H  H5           2.1307443     0.0116507    -1.2355918
    C  C9           0.0000000    -0.0124158    -2.9456908
    H  H2           2.6368885    -0.8657828     2.0870378
    H  H7           2.6420501     0.8779591     2.0770403
    H  H8           3.4010570    -0.0036080     0.7583538
    H  H3          -2.6368885    -0.8657828     2.0870378
    H  H9          -3.4010570    -0.0036080     0.7583538
    H  H10         -2.6420501     0.8779591     2.0770403
    H  H1           0.0000000    -1.0248155    -3.3569081
    H  H6           0.8766354     0.4879074    -3.3522242
    H  H11         -0.8766354     0.4879074    -3.3522242
  Point Group = CS  Order =  1 Nsymop =  2
  This system has  31 degrees of freedom


SPARTAN AB INITIO PROGRAM: SGI/R10K/32    Release 5.1.3
  (Job run on Swing)

  2,6-DI-TERT-BUTYLPHENOLATE  (1g)
  Calculation started:  Wed Apr 27 01:48:33 2005
```

```
  Run type: Single point energy
  Model: RHF/6-31G*
  Number of shells: 102
    57 S shells
    30 SP shells
    15 6D shells
  Number of basis functions: 267
  Number of electrons: 114
  Use of molecular symmetry enabled
  Molecular charge:  -1
  Spin multiplicity:  1

                    Cartesian Coordinates (Angstroms)
    Atom Label         X             Y             Z
    -- --------  ------------- ------------- -------------
    O  O1           0.0000000     0.0000000     1.4929605
    C  C1           0.0000000     0.0000000     0.2270979
    C  C2           0.0000000     0.0000000    -2.6452328
    C  C3           1.2402930     0.0000000    -0.5648672
    C  C4          -1.2402930     0.0000000    -0.5648672
    C  C5          -1.1955333     0.0000000    -1.9322669
    C  C6           1.1955333     0.0000000    -1.9322669
    C  C7           2.5684086     0.0000000     0.2284899
    C  C11         -2.5684086     0.0000000     0.2284899
    H  H4          -2.1178855     0.0000000    -2.4993398
    H  H5           2.1178855     0.0000000    -2.4993398
    H  H6           0.0000000     0.0000000    -3.7224209
    H  H22         -4.7286574     0.0000000    -0.0574706
    C  C9           2.6253636    -1.2588738     1.1404149
    C  C8           2.6253636     1.2588738     1.1404149
    C  C10          3.8330964     0.0000000    -0.6732564
    H  H7           1.7428512     1.2627803     1.7717214
    H  H9           2.6338562     2.1646379     0.5419008
    H  H10          3.5146187     1.2540950     1.7655215
    H  H2           1.7428512    -1.2627803     1.7717214
    H  H11          3.5146187    -1.2540950     1.7655215
    H  H12          2.6338562    -2.1646379     0.5419008
    H  H8           3.8659653    -0.8793429    -1.3083042
    H  H13          4.7286574     0.0000000    -0.0574706
    H  H14          3.8659653     0.8793429    -1.3083042
    C  C13         -2.6253636    -1.2588738     1.1404149
    C  C14         -3.8330964     0.0000000    -0.6732564
    C  C12         -2.6253636     1.2588738     1.1404149
    H  H16         -1.7428512     1.2627803     1.7717214
    H  H17         -3.5146187     1.2540950     1.7655215
    H  H18         -2.6338562     2.1646379     0.5419008
    H  H3          -1.7428512    -1.2627803     1.7717214
    H  H19         -2.6338562    -2.1646379     0.5419008
    H  H20         -3.5146187    -1.2540950     1.7655215
    H  H15         -3.8659653    -0.8793429    -1.3083042
    H  H21         -3.8659653     0.8793429    -1.3083042

  Point Group = CNV Order =  2 Nsymop =  4
  This system has  30 degrees of freedom

SPARTAN AB INITIO PROGRAM: SGI/R10K/32    Release 5.1.3
  (Job run on Swing)

  2,6-DI-TERT-BUTYL-4MEPHENOLATE (1f)
  Calculation started:  Wed Apr 27 02:05:20 2005

  Run type: Single point energy
  Model: RHF/6-31G*
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Number of shells: 110
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  32 SP shells
  16 6D shells
Number of basis functions: 286
Number of electrons: 122
Use of molecular symmetry enabled
Molecular charge:  -1
Spin multiplicity:  1
                  Cartesian Coordinates (Angstroms)
  Atom Label          X             Y             Z
  -- --------  ------------- ------------- -------------
  O  O1           0.0015890     0.0000000     1.8631649
  C  C1           0.0020493     0.0000000     0.5974137
  C  C2           0.0006024     0.0000000    -2.2882626
  C  C3           1.2381610     0.0000000    -0.1967317
  C  C4          -1.2378574     0.0000000    -0.1963782
  C  C5          -1.1933393     0.0000000    -1.5614525
  C  C6           1.1919075     0.0000000    -1.5642805
  C  C7           2.5696944     0.0000000     0.5908031
  C  C11         -2.5679807     0.0000000     0.5942607
  H  H4          -2.1171465     0.0000000    -2.1257257
  H  H5           2.1158565     0.0000000    -2.1279380
  C  C15         -0.0090820     0.0000000    -3.8113019
  H  H22         -4.7277464     0.0000000     0.3072646
  C  C9           2.6280591    -1.2592962     1.5015718
  C  C8           2.6280591     1.2592962     1.5015718
  C  C10          3.8317962     0.0000000    -0.3145371
  H  H7           1.7466298     1.2633735     2.1340210
  H  H9           2.6352465     2.1644014     0.9018680
  H  H10          3.5178835     1.2564420     2.1257238
  H  H2           1.7466298    -1.2633735     2.1340210
  H  H11          3.5178835    -1.2564420     2.1257238
  H  H12          2.6352465    -2.1644014     0.9018680
  H  H8           3.8634908    -0.8792719    -0.9498822
  H  H13          4.7291378     0.0000000     0.2986460
  H  H14          3.8634908     0.8792719    -0.9498822
  C  C13         -2.6242273    -1.2591144     1.5053076
  C  C14         -3.8320076     0.0000000    -0.3083297
  C  C12         -2.6242273     1.2591144     1.5053076
  H  H16         -1.7415931     1.2628589     2.1361078
  H  H17         -3.5130181     1.2556762     2.1309761
  H  H18         -2.6326863     2.1644742     0.9060364
  H  H3          -1.7415931    -1.2628589     2.1361078
  H  H19         -2.6326863    -2.1644742     0.9060364
  H  H20         -3.5130181    -1.2556762     2.1309761
  H  H15         -3.8651496    -0.8792835    -0.9435939
  H  H21         -3.8651496     0.8792835    -0.9435939
  H  H1           1.0039159     0.0000000    -4.2047998
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This system has  64 degrees of freedom
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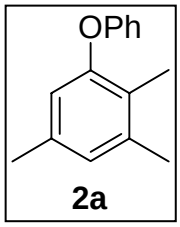

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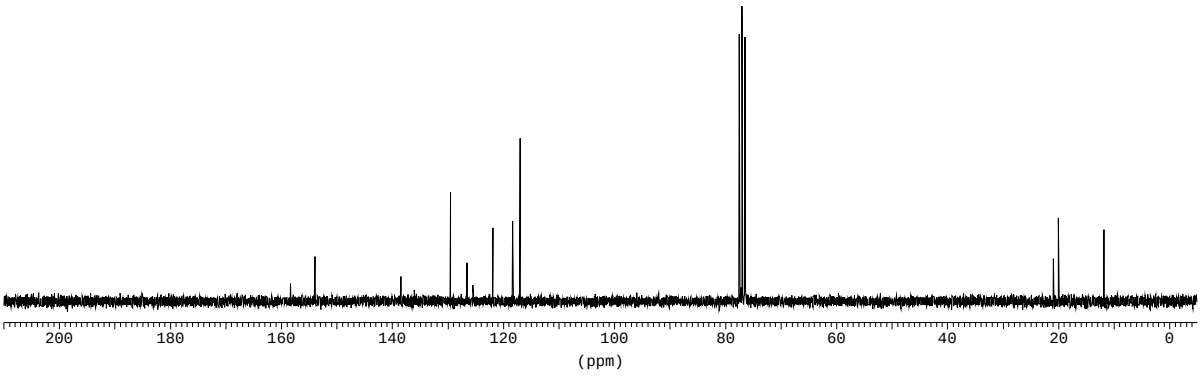
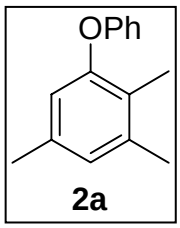
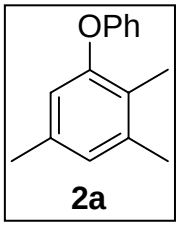


AOA157/CDCl3/250MHz





Peak List

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Peak Results saved in File : C:\WIN1D\TMP\EDIT.ASC

Nucleus : 1H

SF : 250.132853 MHz

OFFSET: 15.7781 ppm, SW_p : 5000.00 Hz, SI : 16384

Peak Picking Parameter

Peak constant PC = 1.00, Noise = 2, Sens. level = 9

Peak Picking region

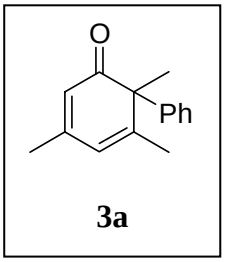
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
7.43/ 1859.2	7.32/ 1830.8	11.78	15.29
7.33/ 1834.2	7.29/ 1824.1	24.92	27.21
7.28/ 1821.4	7.24/ 1812.2	21.25	23.06
7.11/ 1779.3	7.05/ 1763.4	9.33	13.22
7.07/ 1768.6	7.01/ 1754.2	15.08	16.62
7.02/ 1754.8	7.00/ 1750.3	6.73	7.90
6.93/ 1732.9	6.89/ 1722.8	25.24	26.99
6.90/ 1724.9	6.87/ 1717.9	24.60	25.29
3.60/ 901.0	1.46/ 366.3	80.65	113.42

Peak Picking results

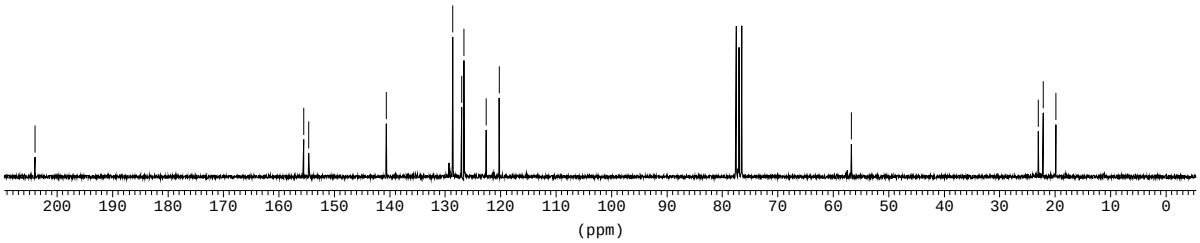
Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	6923	1833.88	7.3316	754	12.4
2	6947	1826.55	7.3023	1530	25.2
3	6981	1816.18	7.2609	1313	21.6
4	7144	1766.43	7.0620	568	9.3
5	7146	1765.82	7.0595	577	9.5
6	7170	1758.50	7.0303	927	15.2
7	7192	1751.79	7.0034	414	6.8
8	7269	1728.29	6.9095	1548	25.5
9	7297	1719.74	6.8753	1503	24.7
10	7336	1707.84	6.8277	1238	20.4
11	7496	1659.01	6.6325	1180	19.4
12	11050	574.42	2.2964	6081	100.0
13	11083	564.35	2.2562	5751	94.6
14	11199	528.95	2.1147	5625	92.5

AOA179.3

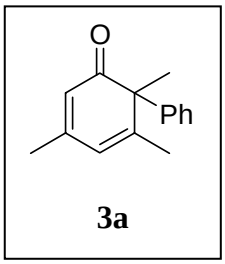
203.9727
155.5278
154.5725
140.6228
128.5836
126.9763
126.5821
122.5488
120.2289
56.7123
22.9752
22.1261
19.8365



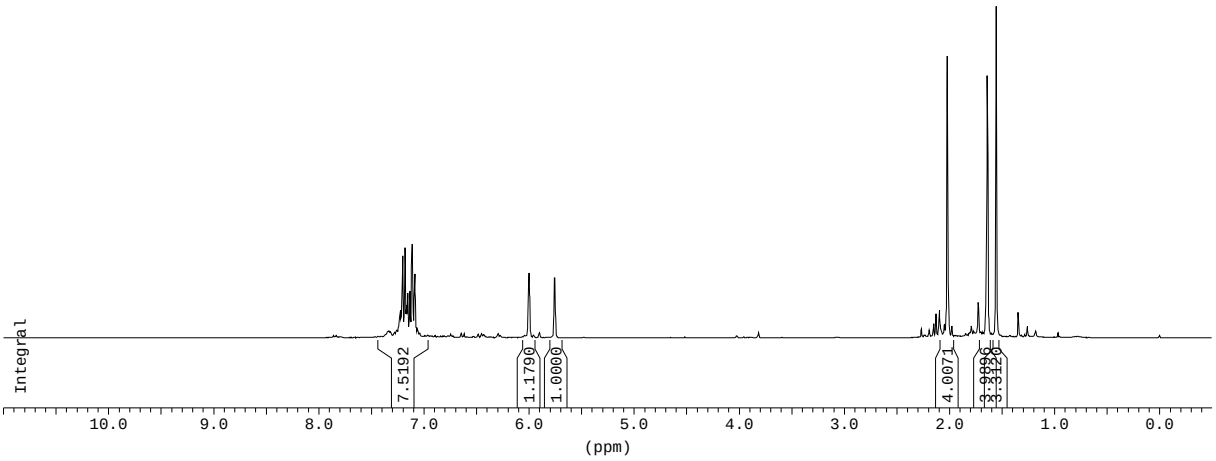
3a



AOA179.3/CDCl3/2409031/300MHz



3a



Peak List

File Name : d:\profes~1\nmr\2003\sept2003\aoa179\2409031\001001.1R

Peak Results saved in File : D:\PROFES~1\NMR\2003\SEPT2003\AOA179\2409031\001001.TXT

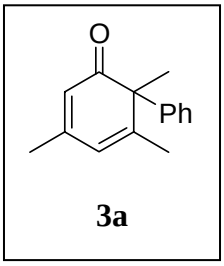
Nucleus : off

SF : 300.130034 MHz

OFFSET : 19.6688 ppm

SW_p : 6172.84 Hz

SI : 16384



3a

Peak Picking Parameter

Peak constant PC = 1.00, Noise = 136, Sens. level = 545

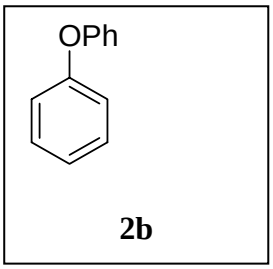
Peak Picking region

Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
5.86/ 1758.1	5.54/ 1662.0	16.63	23.88
6.18/ 1854.5	5.95/ 1785.6	17.32	26.64
8.63/ 2590.0	6.87/ 2060.6	5.23	52.89
2.70/ 809.4	1.16/ 349.0	72.57	124.72

Peak Picking results

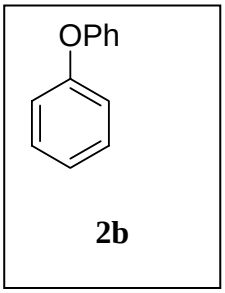
Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	9914	2167.98	7.2235	14689	8.3
2	9919	2166.10	7.2172	11385	6.4
3	9931	2161.58	7.2021	43970	24.7
4	9951	2154.04	7.1770	48331	27.2
5	9962	2149.90	7.1632	17338	9.7
6	9971	2146.51	7.1519	23962	13.5
7	9988	2140.10	7.1306	24958	14.0
8	10003	2134.45	7.1118	50275	28.3
9	10006	2133.32	7.1080	48837	27.5
10	10024	2126.54	7.0854	34173	19.2
11	10888	1801.02	6.0008	33171	18.6
12	10891	1799.89	5.9970	34694	19.5
13	11083	1727.55	5.7560	32075	18.0
14	14059	606.31	2.0202	151256	85.0
15	14363	491.78	1.6385	140738	79.1
16	14430	466.53	1.5544	177869	100.0

aoa190/CDCl3/300MHz

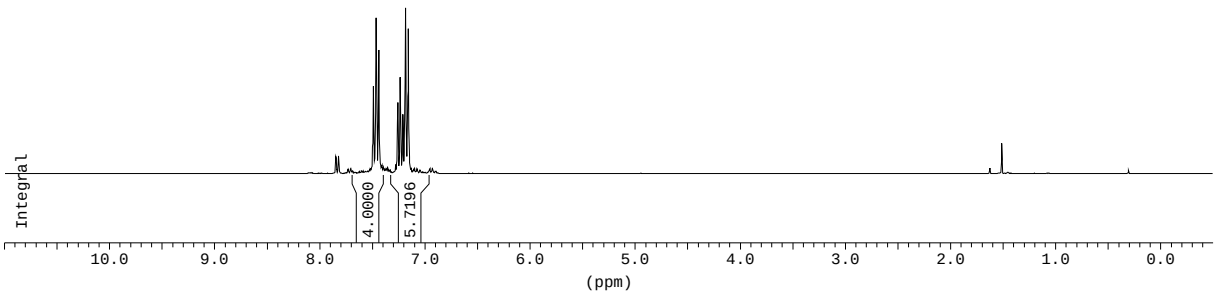


2b

aoa190/CDCl3/300Mhz



2b



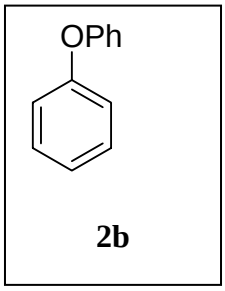
Peak List

File Name : d:\nmr\aoa\aoa190\aoa190\10100326\001001.1R

Peak Results saved in File : D:\NMR\AOA\AOA190\AOA190\10100326\001001.TXT

Nucleus : off, SF : 300.130000 MHz

OFFSET: 19.7835 ppm, SW_p : 6172.84 Hz, SI : 16384



2b

Peak Picking Parameter

Peak constant PC = 1.00, Noise = 58, Sens. level = 231

Peak Picking region

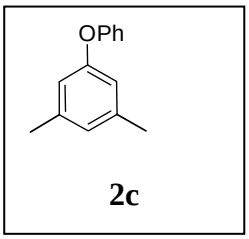
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
7.86/ 2357.6	7.06/ 2119.5	11.63	114.40
9.74/ 2924.7	9.48/ 2844.0	462.00	470.79

Peak Picking results

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	9794	2247.64	7.4889	120211	52.6
2	9800	2245.37	7.4813	50695	22.2
3	9814	2240.10	7.4638	214686	94.0
4	9817	2238.97	7.4600	168996	74.0
5	9823	2236.71	7.4525	38371	16.8
6	9832	2233.32	7.4412	96003	42.0
7	9837	2231.43	7.4349	170183	74.5
8	9843	2229.17	7.4274	34486	15.1
9	9976	2179.06	7.2604	69953	30.6
10	9979	2177.93	7.2566	97731	42.8
11	9982	2176.80	7.2529	55359	24.2
12	9998	2170.78	7.2328	132580	58.1
13	10015	2164.37	7.2114	55148	24.2
14	10018	2163.24	7.2077	81495	35.7
15	10021	2162.11	7.2039	61637	27.0
16	10032	2157.97	7.1901	95207	41.7
17	10036	2156.46	7.1851	225100	98.6
18	10039	2155.33	7.1813	228336	100.0
19	10045	2153.07	7.1738	64763	28.4
20	10056	2148.92	7.1600	142406	62.4
21	10059	2147.79	7.1562	199736	87.5

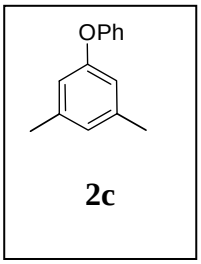
22	10062	2146.66	7.1524	152287	66.7

AOB134/CDCl3/250MHz



2c

AOB134/CDCl3/400MHz

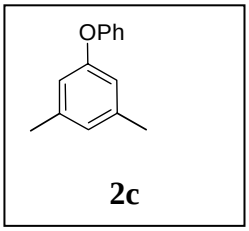


2c

Peak List

File Name : d:\profes~1\nmr\2004\05\aob134\aob134.1\1\FID.1R

Peak Results saved in File : C:\WIN1D\TMP\EDIT.ASC



2c

Nucleus : off

SF : 400.130019 MHz

OFFSET : 15.0116 ppm

SW_p : 8012.82 Hz

SI : 32768

Peak Picking Parameter

Peak constant PC = 1.00, Noise = 30

Sens. level = 122

Peak Picking region

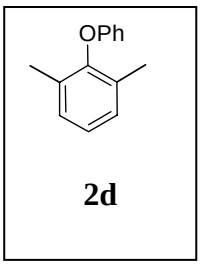
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
7.36/ 2946.3	7.35/ 2940.2	6.84	7.42
7.35/ 2939.9	7.33/ 2932.8	12.58	14.21
7.32/ 2930.1	7.31/ 2923.5	7.33	8.16
7.12/ 2850.7	7.11/ 2844.1	4.05	5.37
7.10/ 2839.9	7.09/ 2835.5	5.86	6.78
7.08/ 2833.3	7.07/ 2827.2	2.51	3.92
7.03/ 2813.7	7.01/ 2803.5	11.32	13.04
7.00/ 2802.0	6.98/ 2793.9	8.96	10.37
6.96/ 2785.4	6.69/ 2678.3	6.22	12.10

Peak Picking results

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	12536	2941.13	7.3504	33902	7.0
2	12566	2933.80	7.3321	61357	12.6
3	12601	2925.24	7.3107	36476	7.5
4	12930	2844.79	7.1097	20328	4.2
5	12960	2837.45	7.0913	29851	6.1
6	12991	2829.87	7.0724	12796	2.6
7	13079	2808.35	7.0186	55910	11.5
8	13115	2799.55	6.9966	45406	9.4
9	13514	2701.98	6.7528	43068	8.9

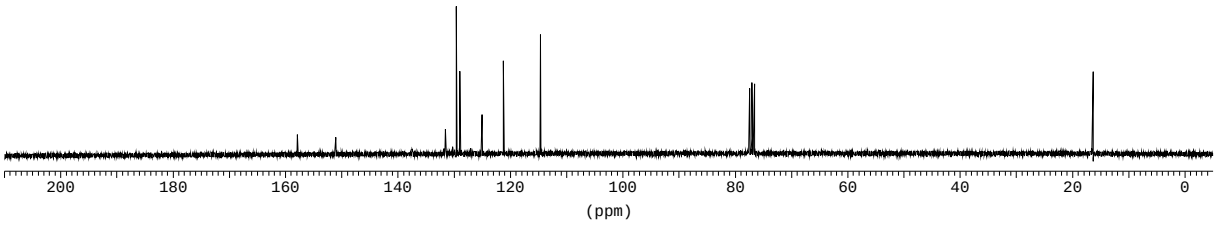
10	13692	2658.46	6.6440	90816	18.7
11	20813	917.14	2.2921	485540	100.0

AOB105.F1/CDCl3/22030420/300MHz

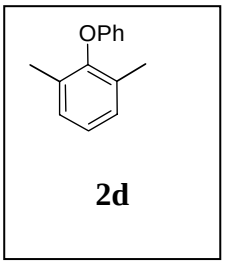


2d

157.8322
151.0537
131.5039
129.5911
128.9438
125.0018
121.2126
114.5869
16.3213



AOB105.F1/CDCl3/22030420/300MHz



2d

Peak List

File Name : d:\profes~1\nmr\2004\03\aob105~2\22030420\001001.1R

Peak Results saved in File : D:\PROFES~1\NMR\2004\03\AOB105~2\22030420\001001.TXT

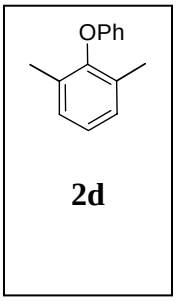
Nucleus : off

SF : 300.130037 MHz

OFFSET : 19.6611 ppm

SW_p : 6172.84 Hz

SI : 16384



2d

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 98

Sens. level = 394

Peak Picking region

Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
7.19/ 2157.0	7.18/ 2155.5	2.96	3.58
7.20/ 2161.6	7.18/ 2155.1	8.22	9.34

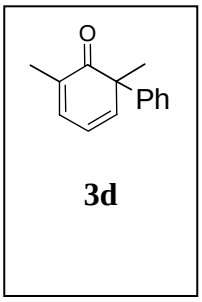
7.17/ 2151.8	7.16/ 2148.4	11.86	12.86
7.15/ 2145.7	7.14/ 2143.8	3.50	4.36
7.15/ 2146.9	7.14/ 2143.8	3.37	4.87
7.22/ 2165.7	7.13/ 2138.9	0.61	14.52
7.09/ 2126.5	6.94/ 2082.4	0.32	20.67
6.93/ 2078.7	6.90/ 2070.8	5.21	6.45
2.94/ 882.8	1.77/ 532.4	85.98	115.95

Peak Picking results

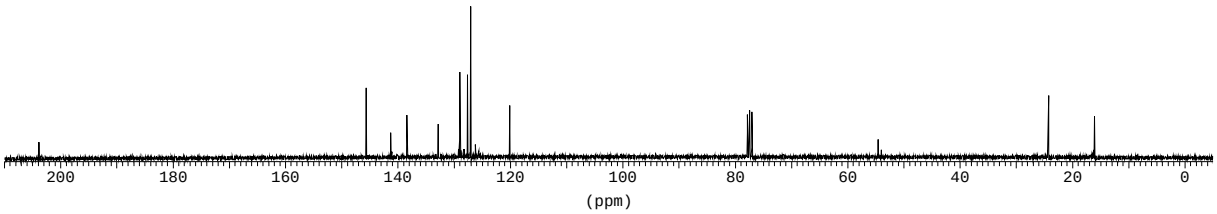
Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	9927	2160.80	7.1995	6836	1.0
2	9934	2158.16	7.1907	56419	8.4
3	9939	2156.28	7.1845	21538	3.2
4	9947	2153.26	7.1744	9119	1.4
5	9953	2151.00	7.1669	83111	12.3
6	9957	2149.49	7.1619	82766	12.3
7	9963	2147.23	7.1543	11969	1.8
8	9971	2144.22	7.1443	26411	3.9
9	9976	2142.34	7.1380	74062	11.0
10	9983	2139.70	7.1292	8850	1.3
11	10050	2114.46	7.0451	3027	0.4
12	10059	2111.06	7.0338	20461	3.0
13	10069	2107.30	7.0213	31288	4.6
14	10083	2102.02	7.0037	135092	20.0
15	10094	2097.88	6.9899	116093	17.2
16	10107	2092.98	6.9736	34932	5.2
17	10119	2088.46	6.9585	21636	3.2
18	10132	2083.56	6.9422	12012	1.8
19	10163	2071.88	6.9033	38098	5.7
20	10182	2064.72	6.8794	54204	8.0
21	10202	2057.19	6.8543	26774	4.0
22	10334	2007.46	6.6886	98763	14.7
23	10357	1998.79	6.6597	74772	11.1
24	14032	614.20	2.0464	673806	100.0

AOB105.F2/300MHz/22030419

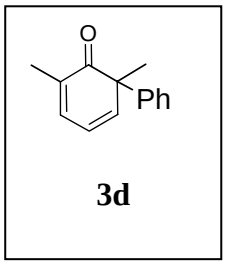
203.8558
145.6281
141.2497
138.3769
132.8058
128.9656
127.5547
127.0092
120.1362
54.5773
24.2052
16.0304



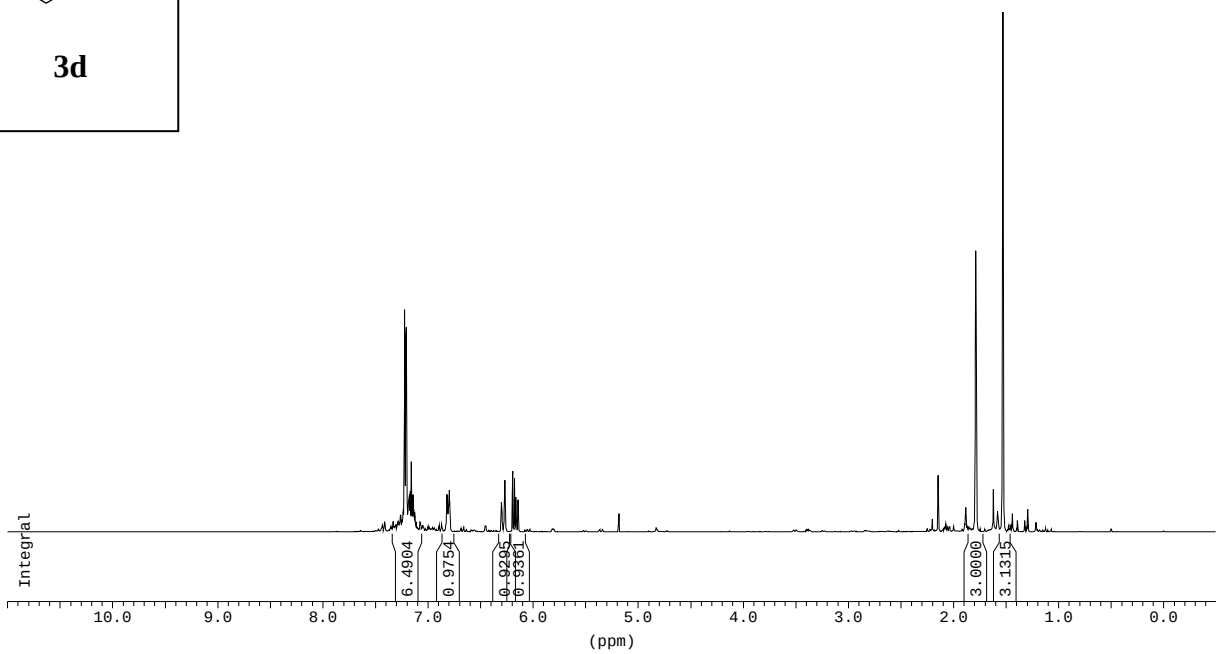
3d

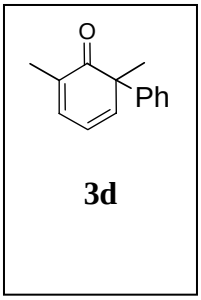


AOB105.F2/CDCl3/400MHz



3d





3d

Peak List

File Name : d:\profes~1\nmr\aob\aob105.2\22030419\001001.1R

Peak Results saved in File : C:\WIN1D\TMP\EDIT.ASC

Nucleus : off

SF : 300.130009 MHz

OFFSET : 19.7519 ppm

SW_p : 6172.84 Hz

SI : 16384

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 113

Sens. level = 453

Peak Picking region

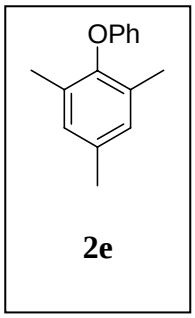
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
2.58/ 772.9	1.47/ 441.0	35.71	142.91
6.24/ 1873.8	6.23/ 1870.1	6.11	6.50
6.26/ 1878.3	6.25/ 1876.1	6.45	7.14
6.27/ 1881.7	6.27/ 1880.6	10.11	10.61
6.27/ 1882.1	6.26/ 1879.8	9.94	10.87
6.29/ 1887.8	6.28/ 1885.5	11.43	12.33
6.37/ 1910.4	6.35/ 1906.6	9.27	10.31
6.40/ 1920.5	6.38/ 1916.0	5.21	6.56
7.41/ 2223.5	7.20/ 2159.8	0.00	46.19

Peak Picking results

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	9844	2219.31	7.3945	4238	1.4
2	9854	2215.54	7.3819	5132	1.7
3	9859	2213.66	7.3757	6176	2.0
4	9864	2211.77	7.3694	4804	1.5
5	9879	2206.12	7.3506	9845	3.2
6	9891	2201.60	7.3355	7189	2.3
7	9897	2199.34	7.3280	11790	3.8
8	9910	2194.44	7.3116	132708	42.8
9	9919	2191.05	7.3003	116354	37.5

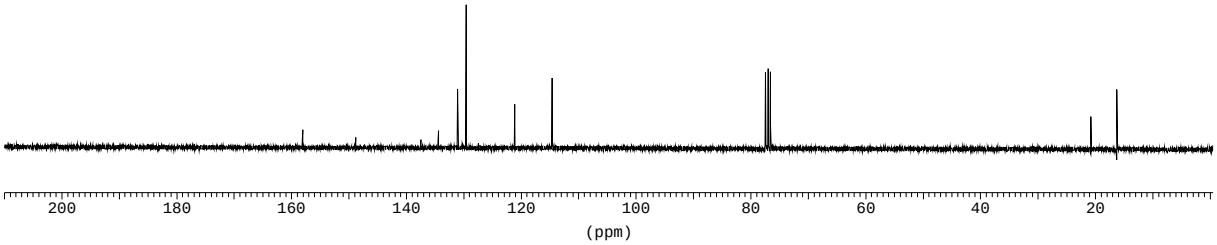
10	9922	2189.92	7.2966	122080	39.3
11	9941	2182.76	7.2727	18573	6.0
12	9946	2180.88	7.2664	22173	7.1
13	9952	2178.62	7.2589	24314	7.8
14	9960	2175.60	7.2489	41910	13.5
15	9969	2172.21	7.2376	17243	5.6
16	9975	2169.95	7.2300	22042	7.1
17	9981	2167.69	7.2225	11646	3.8
18	9986	2165.81	7.2162	9634	3.1
19	9996	2162.04	7.2037	5771	1.9
20	10231	2073.50	6.9087	22361	7.2
21	10247	2067.47	6.8886	24872	8.0
22	10642	1918.65	6.3927	16442	5.3
23	10644	1917.90	6.3902	17556	5.7
24	10646	1917.15	6.3877	17304	5.6
25	10667	1909.23	6.3614	29467	9.5
26	10669	1908.48	6.3588	30627	9.9
27	10671	1907.73	6.3563	29152	9.4
28	10728	1886.25	6.2848	36049	11.6
29	10743	1880.60	6.2660	31706	10.2
30	10753	1876.83	6.2534	20833	6.7
31	10769	1870.80	6.2333	19056	6.1
32	14238	563.82	1.8786	167874	54.1
33	14444	486.21	1.6200	310363	100.0

AOB111A/CDCl3/300MHz/26030425

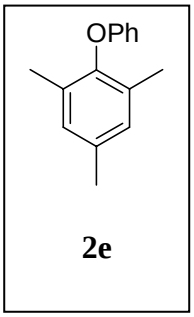


2e

158.0140
148.7773
134.3622
131.0384
129.5475
129.5256
121.0890
114.5723
20.7651
16.2340



AOB111a/CDCl3/300MHz/26030425



2e

Peak List

File Name : d:\profes~1\nmr\2004\03\aob111\26030425\001001.1R

Peak Results saved in File : D:\PROFES~1\NMR\2004\03\AOB111\26030425\001001.TXT

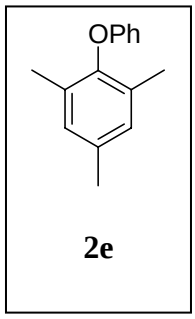
Nucleus : off

SF : 300.130034 MHz

OFFSET : 19.6714 ppm

SW_p : 6172.84 Hz

SI : 16384



2e

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 143

Sens. level = 571

Peak Picking region

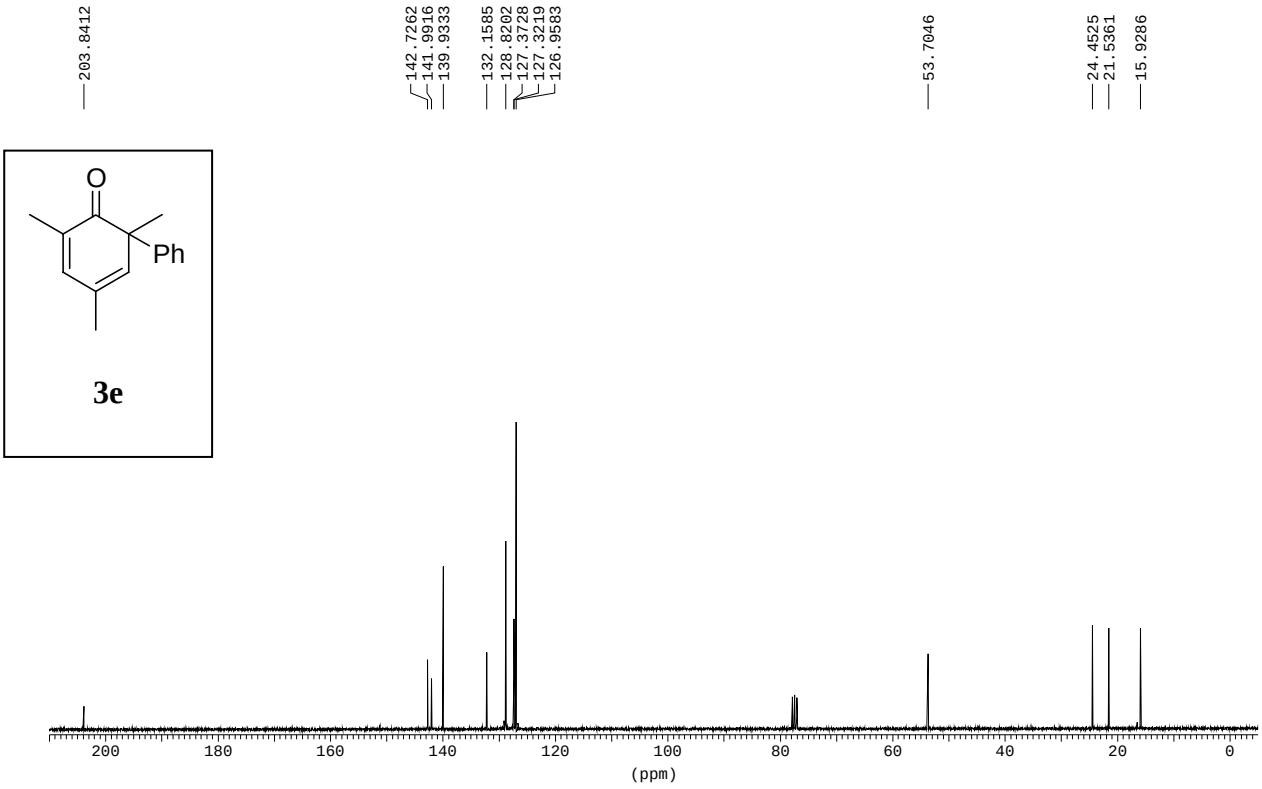
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
6.73/ 2020.0	6.61/ 1984.6	10.81	14.11
6.86/ 2060.3	6.81/ 2043.3	22.33	23.86
6.93/ 2079.5	6.83/ 2049.4	7.47	8.75
6.94/ 2081.8	6.88/ 2066.3	3.87	5.40
7.15/ 2146.2	7.12/ 2136.0	9.39	10.62
7.18/ 2155.2	7.15/ 2145.4	11.45	12.69
7.22/ 2166.5	7.18/ 2156.4	6.63	8.25
7.22/ 2166.5	7.18/ 2156.4	5.74	8.25
2.27/ 679.8	1.49/ 445.9	87.32	108.34

Peak Picking results

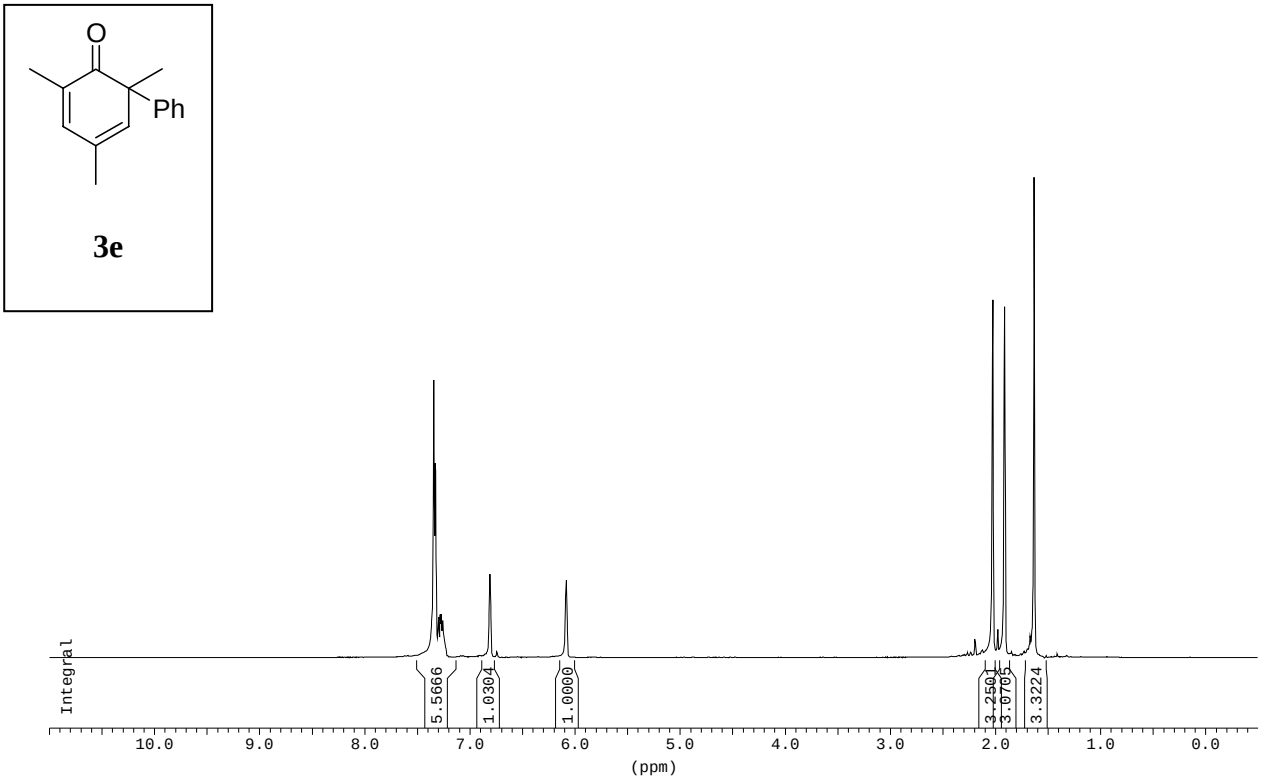
Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	9945	2157.11	7.1872	39209	7.0
2	9965	2149.57	7.1621	64275	11.5
3	9988	2140.91	7.1333	56667	10.1
4	10177	2069.70	6.8960	25650	4.6
5	10197	2062.16	6.8709	43399	7.8
6	10236	2047.47	6.8219	125697	22.5
7	10339	2008.66	6.6926	73723	13.2
8	10360	2000.75	6.6663	62926	11.3
9	13900	667.02	2.2224	271427	48.6

10 14072 602.22 2.0065 558782 100.0

AOB111B/CDCl3/300MHz



AOB111b/CDCl3/300MHz



Peak List

File Name : d:\profes~1\nmr\2004\03\aob111\26030426\001001.1R

Peak Results saved in File : D:\PROFES~1\NMR\2004\03\AOB111\26030426\001001.TXT

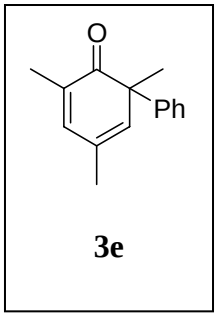
Nucleus : off

SF : 300.130000 MHz

OFFSET : 19.7835 ppm

SW_p : 6172.84 Hz

SI : 16384



3e

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 124

Sens. level = 494

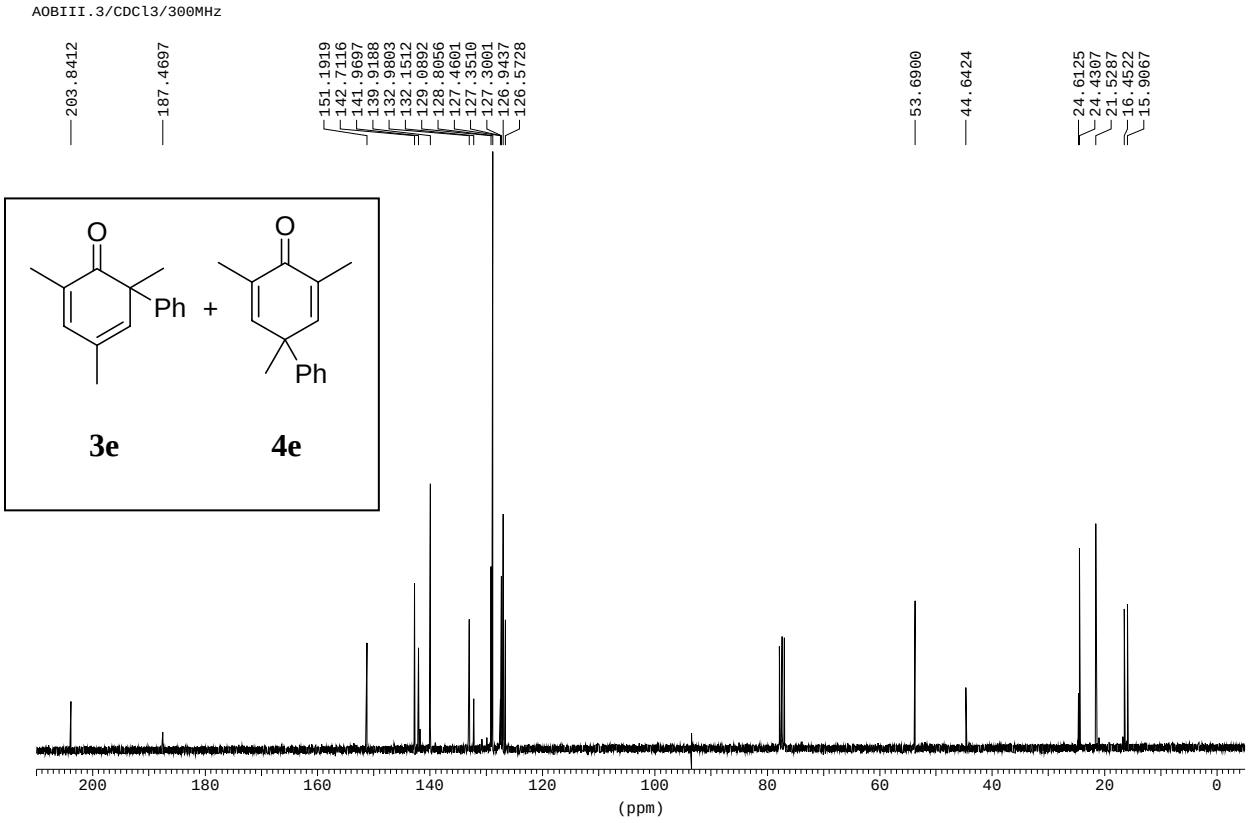
Peak Picking region

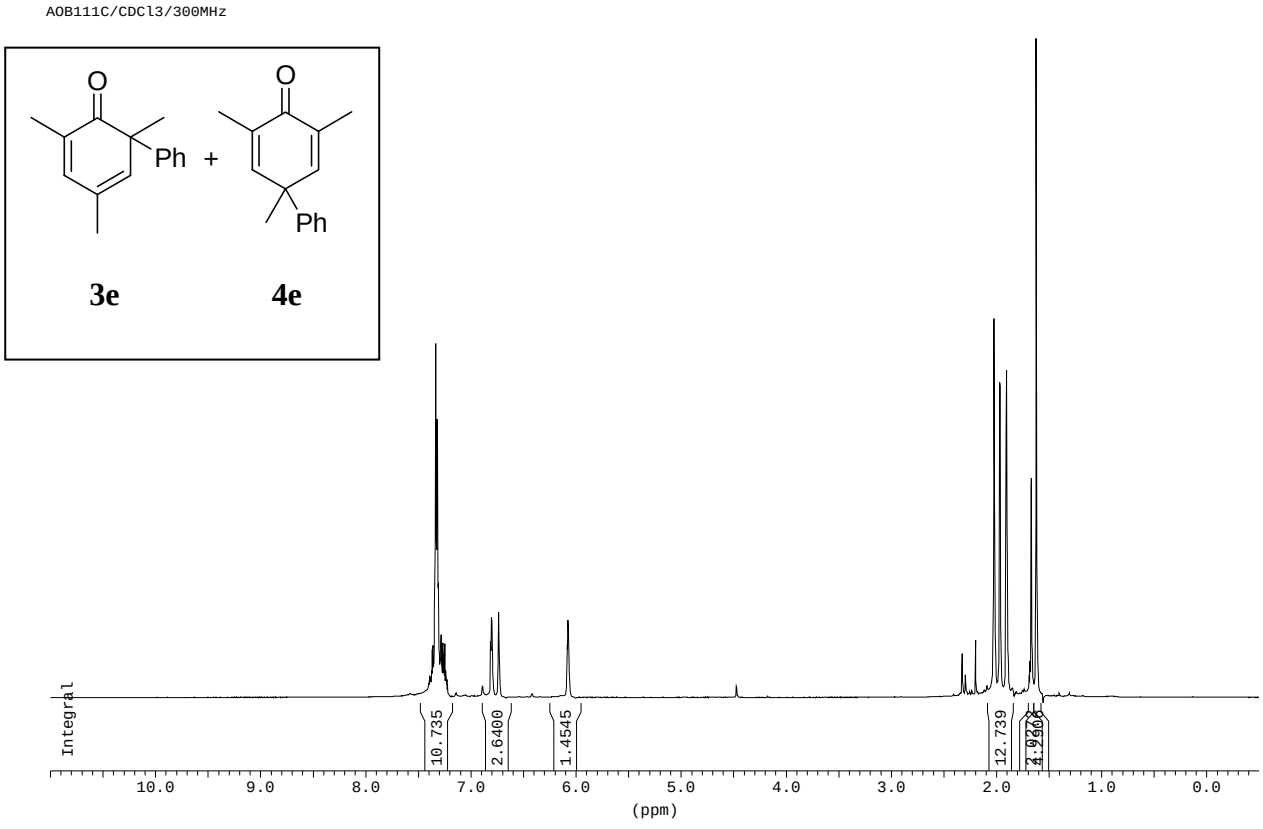
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
7.65/ 2294.7	7.16/ 2148.2	4.00	61.78
6.86/ 2057.7	6.67/ 2001.6	15.20	20.32
6.23/ 1869.0	5.98/ 1795.9	14.60	20.56
2.31/ 694.3	1.31/ 392.8	90.92	108.55
2.17/ 652.1	1.84/ 553.3	70.66	78.05

Peak Picking results

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	9912	2203.18	7.3407	108683	57.7
2	9920	2200.16	7.3307	76009	40.4
3	9925	2198.28	7.3244	72996	38.8
4	9948	2189.61	7.2956	15637	8.3
5	9959	2185.47	7.2817	16790	8.9
6	9967	2182.46	7.2717	16975	9.0
7	9975	2179.44	7.2617	14290	7.6
8	9981	2177.18	7.2541	14285	7.6
9	9985	2175.67	7.2491	10638	5.6
10	10335	2043.81	6.8097	32648	17.3
11	10915	1825.29	6.0817	30251	16.1
12	14146	607.97	2.0257	140235	74.5

13	14237	573.69	1.9115	137480	73.0
14	14460	489.67	1.6315	188350	100.0





Peak List

File Name : d:\profes~1\nmr\2004\03\aob111\26030427\001001.1R

Peak Results saved in File : D:\PROFES~1\NMR\2004\03\AOB111\26030427\001001.TXT

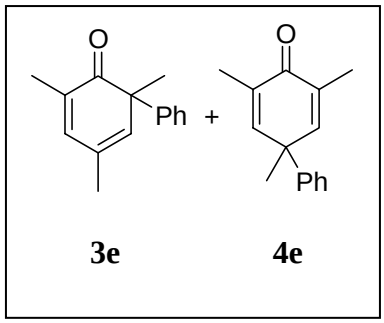
Nucleus : off

SF : 300.130000 MHz

OFFSET : 19.7835 ppm

SW_p : 6172.84 Hz

SI : 16384



Peak Picking Parameter

Peak constant PC = 1.00

Noise = 117

Sens. level = 466

Peak Picking region

Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
6.87/ 2061.9	6.79/ 2037.4	11.98	13.86
6.77/ 2031.4	6.71/ 2014.8	12.66	13.90
6.13/ 1839.6	6.06/ 1819.3	11.59	13.18
7.90/ 2370.1	7.16/ 2150.1	1.77	60.95
2.05/ 614.4	2.00/ 599.3	55.44	61.44
1.98/ 595.5	1.97/ 590.3	46.89	51.44
1.98/ 594.4	1.94/ 581.6	47.62	51.44
1.92/ 575.6	1.90/ 569.2	48.71	56.17
1.63/ 490.4	1.61/ 483.6	96.55	104.01

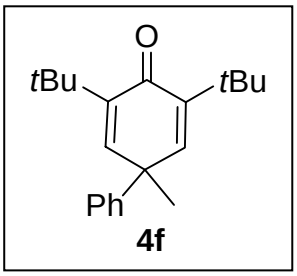
Peak Picking results

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	9869	2219.38	7.3947	4836	2.7
2	9872	2218.25	7.3910	5717	3.2
3	9877	2216.36	7.3847	5486	3.1
4	9888	2212.22	7.3709	7471	4.2
5	9892	2210.71	7.3659	12531	7.0
6	9896	2209.21	7.3608	13985	7.8
7	9904	2206.19	7.3508	11702	6.6

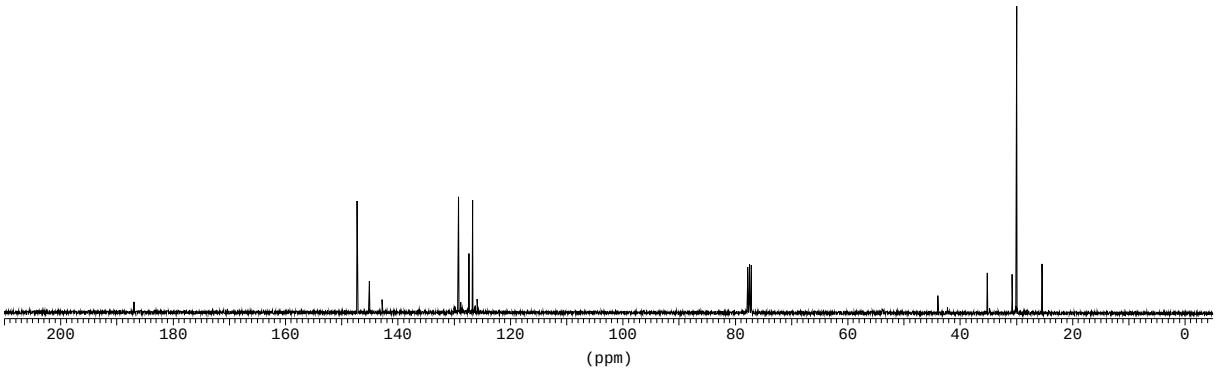
8	9913	2202.80	7.3395	34297	19.2	
9	9919	2200.54	7.3320	95783	53.6	
10	9927	2197.53	7.3219	75323	42.2	
11	9930	2196.40	7.3181	72381	40.5	
12	9932	2195.64	7.3156	70816	39.7	
13	9945	2190.74	7.2993	12209	6.8	
14	9951	2188.48	7.2918	13239	7.4	
15	9953	2187.73	7.2893	12897	7.2	
16	9956	2186.60	7.2855	13946	7.8	
17	9959	2185.47	7.2817	17009	9.5	
18	9963	2183.96	7.2767	15436	8.6	
19	9971	2180.95	7.2667	13344	7.5	
20	9973	2180.20	7.2642	14790	8.3	
21	9975	2179.44	7.2617	12854	7.2	
22	9981	2177.18	7.2541	11601	6.5	
23	9986	2175.30	7.2479	14475	8.1	
24	9993	2172.66	7.2391	7233	4.1	
25	9997	2171.15	7.2340	6318	3.5	
26	10002	2169.27	7.2278	4794	2.7	
27	10340	2041.92	6.8035	21608	12.1	
28	**10395**	**2021.20**	**6.7344**	**23051**	**12.9**	**4e**
29	10920	1823.40	6.0754	20925	11.7	
30	14149	606.84	2.0219	102573	57.4	
31	**14192**	**590.64**	**1.9680**	**85308**	**47.8**	**4e**
32	14245	570.68	1.9014	88652	49.6	
33	**14431**	**500.60**	**1.6679**	**59436**	**33.3**	**4e**
34	14467	487.03	1.6227	178570	100.0	

AOB169.2/CDCl3/400MHz

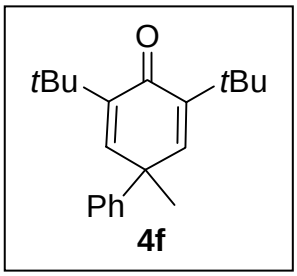
186.8981
147.2207
145.0689
142.7821
129.2122
127.3621
126.6793
43.9181
35.1283
30.7532
29.9274



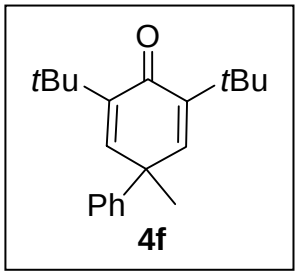
4f



AOB169.2/CDCl3/400MHz



4f



4f

Peak List

File Name : d:\profes~1\nmr\2004\07\aob169.2\1\FID.1R

Peak Results saved in File : C:\WIN1D\TMP\EDIT.ASC

Nucleus : off

SF : 400.130000 MHz

OFFSET : 16.5197 ppm

SW_p : 8278.15 Hz

SI : 32768

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 34

Sens. level = 137

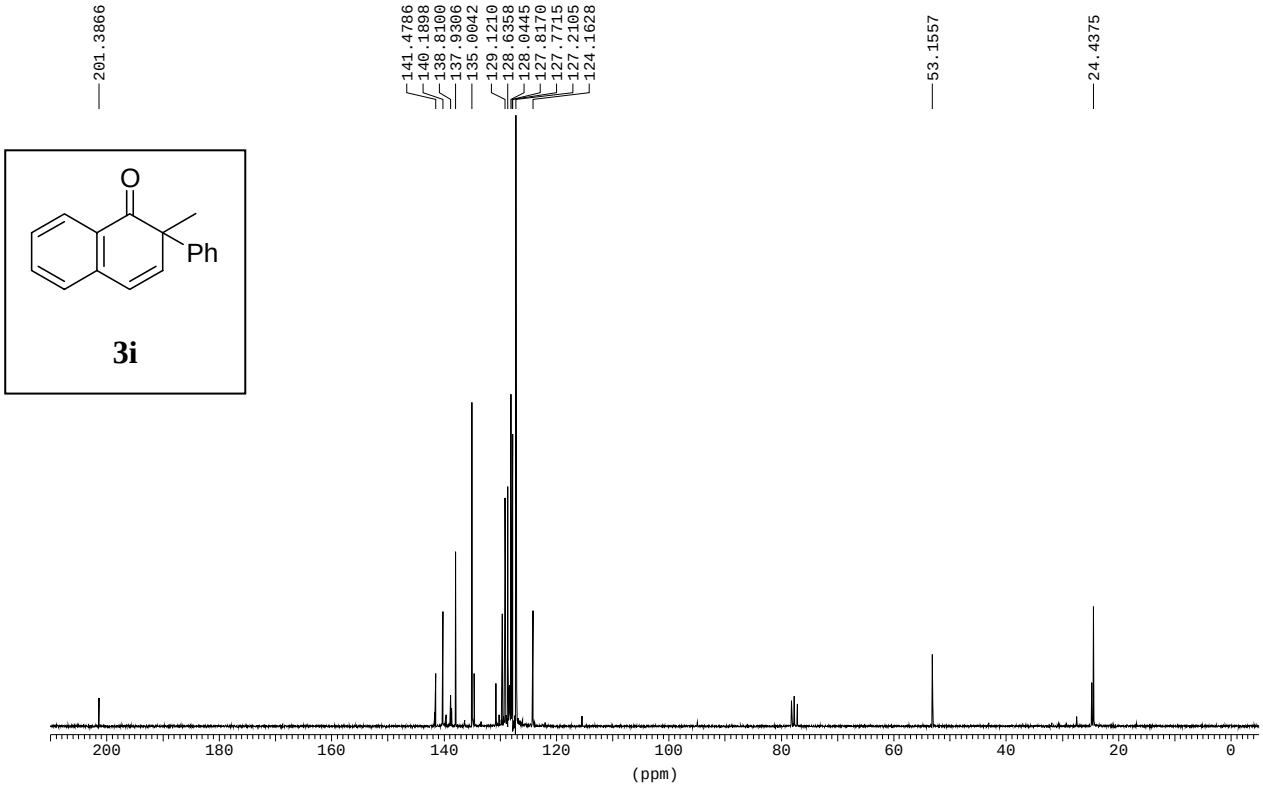
Peak Picking region

Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
6.73/ 2691.0	6.29/ 2517.5	9.05	11.90
7.52/ 3008.8	6.96/ 2786.5	2.66	6.94
2.33/ 931.4	0.76/ 304.7	97.36	116.99
2.26/ 903.9	1.59/ 636.4	14.36	29.17

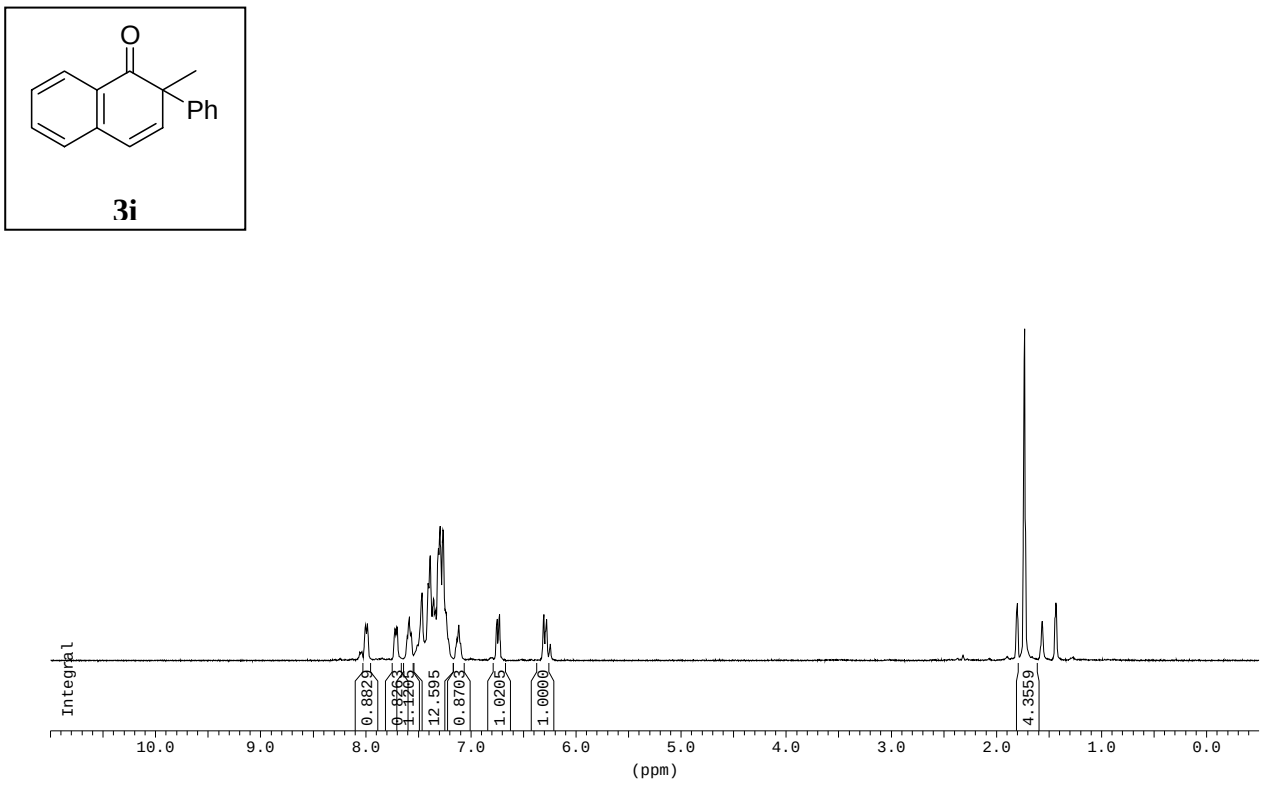
Peak Picking results

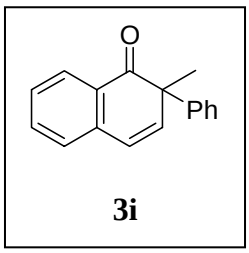
Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	14480	2951.97	7.3775	9157	2.8
2	14506	2945.40	7.3611	9778	3.0
3	14574	2928.22	7.3182	20981	6.5
4	14603	2920.90	7.2999	15131	4.7
5	15645	2657.66	6.6420	36214	11.2
6	23512	670.23	1.6750	52225	16.1
7	24111	518.90	1.2968	324329	100.0

AOC106/CDCl3/250MHz



AOC106/CDCl3/400MHz





3i

Peak List

File Name : d:\profes~1\nmr\aob\aob106\aob106f1\1\FID.1R

Peak Results saved in File : C:\WIN1D\TMP\EDIT.ASC

Nucleus : off

SF : 400.130018 MHz

OFFSET : 15.0128 ppm

SW_p : 8012.82 Hz

SI : 32768

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 29

Sens. level = 118

Peak Picking region

Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
6.37/ 2548.7	6.18/ 2473.3	11.79	18.43
6.90/ 2762.4	6.60/ 2641.3	12.04	18.35
7.13/ 2851.9	7.09/ 2836.0	9.55	13.62
7.56/ 3023.1	7.13/ 2851.9	15.53	47.09
7.66/ 3063.9	7.54/ 3016.7	12.04	15.19
7.84/ 3137.5	7.66/ 3063.9	9.13	13.20
8.08/ 3234.8	7.94/ 3175.2	9.55	13.28
2.68/ 1072.7	0.23/ 91.1	80.29	115.24

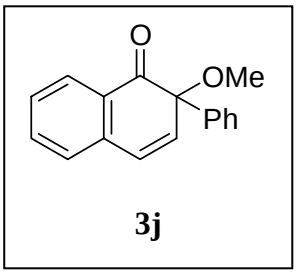
Peak Picking results

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	11476	3200.83	7.9995	7202	10.4
2	11505	3193.74	7.9817	7544	10.9
3	11935	3088.59	7.7190	6432	9.3
4	11964	3081.50	7.7012	6832	9.9
5	12155	3034.79	7.5845	8931	12.9
6	12356	2985.64	7.4617	13963	20.1
7	12450	2962.65	7.4042	16002	23.1
8	12455	2961.43	7.4012	15823	22.8
9	12480	2955.32	7.3859	21756	31.4
10	12534	2942.11	7.3529	12689	18.3

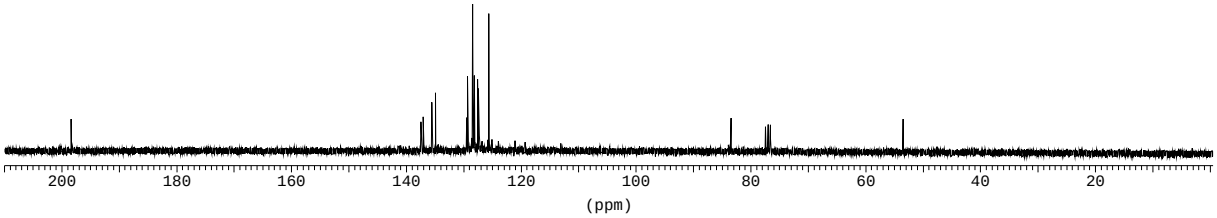
11	12607	2924.26	7.3083	23263	33.6
12	12634	2917.66	7.2918	27948	40.3
13	12669	2909.10	7.2704	24924	36.0
14	12682	2905.92	7.2624	27129	39.1
15	12686	2904.94	7.2600	26753	38.6
16	12926	2846.26	7.1133	7235	10.4
17	13522	2700.52	6.7491	8500	12.3
18	13561	2690.98	6.7253	9445	13.6
19	14251	2522.25	6.3036	9435	13.6
20	14291	2512.47	6.2791	8417	12.1
21	21735	692.18	1.7299	69328	100.0

AOB 114/CDCl3/300MHz/05040413

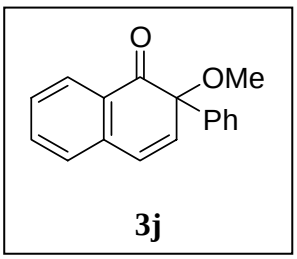
198.3501
137.4605
137.0168
135.5550
134.8786
129.4893
129.2856
128.4347
128.3692
128.1583
127.5692
127.3874
125.5764
83.4657
53.4718



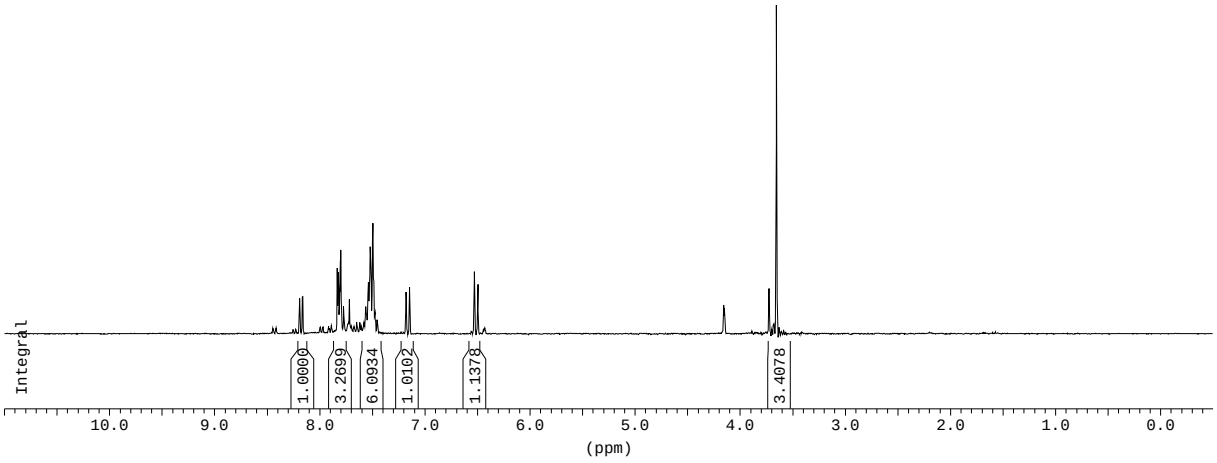
3j



AOB 114/CDCl3/300MHz



3j



Peak List

File Name : d:\profes~1\nmr\aob\aob114~1\05040413\001001.1R

Peak Results saved in File : D:\PROFES~1\NMR\AOB\AOB114~1\05040413\001001.TXT

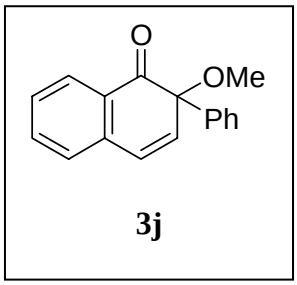
Nucleus : off

SF : 300.129938 MHz

OFFSET : 19.9910 ppm

SW_p : 6172.84 Hz

SI : 16384



3j

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 38

Sens. level = 151

Peak Picking region

Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
6.69/ 2007.7	6.42/ 1927.9	14.65	23.11
7.34/ 2203.7	7.09/ 2129.1	12.05	17.38
8.25/ 2476.8	8.14/ 2442.9	10.11	14.45
8.05/ 2414.6	7.43/ 2230.8	5.72	34.84
4.97/ 1490.5	3.55/ 1064.3	93.88	131.11

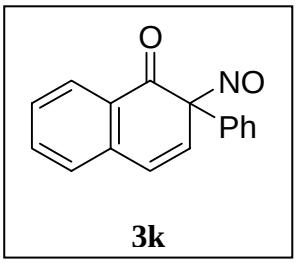
Peak Picking results

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	9400	2458.35	8.1910	12268	10.2
2	9402	2457.60	8.1884	12853	10.7
3	9421	2450.44	8.1646	13283	11.1
4	9423	2449.69	8.1621	13466	11.2
5	9687	2350.22	7.8307	23938	20.0
6	9692	2348.34	7.8244	22496	18.8
7	9694	2347.58	7.8219	19009	15.9
8	9698	2346.08	7.8169	12298	10.3
9	9702	2344.57	7.8118	10948	9.1
10	9704	2343.82	7.8093	13011	10.9
11	9708	2342.31	7.8043	26759	22.3
12	9713	2340.43	7.7980	30509	25.5
13	9735	2332.14	7.7704	10002	8.4

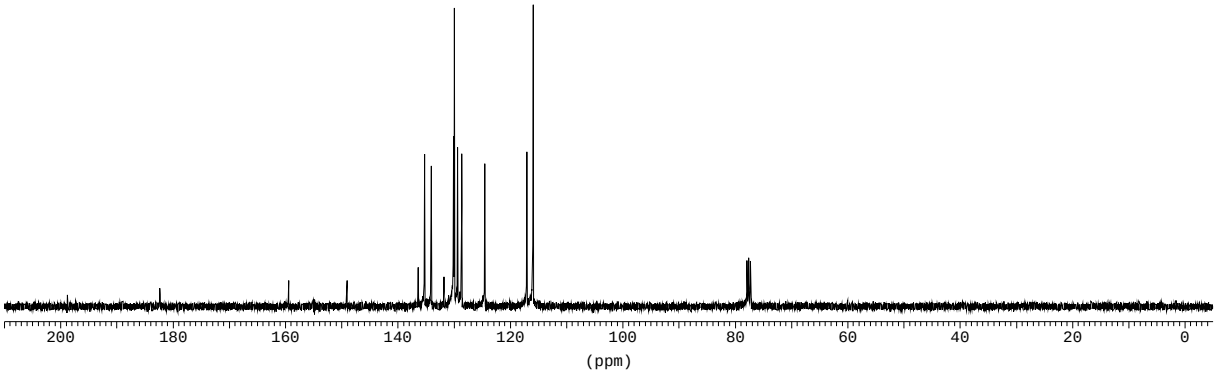
15	9900	2269.97	7.5633	9859	8.2
16	9908	2266.96	7.5533	6992	5.8
17	9913	2265.07	7.5470	7347	6.1
18	9917	2263.57	7.5420	11199	9.4
19	9920	2262.44	7.5382	18360	15.3
20	9922	2261.68	7.5357	18843	15.7
21	9932	2257.91	7.5231	21563	18.0
22	9937	2256.03	7.5168	31579	26.4
23	9954	2249.63	7.4955	33371	27.9
24	9957	2248.50	7.4917	40244	33.6
25	9969	2243.97	7.4767	7614	6.4
26	9972	2242.84	7.4729	7805	6.5
27	10208	2153.93	7.1767	15194	12.7
28	10234	2144.13	7.1440	16996	14.2
29	10725	1959.14	6.5277	22529	18.8
30	10751	1949.35	6.4950	17990	15.0
31	13014	1096.74	3.6542	119760	100.0

AOC45/CDCl3/400MHz

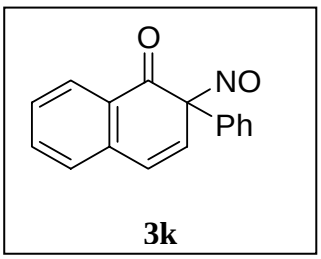
182.3245
159.4169
149.0231
136.4061
135.2468
134.0319
131.7928
130.0856
129.9030
129.3313
128.6326
124.5354
117.0636
115.9282



3k



AOC45/CDCl3/400MHz



3k

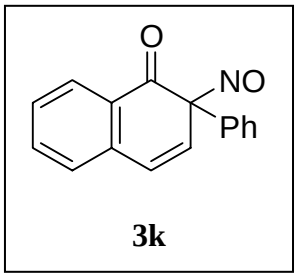
Peak List

File Name : d:\profes~1\nmr\2004\10\aoc45bis\1\FID.1R

Peak Results saved in File : C:\WIN1D\TMP\EDIT.ASC

Nucleus : off, SF : 400.130071 MHz; OFFSET : 14.8808 ppm

SW_p : 8012.82 Hz; SI : 32768



3k

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 27

Sens. level = 108

Peak Picking region

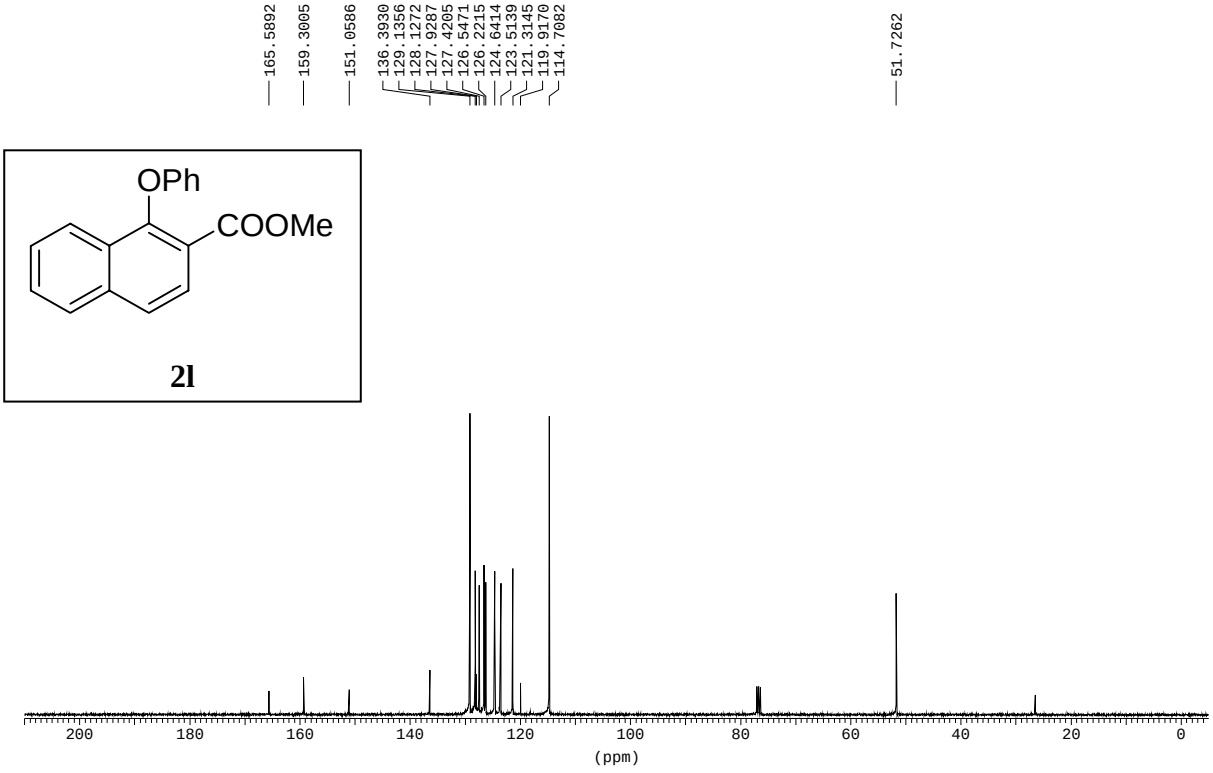
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
8.16/ 3265.6	8.03/ 3213.5	13.38	24.08
7.62/ 3047.8	7.45/ 2981.0	6.88	25.22
7.42/ 2969.7	7.31/ 2923.5	6.69	23.12
6.89/ 2755.3	6.73/ 2691.0	16.82	31.91
7.08/ 2832.1	6.95/ 2782.4	0.96	14.14
7.29/ 2918.9	7.11/ 2846.7	5.54	45.48

Peak Picking results

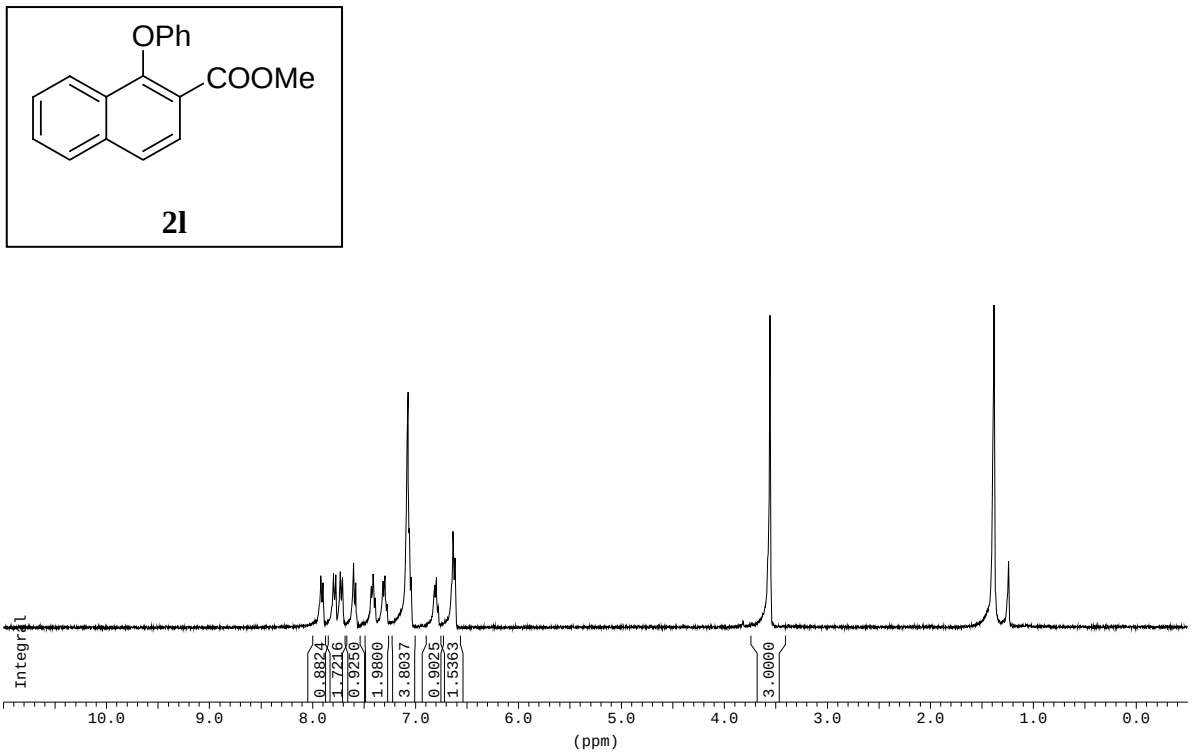
Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	11101	3239.71	8.0966	26050	32.1
2	11103	3239.22	8.0954	26493	32.6
3	11133	3231.88	8.0771	25459	31.4
4	11135	3231.39	8.0759	25668	31.6
5	12068	3003.25	7.5057	14708	18.1
6	12073	3002.02	7.5026	14660	18.1
7	12098	2995.91	7.4873	31579	38.9
8	12104	2994.44	7.4837	29795	36.7
9	12129	2988.33	7.4684	20250	25.0
10	12135	2986.86	7.4647	17617	21.7
11	12310	2944.07	7.3578	20380	25.1
12	12314	2943.09	7.3553	20350	25.1
13	12341	2936.49	7.3388	31948	39.4
14	12345	2935.51	7.3364	30623	37.7

15	12372	2928.91	7.3199	14613	18.0
16	12376	2927.93	7.3174	13479	16.6
17	12443	2911.55	7.2765	23462	28.9
18	12454	2908.86	7.2698	23950	29.5
19	12479	2902.74	7.2545	81159	100.0
20	12495	2898.83	7.2447	68009	83.8
21	12507	2895.90	7.2374	21744	26.8
22	12520	2892.72	7.2294	41802	51.5
23	12532	2889.78	7.2221	19536	24.1
24	12550	2885.38	7.2111	32489	40.0
25	12575	2879.27	7.1958	44941	55.4
26	12616	2869.24	7.1708	50620	62.4
27	12684	2852.61	7.1292	40406	49.8
28	12815	2820.58	7.0492	2211	2.7
29	12825	2818.14	7.0430	2912	3.6
30	12843	2813.73	7.0320	11071	13.6
31	12852	2811.53	7.0265	16650	20.5
32	12864	2808.60	7.0192	13946	17.2
33	12868	2807.62	7.0168	17354	21.4
34	12874	2806.15	7.0131	14293	17.6
35	12878	2805.18	7.0107	18946	23.3
36	12888	2802.73	7.0045	14103	17.4
37	12902	2799.31	6.9960	11202	13.8
38	12912	2796.86	6.9899	6786	8.4
39	13136	2742.09	6.8530	45373	55.9
40	13177	2732.06	6.8279	39806	49.0

AOC46.2/CDCl3/400MHz



AOC46.2/CDCl3/400MHz



Peak List

File Name : d:\profes~1\nmr\2004\10\aoc46.2\1\FID.1R

Peak Results saved in File : C:\WIN1D\TMP\EDIT.ASC

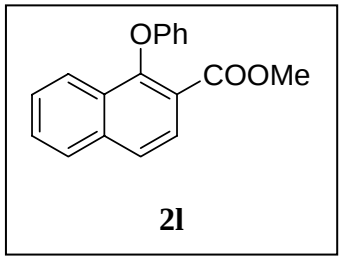
Nucleus : off

SF : 400.130015 MHz

OFFSET : 15.0216 ppm

SW_p : 8012.82 Hz

SI : 32768



2l

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 74

Sens. level = 294

Peak Picking region

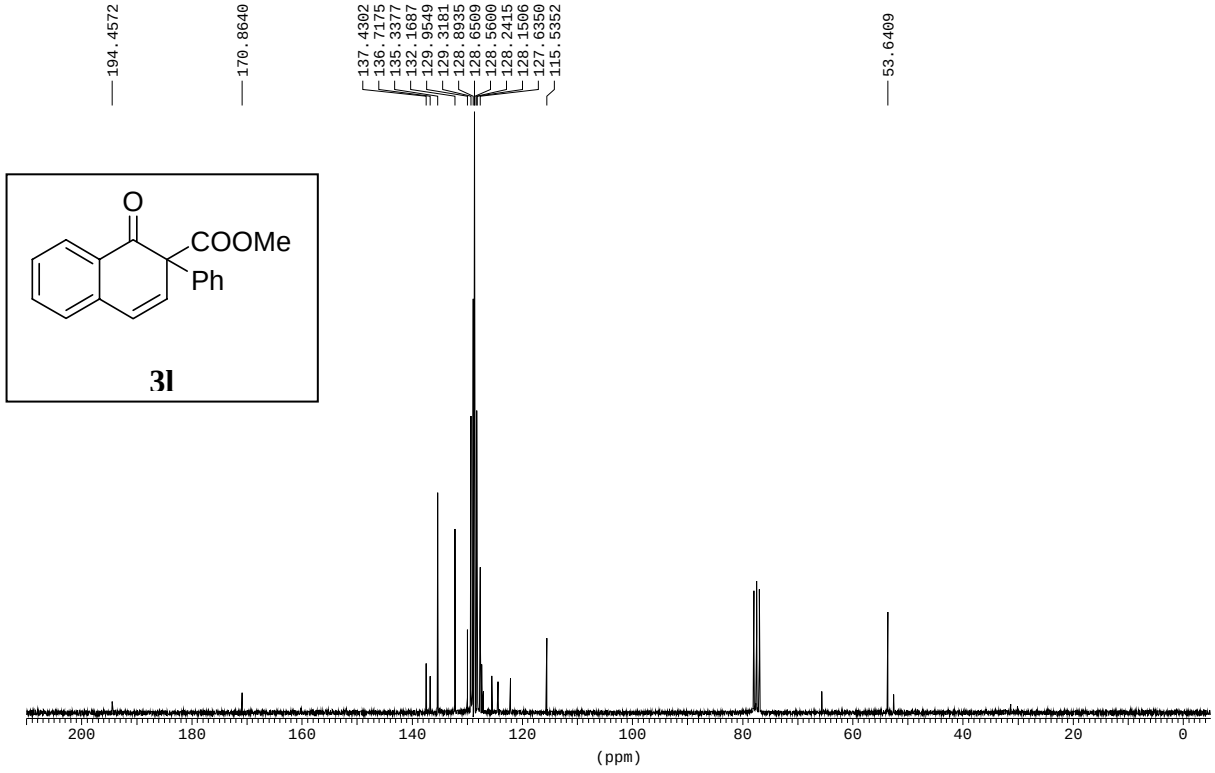
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
4.21/ 1682.9	3.60/ 1442.0	91.24	112.20
6.92/ 2770.1	6.74/ 2695.5	20.17	36.62
7.09/ 2837.1	6.93/ 2774.7	4.15	17.86
7.33/ 2932.4	7.18/ 2874.0	10.07	43.11
7.53/ 3013.6	7.47/ 2987.2	5.45	18.44
7.67/ 3069.4	7.57/ 3027.8	6.32	19.74
7.82/ 3129.8	7.75/ 3100.4	12.09	24.06
8.21/ 3286.5	7.87/ 3149.6	11.80	23.63

Peak Picking results

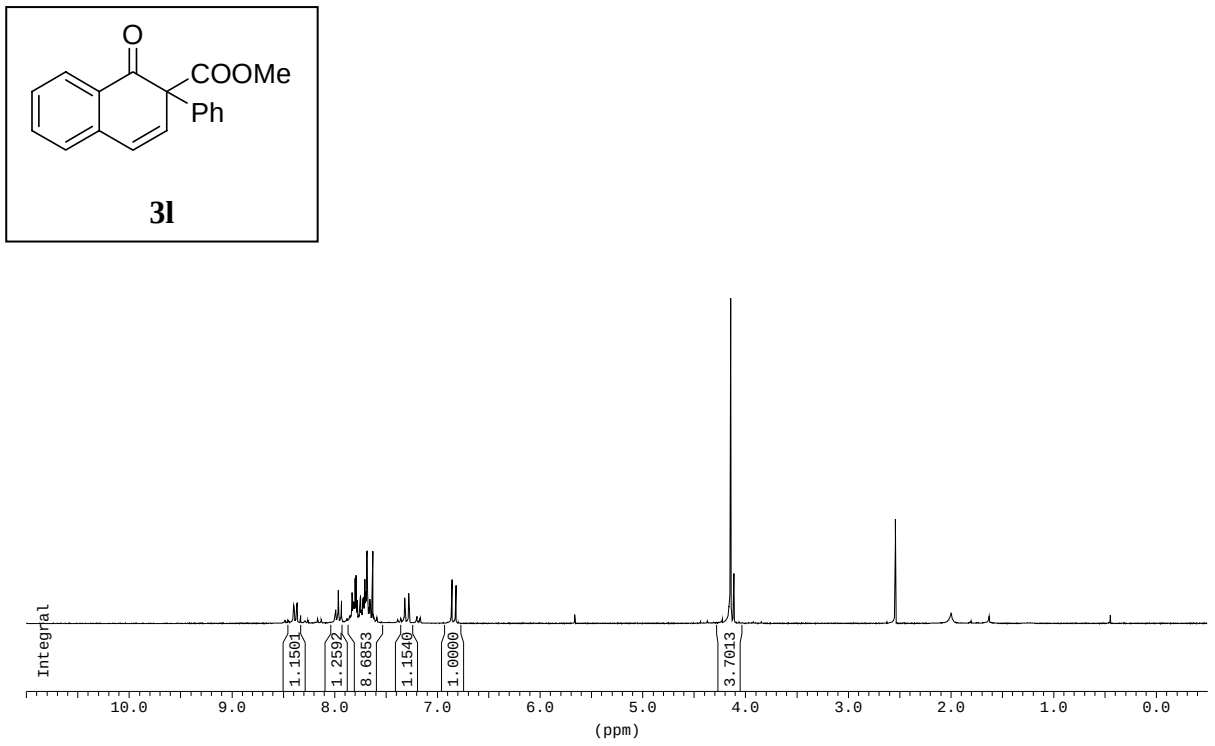
Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	11299	3247.62	8.1164	7373	16.3
2	11333	3239.31	8.0956	6347	14.1
3	11502	3197.98	7.9924	7683	17.0
4	11537	3189.42	7.9710	7501	16.6
5	11610	3171.57	7.9264	7949	17.6
6	11643	3163.50	7.9062	7155	15.9
7	11820	3120.22	7.7980	9271	20.5
8	11853	3112.15	7.7779	6404	14.2
9	12102	3051.26	7.6257	5802	12.9
10	12129	3044.66	7.6092	7668	17.0

11	12161	3036.84	7.5896	4146	9.2
12	12289	3005.54	7.5114	6590	14.6
13	12319	2998.20	7.4931	7434	16.5
14	12351	2990.37	7.4735	3284	7.3
15	12704	2904.05	7.2578	14667	32.5
16	12733	2896.96	7.2401	7314	16.2
17	13105	2806.00	7.0127	6057	13.4
18	13134	2798.91	6.9950	7132	15.8
19	13163	2791.81	6.9773	2868	6.4
20	13400	2733.86	6.8324	13898	30.8
21	13433	2725.79	6.8123	9995	22.1
22	18439	1501.66	3.7529	45134	100.0

AOC46.3/CDCl3/400



AOC46.3/CDCl3/250MHz



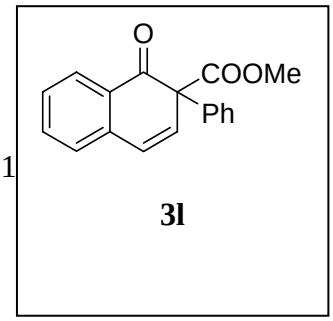
Peak List

File Name : d:\profes~1\nmr\2004\10\aoc46~1.3ca\ot200f\101001.1R

Peak Results saved in File : C:\WIN1D\TMP\EDIT.ASC, Nucleus : 1H

SF : 250.132754 MHz, OFFSET : 16.1734 ppm, SW_p : 5000.00 Hz

SI : 16384



3l

Peak Picking Parameter

Peak constant PC = 1.00, Noise = 3, Sens. level = 11

Peak Picking region

Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
4.48/ 1120.7	3.84/ 961.1	95.19	110.96
7.03/ 1758.8	6.64/ 1661.5	9.44	21.52
7.45/ 1863.5	7.22/ 1806.1	5.99	25.46
7.89/ 1973.7	7.58/ 1897.1	5.94	26.46
7.97/ 1992.6	7.95/ 1987.7	4.43	8.00
8.01/ 2004.2	7.97/ 1994.4	8.02	11.15
8.07/ 2017.6	8.01/ 2003.3	3.87	5.54
8.45/ 2112.8	8.37/ 2094.8	4.21	7.45

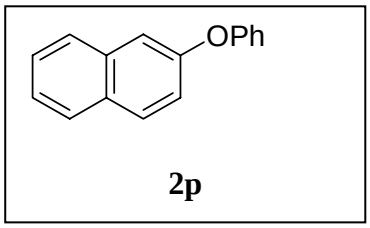
Peak Picking results

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	6350	2107.63	8.4261	545	5.3
2	6352	2107.02	8.4236	574	5.6
3	6354	2106.41	8.4212	503	4.9
4	6375	2100.00	8.3956	616	6.0
5	6378	2099.09	8.3919	640	6.3
6	6682	2006.31	8.0210	424	4.2
7	6686	2005.09	8.0161	430	4.2
8	6706	1998.99	7.9917	1043	10.2
9	6711	1997.46	7.9856	901	8.8
10	6731	1991.36	7.9612	699	6.8
11	6735	1990.14	7.9563	500	4.9
12	6817	1965.11	7.8563	965	9.5
13	6824	1962.98	7.8477	719	7.0
14	6828	1961.76	7.8429	649	6.4

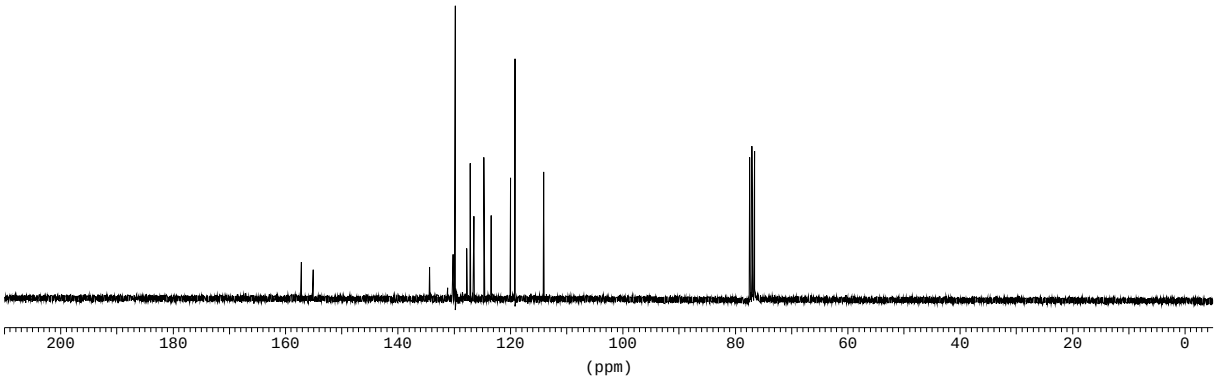
15	6834	1959.93	7.8355	609	6.0
16	6836	1959.32	7.8331	659	6.5
17	6843	1957.18	7.8246	1413	13.8
18	6849	1955.35	7.8172	1515	14.9
19	6856	1953.21	7.8087	613	6.0
20	6860	1951.99	7.8038	731	7.2
21	6881	1945.58	7.7782	839	8.2
22	6885	1944.36	7.7733	874	8.6
23	6903	1938.87	7.7514	768	7.5
24	6906	1937.95	7.7477	715	7.0
25	6909	1937.04	7.7440	795	7.8
26	6917	1934.60	7.7343	1390	13.6
27	6919	1933.99	7.7318	1390	13.6
28	6925	1932.16	7.7245	956	9.4
29	6929	1930.94	7.7196	1082	10.6
30	6935	1929.10	7.7123	2094	20.5
31	6938	1928.19	7.7087	2275	22.3
32	6943	1926.66	7.7026	2180	21.4
33	6959	1921.78	7.6830	761	7.5
34	6962	1920.86	7.6794	679	6.7
35	6982	1914.76	7.6550	2263	22.2
36	7238	1836.64	7.3426	804	7.9
37	7270	1826.87	7.3036	940	9.2
38	7613	1722.20	6.8851	1373	13.5
39	7645	1712.43	6.8461	1196	11.7
40	9838	1043.18	4.1705	10202	100.0

AOB121.1a/CDCl3/300MHz

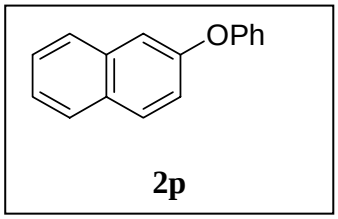
157.1631
155.0685
134.3186
130.1439
129.8457
129.8021
127.7220
127.1038
126.4928
124.6673
123.4164
119.9689
119.1107
114.0633



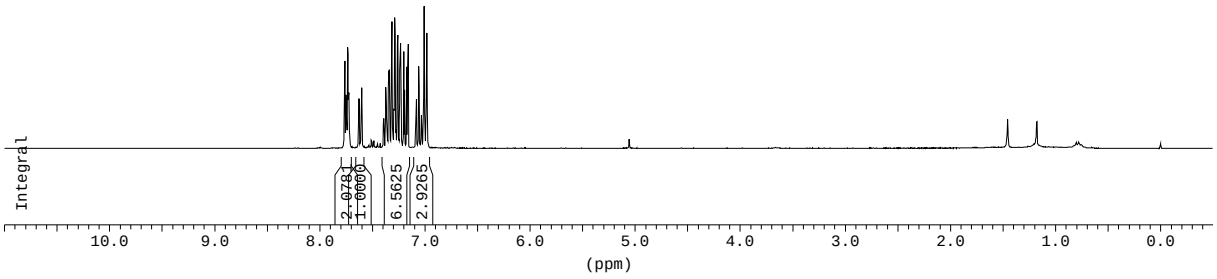
2p



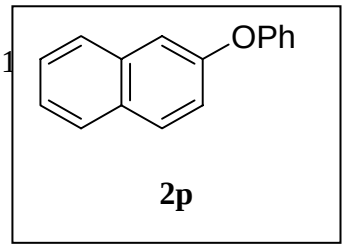
AOB121.1a/CDCl3/300MHz



2p



Peak List



2p

File Name : d:\profes~1\nmr\aob\aob121.1a\26040415\001001.1

Peak Results saved in File : C:\WIN1D\TMP\EDIT.ASC

Nucleus : off

SF : 300.130037 MHz

OFFSET : 19.6609 ppm

SW_p : 6172.84 Hz

SI : 16384

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 52

Sens. level = 207

Peak Picking region

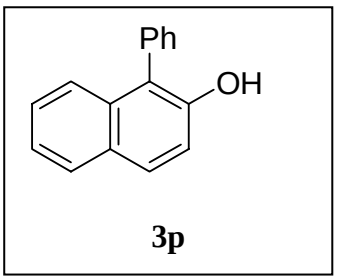
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
7.02/ 2108.4	6.97/ 2091.4	95.91	109.61
7.00/ 2100.1	6.94/ 2083.9	71.60	93.52
7.04/ 2113.6	7.02/ 2108.0	21.94	29.48
7.08/ 2124.6	7.03/ 2109.5	56.53	62.70
7.09/ 2128.0	7.08/ 2123.4	34.27	46.26
7.17/ 2152.1	7.16/ 2147.6	71.26	83.24
7.19/ 2156.6	7.17/ 2152.1	55.50	71.94
7.18/ 2154.7	7.16/ 2150.2	54.48	69.54
7.76/ 2328.0	7.74/ 2323.5	35.99	43.86

Peak Picking results

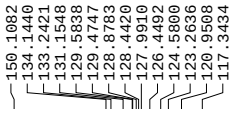
Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	9479	2329.53	7.7617	48023	61.3
2	9489	2325.76	7.7492	29395	37.5
3	9502	2320.86	7.7328	55708	71.1
4	9509	2318.22	7.7241	32891	42.0
5	9588	2288.46	7.6249	27383	34.9
6	9608	2280.92	7.5998	33414	42.6
7	9772	2219.13	7.3939	13785	17.6
8	9776	2217.63	7.3889	16443	21.0
9	9790	2212.35	7.3713	33623	42.9

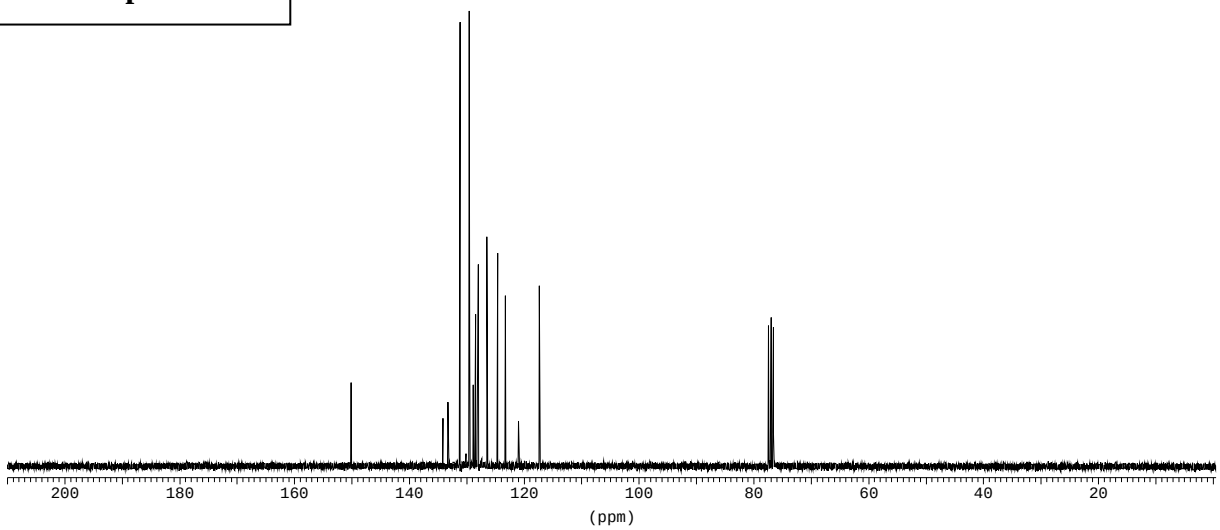
10	9794	2210.85	7.3663	31364	40.0
11	9811	2204.44	7.3450	40386	51.5
12	9813	2203.69	7.3424	42290	54.0
13	9818	2201.80	7.3362	43272	55.2
14	9835	2195.40	7.3148	34699	44.3
15	9838	2194.27	7.3111	69944	89.3
16	9844	2192.01	7.3035	17168	21.9
17	9853	2188.62	7.2922	21357	27.3
18	9858	2186.73	7.2860	72016	91.9
19	9861	2185.60	7.2822	63262	80.7
20	9867	2183.34	7.2747	10269	13.1
21	9876	2179.95	7.2634	24436	31.2
22	9881	2178.07	7.2571	62370	79.6
23	9887	2175.81	7.2495	10095	12.9
24	9897	2172.04	7.2370	42853	54.7
25	9904	2169.40	7.2282	57996	74.0
26	9925	2161.49	7.2018	53471	68.2
27	9932	2158.85	7.1931	32022	40.9
28	9949	2152.45	7.1717	44843	57.2
29	9960	2148.30	7.1579	57450	73.3
30	10021	2125.32	7.0813	27149	34.7
31	10041	2117.79	7.0562	45008	57.4
32	10061	2110.25	7.0311	18055	23.0
33	10081	2102.72	7.0060	78351	100.0
34	10101	2095.18	6.9809	63605	81.2

AOB121.2/CDCl3/300MHz

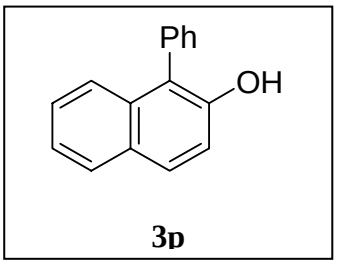


3p

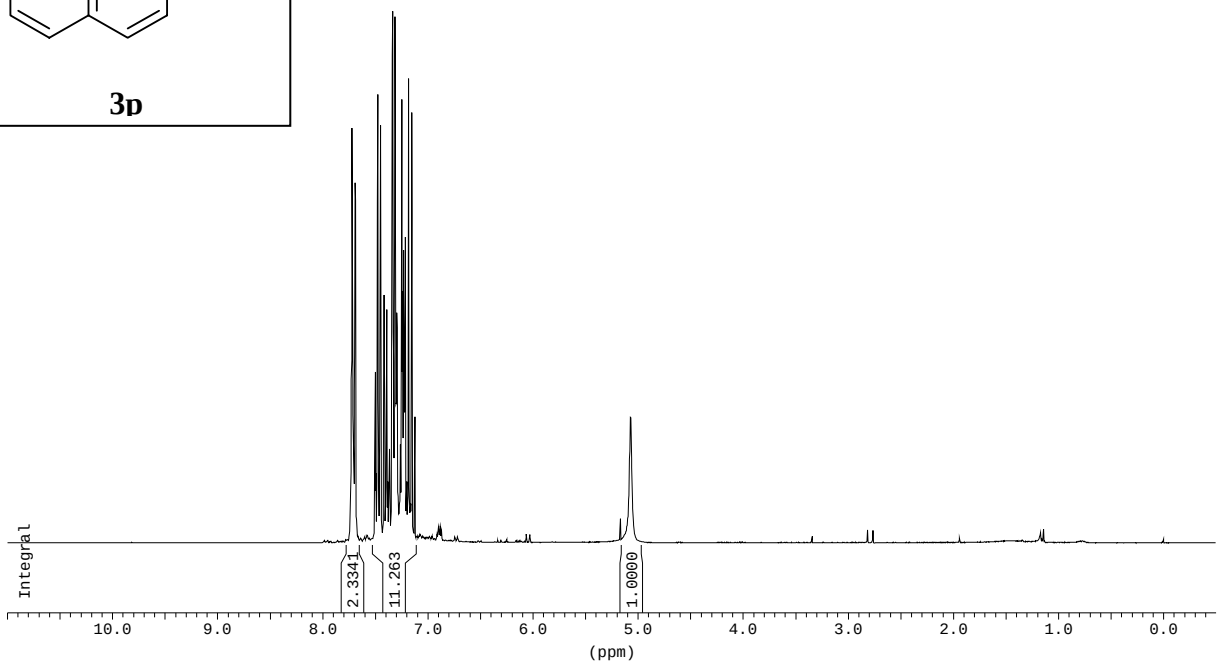




AOB121.2/CDCl3/300MHz



3p



Peak List

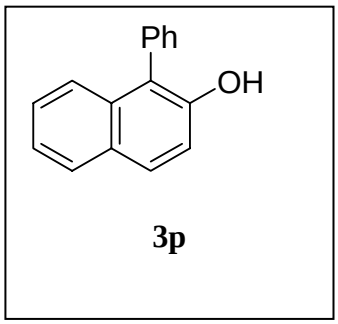
File Name : d:\nmr\aob\aob121~1.2-c\26040414\001001.1R

Peak Results saved in File : D:\NMR\AOB\AOB121~1.2-C\26040414\001001.TXT

Nucleus : off; SF : 300.130047 MHz

OFFSET : 19.6267 ppm; SW_p : 6172.84 Hz

SI : 16384



3p

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 25

Sens. level = 100

Peak Picking region

Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
8.23/ 2469.2	7.02/ 2107.5	11.26	114.59
5.53/ 1658.8	4.94/ 1483.2	15.79	46.64

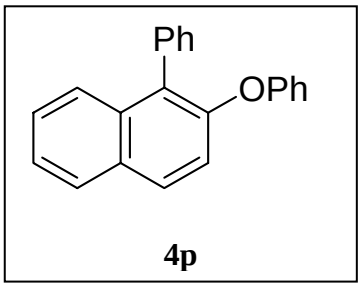
Peak Picking results

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
2	9486	2316.62	7.7187	82435	78.0
4	9510	2307.58	7.6886	71514	67.7
5	9658	2251.82	7.5028	26777	25.3
6	9662	2250.31	7.4978	33763	31.9
7	9666	2248.80	7.4928	13561	12.8
8	9680	2243.53	7.4752	89063	84.3
9	9684	2242.02	7.4702	53101	50.2
10	9696	2237.50	7.4551	58380	55.2
11	9699	2236.37	7.4513	82941	78.5
12	9702	2235.24	7.4476	52353	49.5
13	9705	2234.11	7.4438	13613	12.9
14	9726	2226.20	7.4174	31507	29.8
15	9729	2225.07	7.4137	49112	46.5
16	9733	2223.56	7.4086	28981	27.4
17	9742	2220.17	7.3974	15656	14.8
18	9747	2218.28	7.3911	46237	43.7
19	9756	2214.89	7.3798	11928	11.3
20	9765	2211.50	7.3685	13541	12.8

21	9768	2210.37	7.3647	18421	17.4
22	9790	2202.08	7.3371	96867	91.7
23	9794	2200.58	7.3321	105691	100.0
24	9799	2198.69	7.3258	35775	33.8
25	9812	2193.79	7.3095	104672	99.0
26	9816	2192.29	7.3045	52059	49.3
27	9825	2188.90	7.2932	45657	43.2
28	9831	2186.64	7.2856	12638	12.0
29	9851	2179.10	7.2605	19356	18.3
30	9862	2174.96	7.2467	88141	83.4
31	9869	2172.32	7.2379	49870	47.2
32	9872	2171.19	7.2342	28131	26.6
33	9875	2170.06	7.2304	58080	55.0
34	9878	2168.93	7.2266	40195	38.0
35	9880	2168.17	7.2241	32182	30.4
36	9883	2167.04	7.2204	46536	44.0
37	9889	2164.78	7.2128	60683	57.4
38	9901	2160.26	7.1978	11927	11.3
39	9914	2155.36	7.1814	92268	87.3
40	9938	2146.32	7.1513	85474	80.9
41	9960	2138.03	7.1237	24899	23.6
42	11596	1521.65	5.0700	24810	23.5

AOB121.b/CDCl3/300MHz

158.4795
150.2755
135.3804
133.7367
130.8421
130.5584
129.8602
129.4238
129.2711
128.0565
127.9692
127.2928
126.4419
125.8891
124.8782
122.2163
120.5798
117.6052



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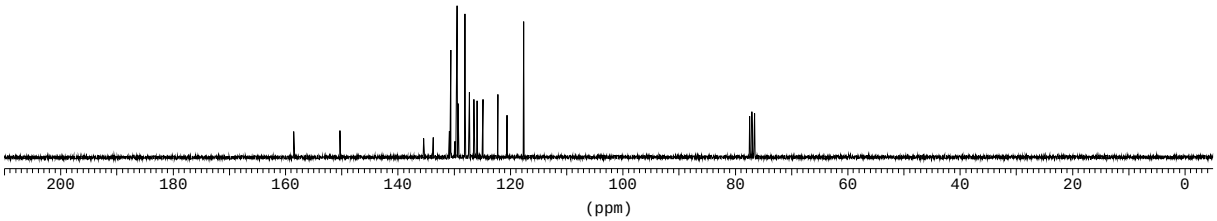
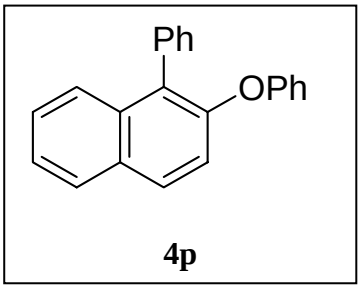
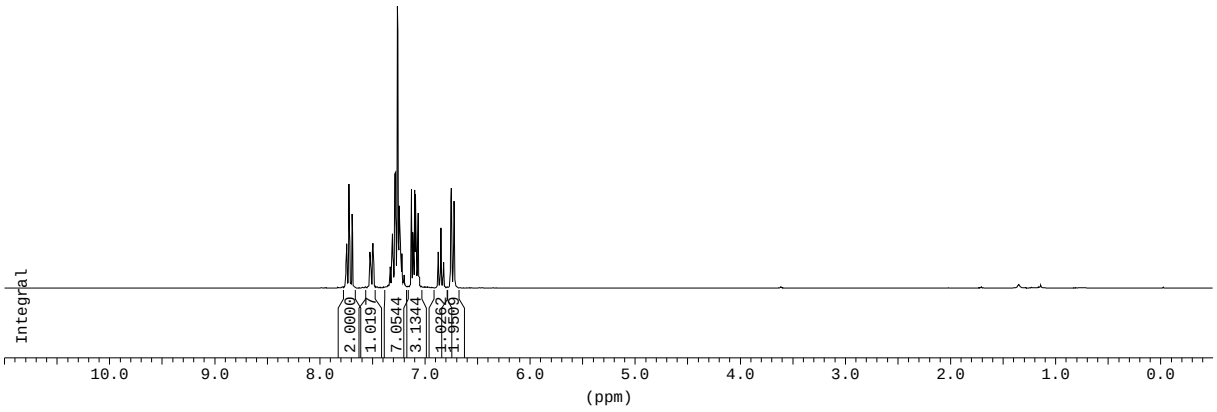


AOB121.b/CDCl3/300MHz



4p



Peak List

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Nucleus : off

SF : 300.130063 MHz, OFFSET : 19.5735 ppm

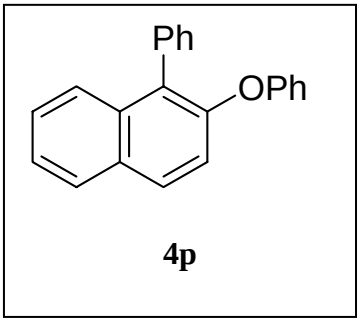
SW_p : 6172.84 Hz, SI : 16384

Peak Picking Parameter

Peak constant PC = 1.00

Noise = 63

Sens. level = 253



4p

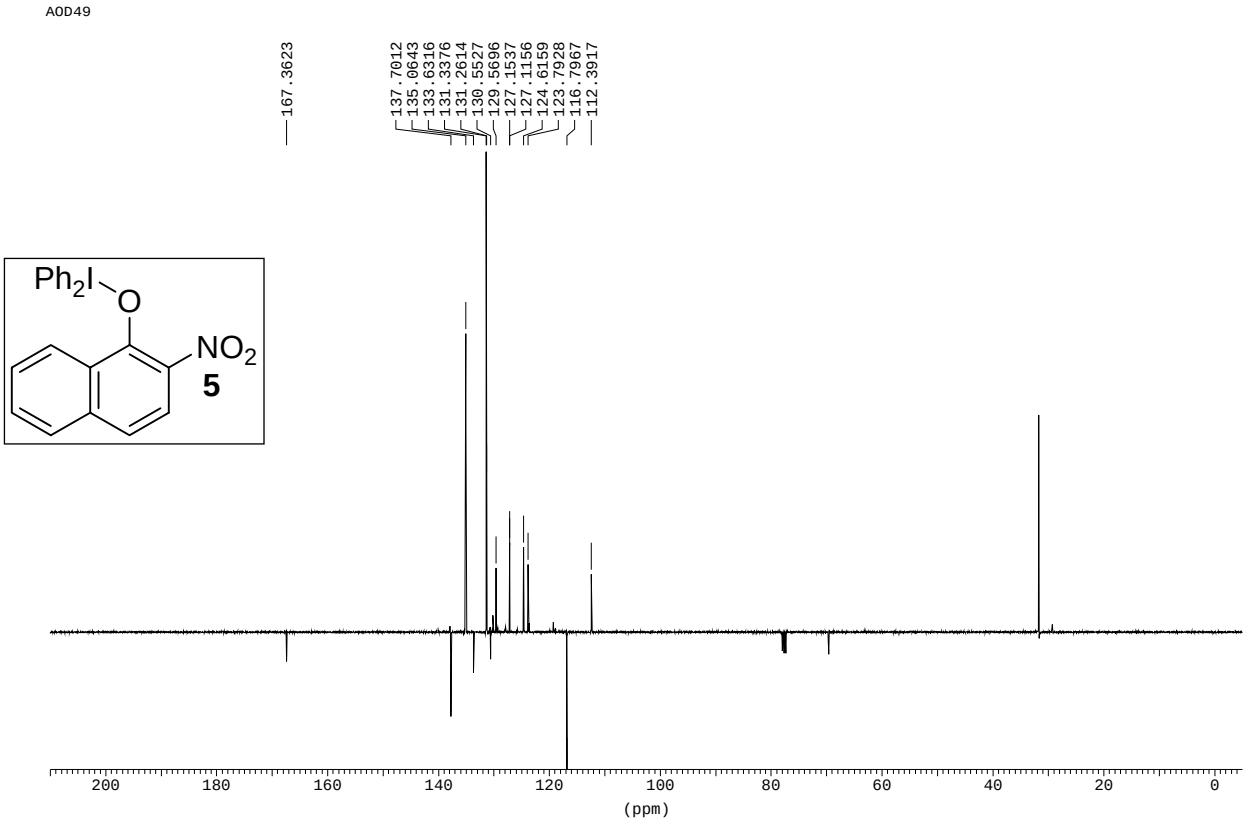
Peak Picking region

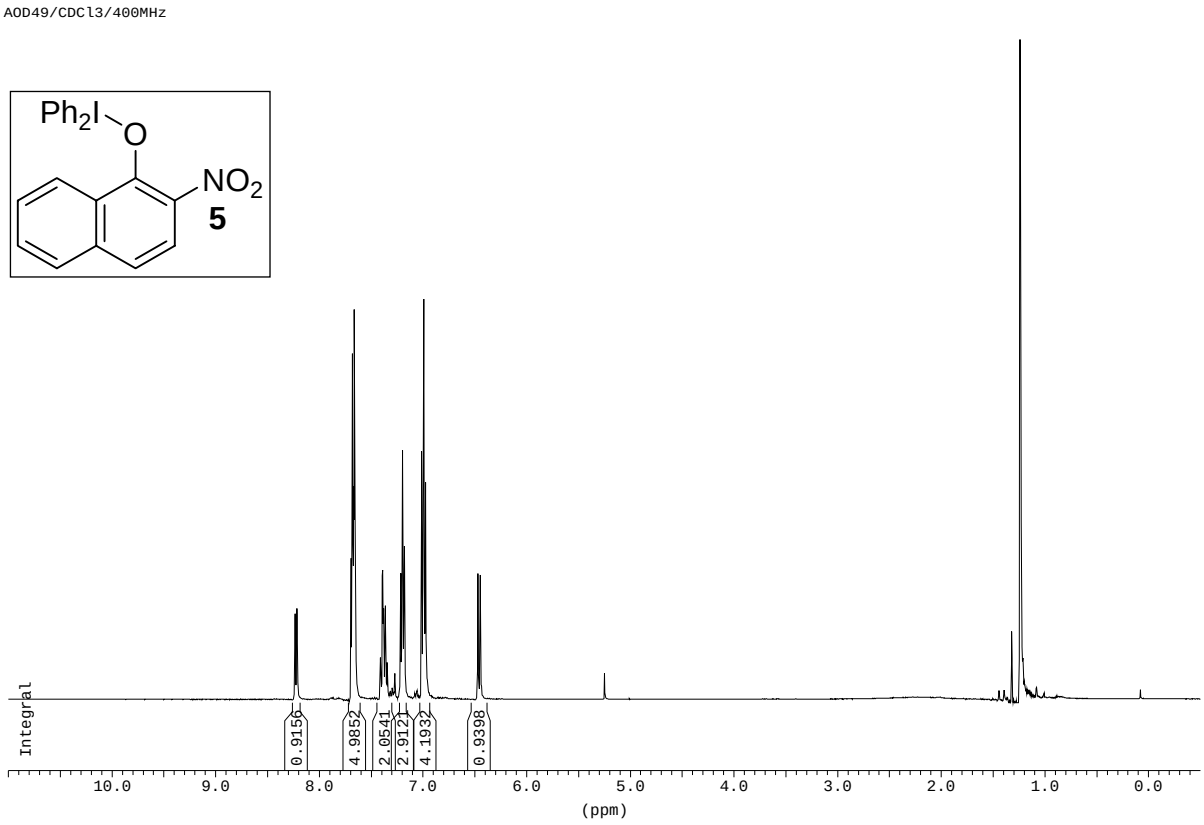
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
8.40/ 2522.5	6.60/ 1980.4	2.35	113.35

Peak Picking results

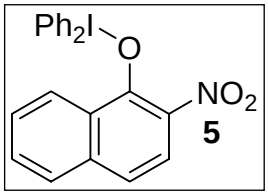
Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	9421	2325.13	7.7471	29378	13.5
2	9426	2323.24	7.7408	34127	15.7
3	9443	2316.84	7.7194	80579	37.0
4	9466	2308.17	7.6906	57546	26.4
5	9601	2257.31	7.5211	28117	12.9
6	9603	2256.56	7.5186	27753	12.7
7	9623	2249.02	7.4935	34476	15.8
8	9625	2248.27	7.4910	32324	14.8
9	9627	2247.51	7.4885	31455	14.4
10	9752	2200.42	7.3316	13024	6.0
11	9755	2199.29	7.3278	16458	7.6
12	9770	2193.64	7.3090	41843	19.2
13	9774	2192.13	7.3039	38959	17.9
14	9789	2186.48	7.2851	88248	40.5
15	9794	2184.60	7.2788	89490	41.1
16	9809	2178.94	7.2600	217950	100.0
17	9813	2177.44	7.2550	188866	86.7
18	9822	2174.05	7.2437	63550	29.2
19	9828	2171.79	7.2361	44201	20.3

20	9839	2167.64	7.2223	14591	6.7
21	9844	2165.76	7.2161	26609	12.2
22	9853	2162.37	7.2048	8729	4.0
23	9855	2161.61	7.2023	7644	3.5
24	9860	2159.73	7.1960	10033	4.6
25	9915	2139.01	7.1269	76224	35.0
26	9926	2134.86	7.1131	43167	19.8
27	9932	2132.60	7.1056	16818	7.7
28	9939	2129.97	7.0968	76125	34.9
29	9946	2127.33	7.0880	72599	33.3
30	9948	2126.57	7.0855	65870	30.2
31	9955	2123.94	7.0767	12323	5.7
32	9960	2122.05	7.0704	28711	13.2
33	9963	2120.92	7.0667	25377	11.6
34	9968	2119.04	7.0604	58003	26.6
35	9975	2116.40	7.0516	8417	3.9
36	10119	2062.15	6.8709	28007	12.9
37	10138	2054.99	6.8470	46562	21.4
38	10158	2047.46	6.8219	19975	9.2
39	10218	2024.85	6.7466	77420	35.5
40	10238	2017.31	6.7215	67050	30.8





Peak List



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SF : 400.130015 MHz
OFFSET : 15.0198 ppm
SW_p : 8012.82 Hz
SI : 32768

Peak Picking Parameter

Peak constant PC = 1.00
Noise = 5
Sens. level = 19

Peak Picking region

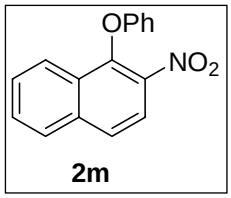
Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
8.56/ 3426.4	8.06/ 3224.9	2.92	6.18

6.63/ 2653.9	6.29/ 2516.7	3.87	7.00
7.74/ 3097.0	7.60/ 3039.8	4.67	16.41
7.54/ 3017.0	7.32/ 2928.0	0.82	10.06
7.24/ 2896.5	7.12/ 2850.3	3.44	11.17
7.04/ 2816.8	6.92/ 2769.1	6.49	17.84

Peak Picking results

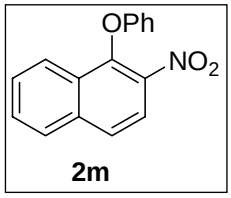
Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	11105	3294.33	8.2331	10289	21.3
2	11138	3286.26	8.2130	10828	22.4
3	11990	3077.92	7.6923	17214	35.6
4	12010	3073.03	7.6801	39010	80.7
5	12013	3072.29	7.6782	41832	86.6
6	12028	3068.62	7.6691	25733	53.3
7	12043	3064.96	7.6599	46991	97.3
8	12047	3063.98	7.6575	41201	85.3
9	12456	2963.96	7.4075	4894	10.1
10	12484	2957.12	7.3904	14853	30.7
11	12488	2956.14	7.3879	15501	32.1
12	12499	2953.45	7.3812	11811	24.4
13	12503	2952.47	7.3788	10793	22.3
14	12526	2946.85	7.3647	10335	21.4
15	12531	2945.62	7.3617	11083	22.9
16	12558	2939.02	7.3452	4229	8.8
17	12563	2937.80	7.3421	4075	8.4
18	12771	2886.94	7.2150	15126	31.3
19	12802	2879.36	7.1961	29966	62.0
20	12832	2872.02	7.1777	18314	37.9
21	13103	2805.75	7.0121	29866	61.8
22	13135	2797.93	6.9925	48312	100.0
23	13167	2790.10	6.9730	26082	54.0
24	13992	2588.36	6.4688	15034	31.1
25	14031	2578.83	6.4450	14919	30.9

AOD50/ J-MOD/400MHz

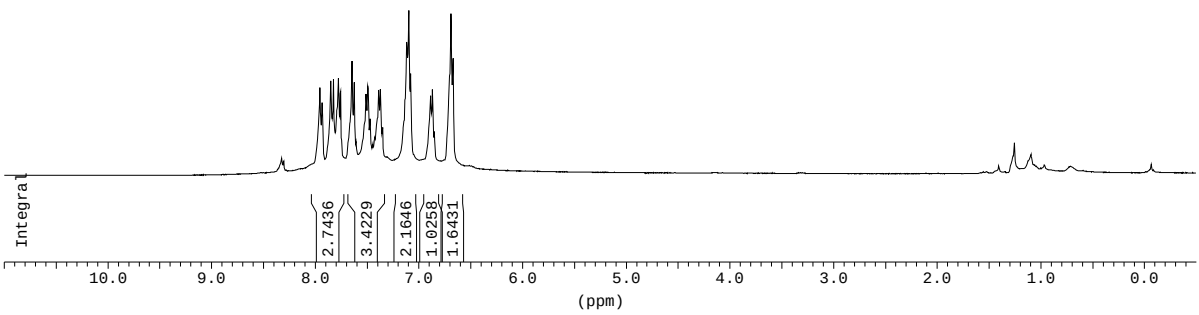


2m

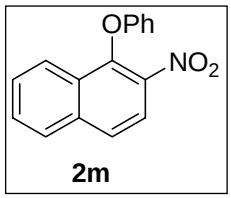
AOD50/CDCl3/400MHz



2m



Peak List



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Nucleus : off
SF : 400.130094 MHz
OFFSET : 14.8228 ppm
SW_p : 8012.82 Hz
SI : 32768

Peak Picking Parameter

Peak constant PC = 1.00
Noise = 24
Sens. level = 98

Peak Picking region

Start(ppm/Hz)	End(ppm/Hz)	MI(%)	MAXI(%)
6.97/ 2790.8	6.84/ 2735.3	47.23	69.91
7.25/ 2900.3	7.02/ 2810.3	51.32	118.20
6.77/ 2707.9	6.55/ 2619.6	59.25	111.85
7.43/ 2972.2	7.32/ 2929.2	50.18	62.42
7.54/ 3017.7	7.46/ 2984.7	51.09	59.93
7.71/ 3084.0	7.59/ 3035.6	53.58	78.97
7.80/ 3119.2	7.73/ 3091.1	48.37	64.69
7.92/ 3168.6	7.81/ 3123.1	59.25	70.81
8.00/ 3202.1	7.90/ 3159.3	42.02	65.37

Peak Picking results

Peak Nr.	Data Point	Frequency	PPM	Intensity	%Int.
1	11240	3182.52	7.9537	20739	58.3
2	11274	3174.21	7.9329	16455	46.3
3	11414	3139.97	7.8474	22444	63.1
4	11450	3131.17	7.8254	22222	62.5
5	11532	3111.12	7.7753	21885	61.5
6	11565	3103.05	7.7551	18061	50.8

7	11743	3059.52	7.6463	25876	72.8
8	11780	3050.48	7.6237	19997	56.2
9	11969	3004.26	7.5082	18497	52.0
10	11998	2997.17	7.4905	19487	54.8
11	12165	2956.33	7.3884	18898	53.1
12	12195	2948.99	7.3701	18202	51.2
13	12610	2847.51	7.1165	30566	86.0
14	12642	2839.69	7.0969	35559	100.0
15	12674	2831.86	7.0774	19835	55.8
16	12983	2756.30	6.8885	17280	48.6
17	13013	2748.97	6.8702	17981	50.6
18	13306	2677.32	6.6911	35384	99.5
19	13338	2669.49	6.6716	22893	64.4

Additional References

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