Supporting Information

Aerobic Homocoupling of Arylboronic Acids Catalysed by Copper Terephthalate Metal Organic Frameworks

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1. Characterization datas

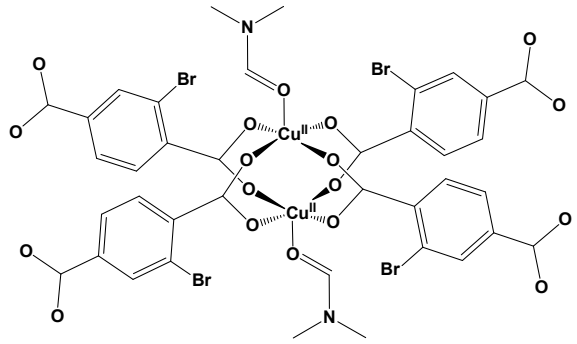


Fig. 1 Structure of MOF-101

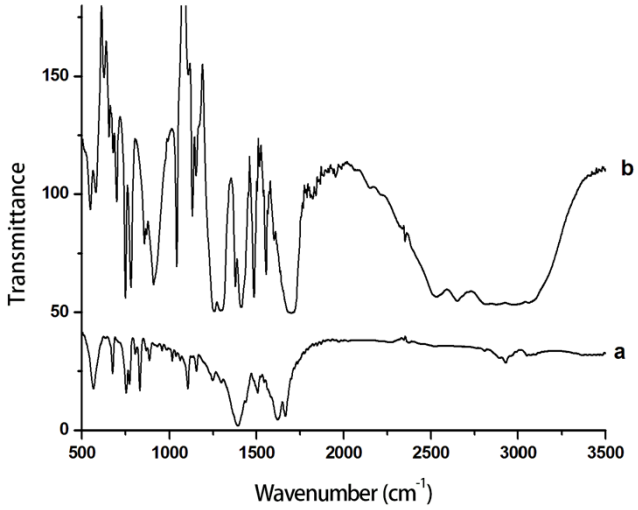


Fig. 2 FT-IR spectra of MOF-101 (a) and 2-bromoterephthalic acid (b)

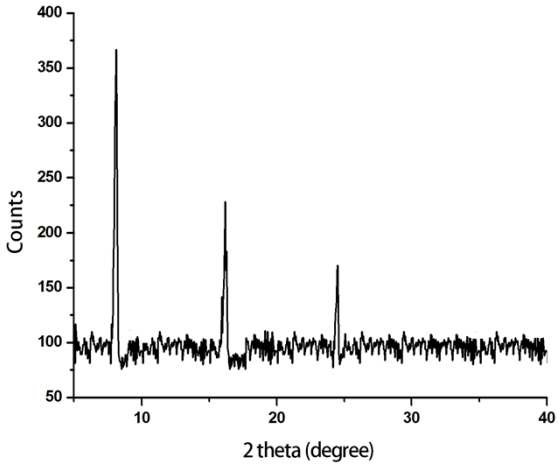


Fig. 3 Powder XRD patterns of MOF-101

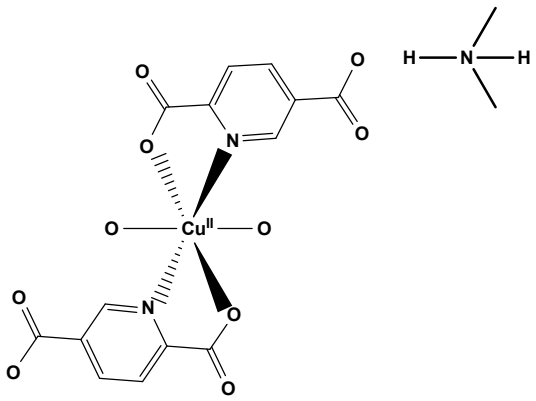


Fig. 4 Structure of $[Cu(pdc)_2]NH_2Me_2$

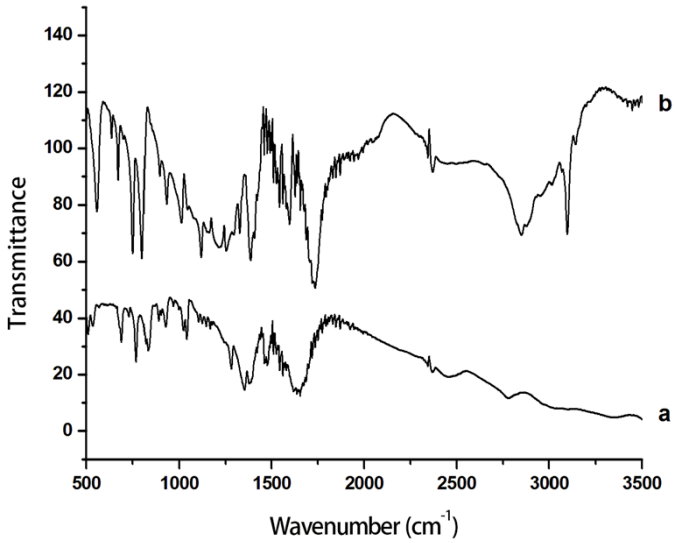


Fig. 5 FT-IR spectra of $[Cu(pdc)_2]NH_2Me_2$ (a) and pyridine-2,5-dicarboxylic acid (b)

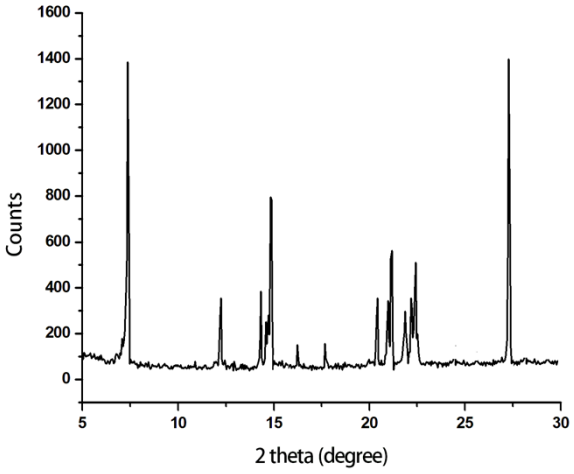


Fig. 6 Powder XRD pattern of $[Cu(pdc)_2]NH_2Me_2$

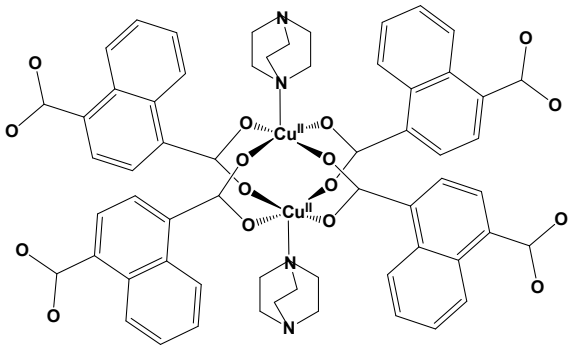


Fig. 7 Structure of $[Cu_2(ndc)_2ted]_n$

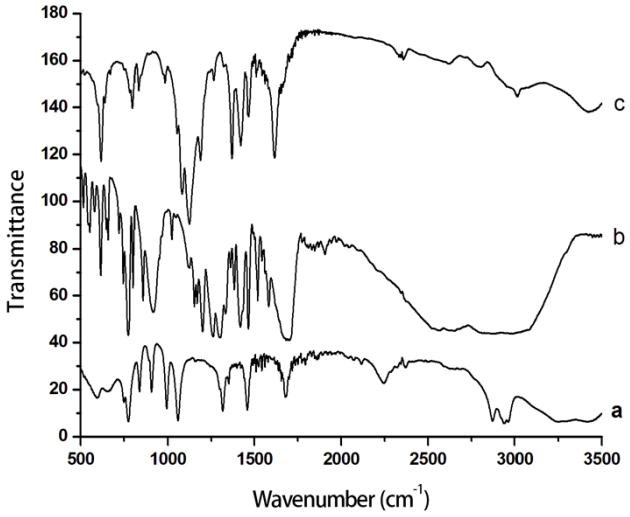


Fig. 8 FT-IR spectra of triethylenediamine (a), 1,4-naphthalenedicarboxylic acid (b) and $[Cu_2(ndc)_2ted]_n$ MOF (c)

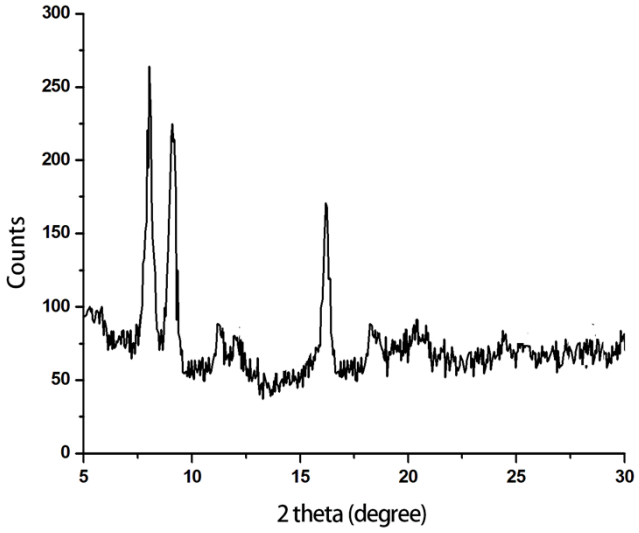


Fig. 9 Powder XRD pattern of $[Cu_2(ndc)_2ted]_n$ MOF

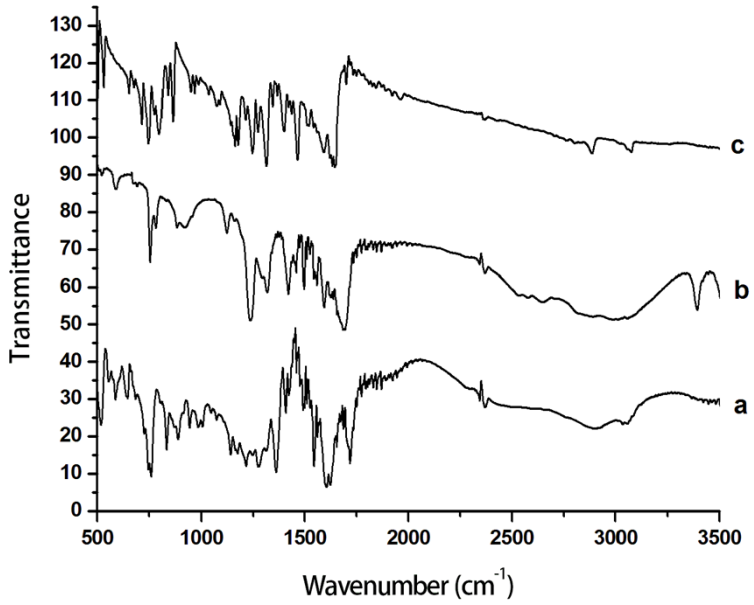


Fig. 10 FT-IR spectra of H_2L=(*Z*)-4-((2-hydroxynaphthalen-1-yl)methyleneamino)benzene-1,3-dioic acid (a), 2-aminoterephthalic acid (b) and 2-hydroxynaphthaldehyde

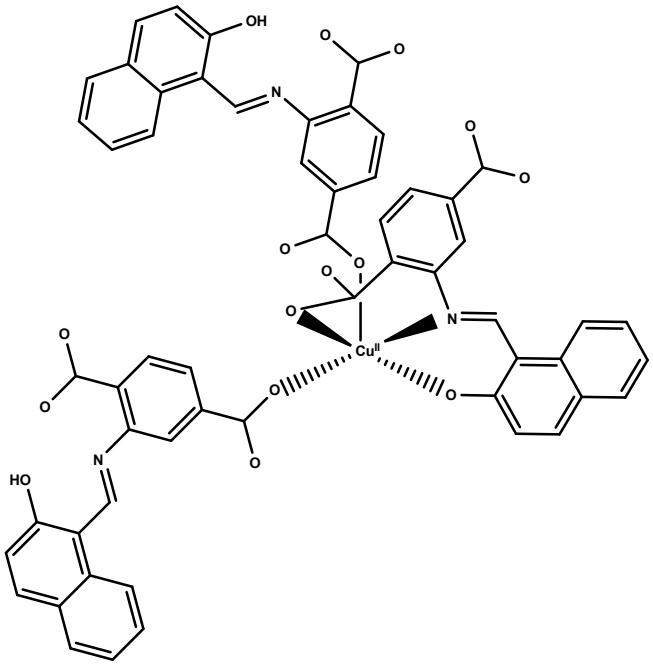


Fig. 11 Structure of $[Cu(H_2L)]_n$

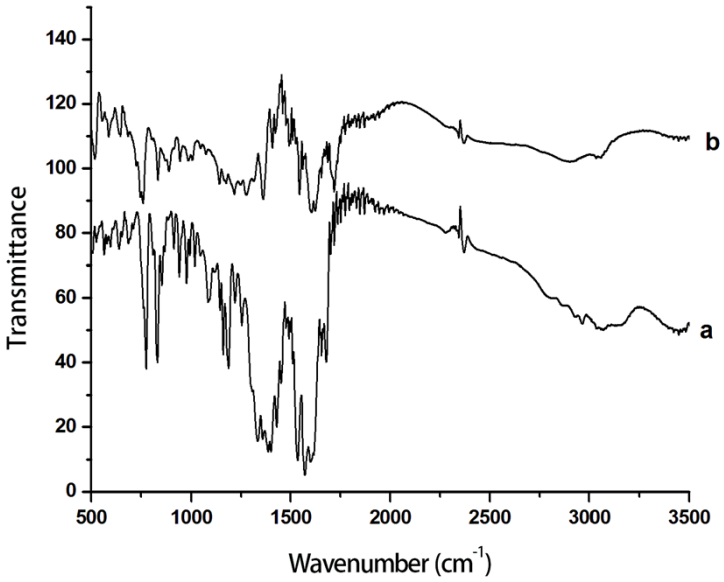


Fig. 12 FT-IR spectra of $[Cu(H_2L)]_n$ (a) and H_2L (b)

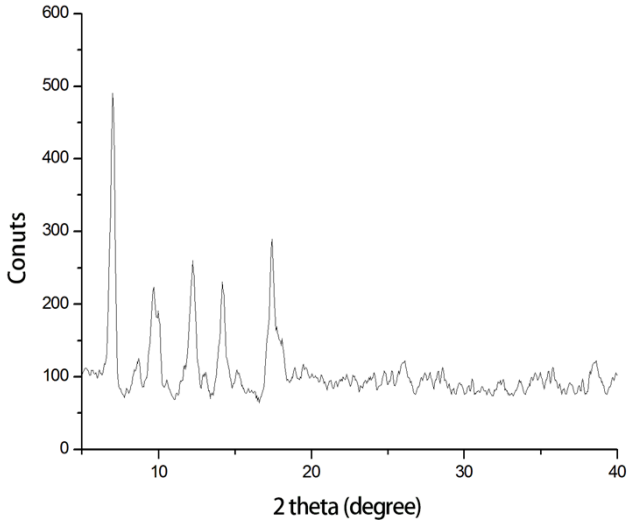
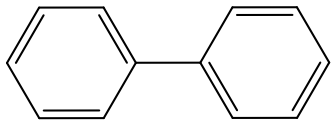


Fig. 13 Powder XRD pattern of $[Cu(H_2L)]_n$

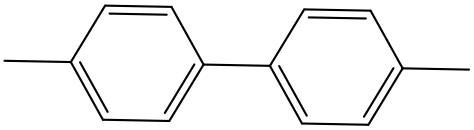
NMR datas of homocoupled products

Biphenyl[1]



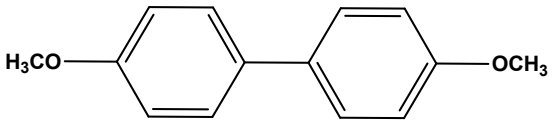
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 68-70°C; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.59 (d, 4H), 7.43-7.39 (t, 4H),7.33-7.30 (d, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 141.3, 128.8, 128.6, 127.3, 127.2 ppm;

4,4'-dimethyl biphenyl[1]



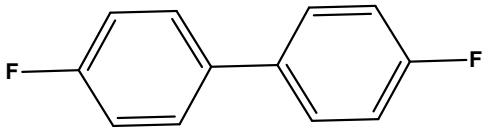
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 124-126°C;^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.48-7.46 (d, 4H), 7.23-7.21 (d, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 138.4, 136.8, 129.6, 126.9, 21.2 ppm;

4,4'-dimethoxy biphenyl[2]



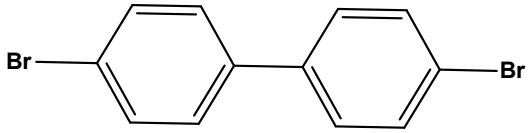
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 172-174°C; ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ 7.49-7.46 (m, 4H), 6.97-6.94 (m, 4H), 3.84 (6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$, 25°C, TMS) δ = 158.7, 133.5, 127.7, 114.2, 55.3 ppm;

4,4'-difluoro biphenyl[1]



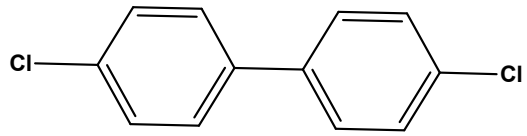
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 88-90°C; ^{1}H NMR (500 MHz, $CDCl_3$, 25°C, TMS): δ 7.51-7.48 (m, 4H), 7.14-7.11 (m, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$, 25°C, TMS) δ = 163.5, 161.6, 136.5, 136.5, 128.7, 128.6, 115.9, 115.7 ppm;

4,4'-dibromo biphenyl[1]



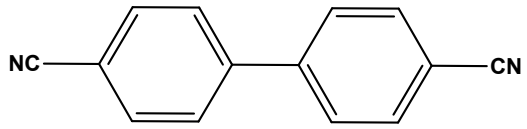
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 162-164°C; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.57-7.54 (m, 4H), 7.42-7.39 (m, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 139.0, 132.1, 128.6, 122.1 ppm;

4,4'-dichloro biphenyl[2]



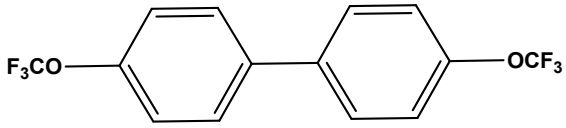
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 148-150°C; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.49-7.46 (m, 4H), 7.42-7.39 (m, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 138.6, 133.9, 129.2, 128.3 ppm;

4,4'-dicyano biphenyl



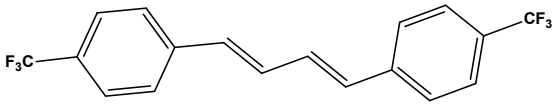
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 235-237°C; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.80-7.77 (m, 4H), 7.71-7.68 (m, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 143.5, 132.9, 127.9, 118.4, 112.5 ppm;

4,4'- bis-(trifluoromethoxy)-biphenyl[3]



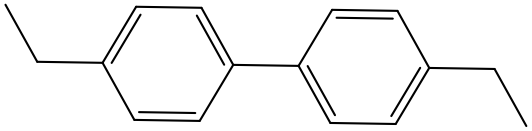
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.58-7.56 (d, 4H), 7.31-7.29 (d, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 149.0, 138.7, 128.6, 121.5, 119.4 ppm;

1,1'-(1*E*,3*E*)-1,3-butadiene-1,4-diylbis[4-(trifluoromethyl)- Benzene[4]



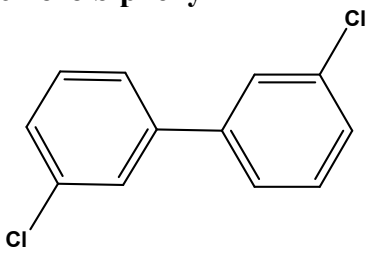
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 144-146°C ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.64-7.48 (m, 8H), 7.06-6.99 (m, 2H), 6.78-6.71 (m, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 140.5, 132.8, 131.1, 129.8, 126.7, 125.8, 125.8 ppm;

4,4'-diethyl biphenyl[5]



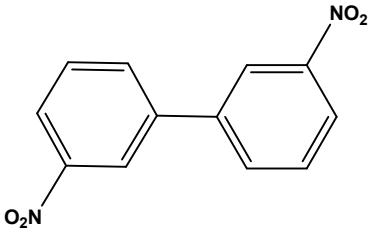
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 78-80°C; ^{1}H NMR (500 MHz, $CDCl_3$, 25°C, TMS): δ 7.51-7.49 (d, 4H), 7.27-7.25 (d, 4H), 2.71-2.66 (q, 4H), 1.29-1.26 (t, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$, 25°C, TMS) δ = 143.0, 138.5, 128.2, 126.9, 28.5, 15.6 ppm;

3,3'-dichloro biphenyl[6]



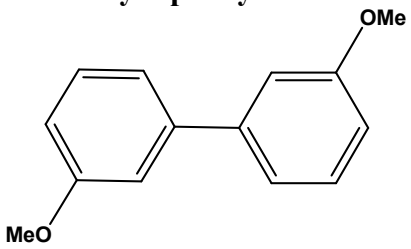
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.54 (s, 2H), 7.44-7.42 (m, 2H), 7.40-7.33 (m, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 141.7, 134.9, 130.2, 128.0, 127.3, 125.3 ppm;

3,3'-dinitro biphenyl[1]



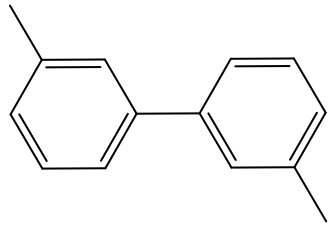
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Yellow solid; m.p. 200-202°C;^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 8.50 (s, 2H), 8.31-8.29 (d, 2H), 7.99-7.97 (d, 2H), 7.73-7.69 (t, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 148.9, 140.3, 133.1, 130.3, 123.3, 122.1 ppm;

3,3'-dimethoxy biphenyl[7]



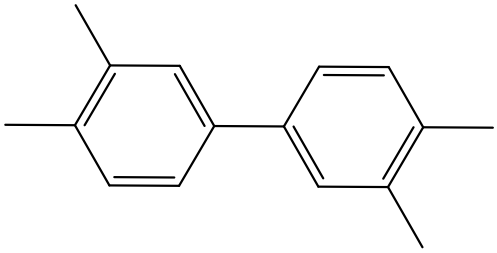
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.38-7.34 (m, 2H), 7.20-7.18 (m, 2H), 7.14-7.13 (m, 2H), 6.92-6.90 (m, 2H), 3.87 (6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 160.0, 142.7, 129.8, 119.8, 113.0, 112.9, 55.4 ppm;

3,3'-dimethyl biphenyl[8]



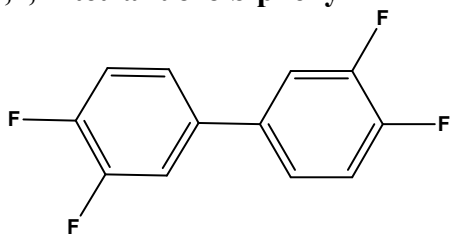
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ 7.40-7.29 (m, 6H), 7.17-7.14 (d, 2H), 2.42 (6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$, 25°C, TMS) δ = 141.3, 138.2, 128.5, 127.9, 127.8, 124.2, 21.5 ppm;

3,3',4,4'-tetramethyl biphenyl



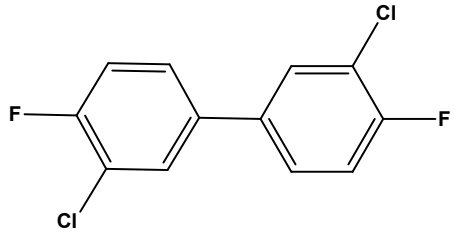
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 72-74°C; ^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ 7.35-7.30 (m, 4H), 7.19-7.16 (2H), 2.31 (6H), 2.29 (6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 139.0, 136.8, 135.4, 130.1, 128.4, 124.5, 20.1, 19.5 ppm;

3,3',4,4'-tetrafluoro biphenyl[9]



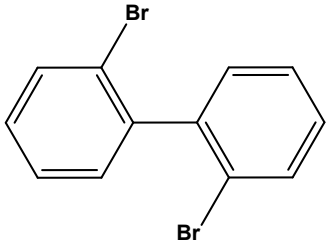
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 80-82°C; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.38-7.33 (m, 2H), 7.30-7.23 (m, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 152.0, 151.8, 151.6, 151.5, 149.5, 149.4, 149.2, 149.0, 136.3, 123.1, 123.1, 123.0, 118.0, 117.8, 116.2, 116.0 ppm;

3,3'-dichloro-4,4'-difluoro biphenyl



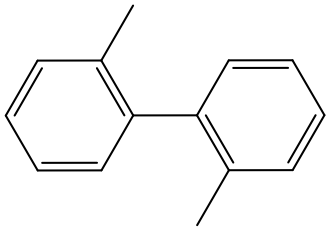
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 138-140°C; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.55-7.53 (m, 2H), 7.38-7.35 (m, 2H), 7.22-7.18 (m, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 159.3, 156.8, 136.3, 129.3, 126.8, 126.7, 121.8, 121.6, 117.3, 117.0 ppm;

2,2'-dibromo biphenyl[10]



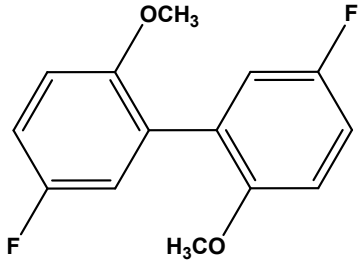
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 78-80°C ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.60-7.58 (d, 2H), 7.32-7.25 (m, 2H), 7.21-7.16 (m, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 142.0, 132.6, 130.9, 129.4, 127.1, 123.5 ppm;

2,2'-dimethyl biphenyl[1]



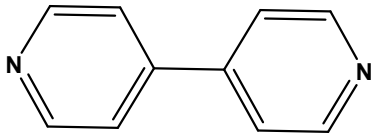
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.32-7.25 (m, 6H), 7.16-7.14 (d, 2H), 2.14 (6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 142.0, 136.0, 129.9, 129.4, 127.2, 125.6, 19.9 ppm;

2,2'-dimethoxy-5,5'-fluoro biphenyl[11]



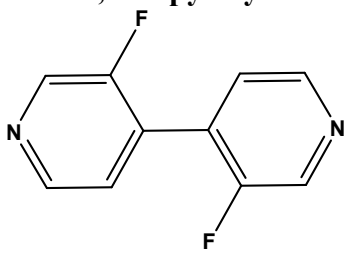
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 122-124°C; ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 7.05-6.97 (m, 4H), 6.92-6.88 (m, 2H), 3.76 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 158.0, 155.6, 153.2, 128.0, 127.9, 118.3, 118.1, 115.0, 114.8, 112.32, 112.2, 56.4 ppm;

4,4'-bipyridyl[12]



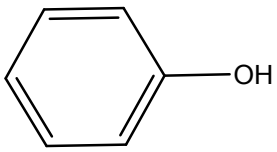
Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 108-110°C ^{1}H NMR (400 MHz, $CDCl_3$, 25°C, TMS): δ 8.75-8.74(d, 4H), 7.55-7.54 (d, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$, 25°C, TMS) δ = 150.6, 145.4, 121.6, 121.3, 121.0 ppm;

3,3'-difluoro-4,4'-bipyridyl[13]



Compound was prepared according to the general procedure. The crude product was purified by column chromatography. Colourless solid; m.p. 170-172°C ^{1}H NMR (500 MHz, $CDCl_3$, 25°C, TMS): δ 8.68-8.59 (m, 4H), 7.43 (s, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$, 25°C, TMS) δ = 157.3, 155.2, 146.1, 139.4, 139.2, 128.4, 124.8 ppm;

Phenol



^{1}H NMR (300 MHz, $CDCl_3$, 25°C, TMS): δ 7.22-7.17 (m, 2H), 6.94-6.83 (m, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$, 25°C, TMS) δ = 155.6, 130.4, 121.5, 116.0 ppm;

2. ESI-MS, ^{1}H & ^{13}C NMR spectral figures

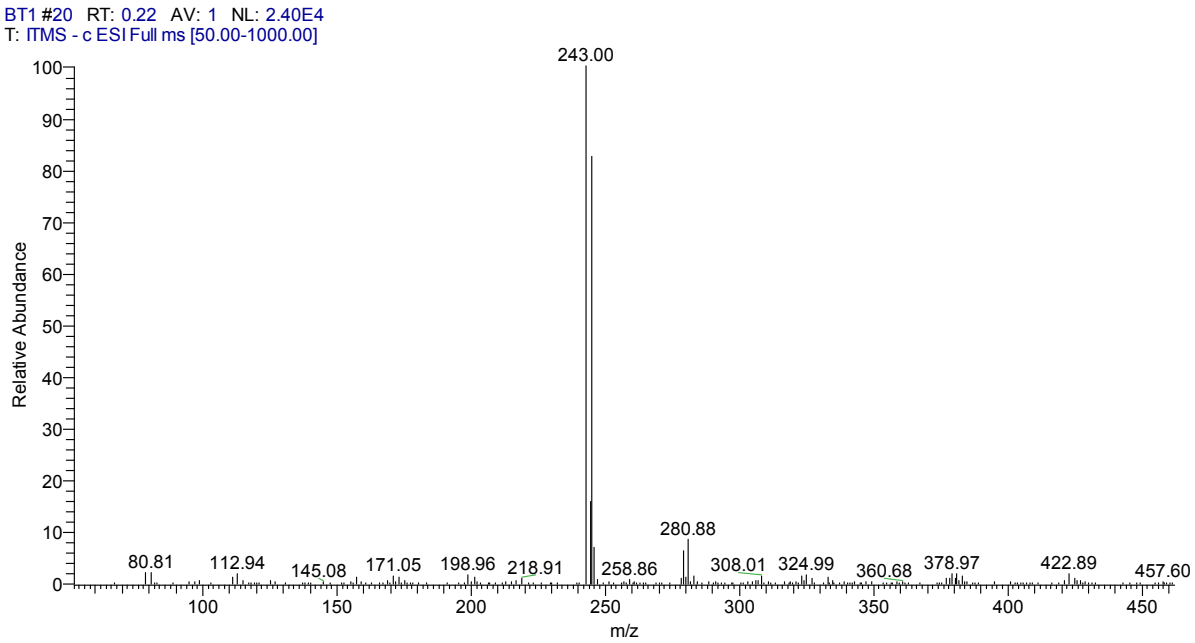


Fig. 14 ESI-MS spectrum of 2-bromoterephthalic acid

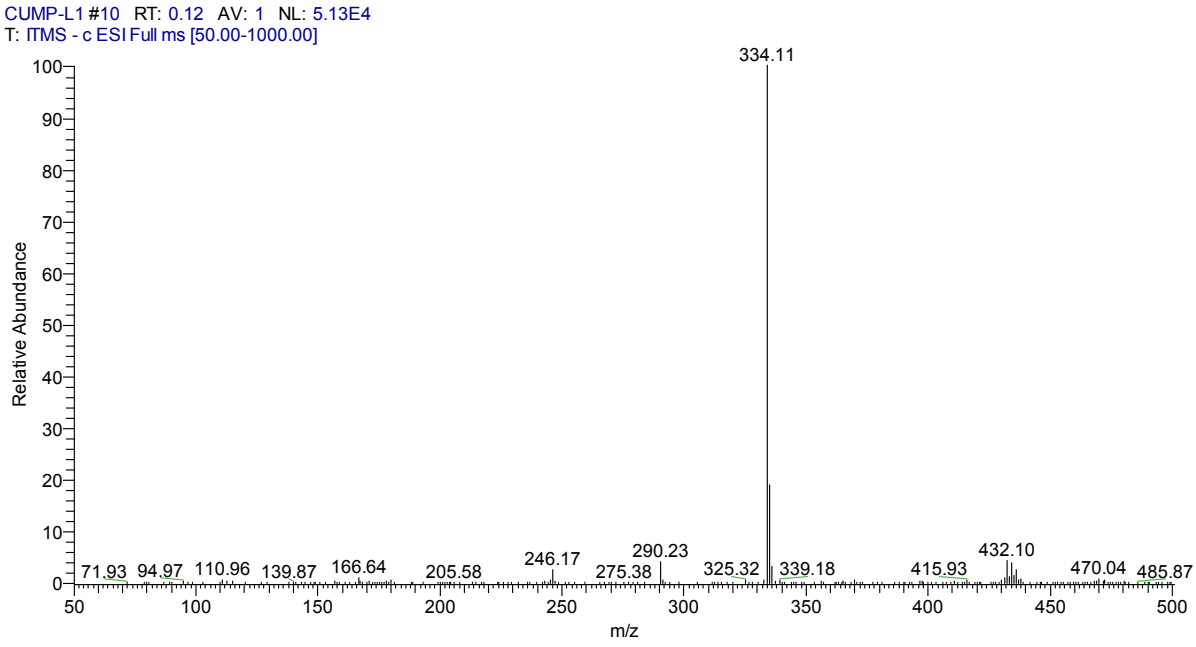


Fig. 15 ESI-MS spectrum of (*Z*)-4-((2-hydroxynaphthalen-1-yl)methyleneamino)benzene-1,3-dioic acid

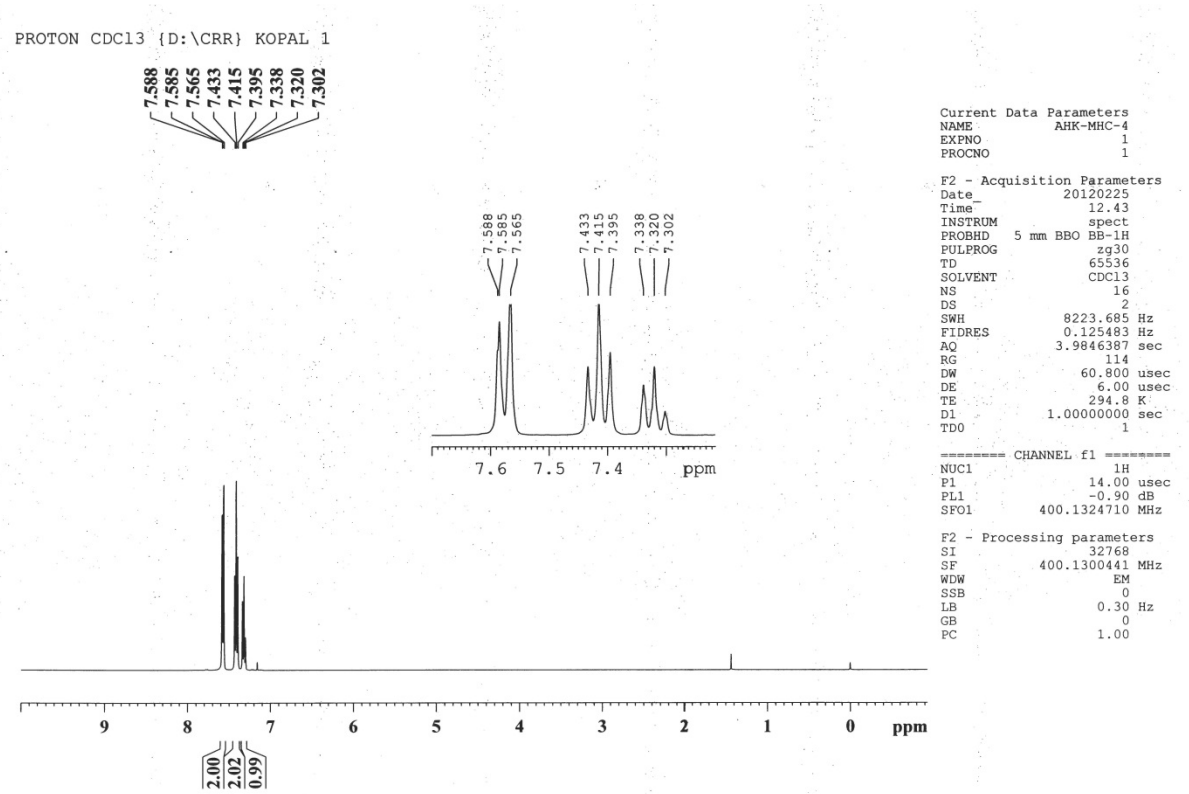


Fig. 16 400 MHz ^{1}H NMR Spectrum of Biphenyl in $CDCl_3$

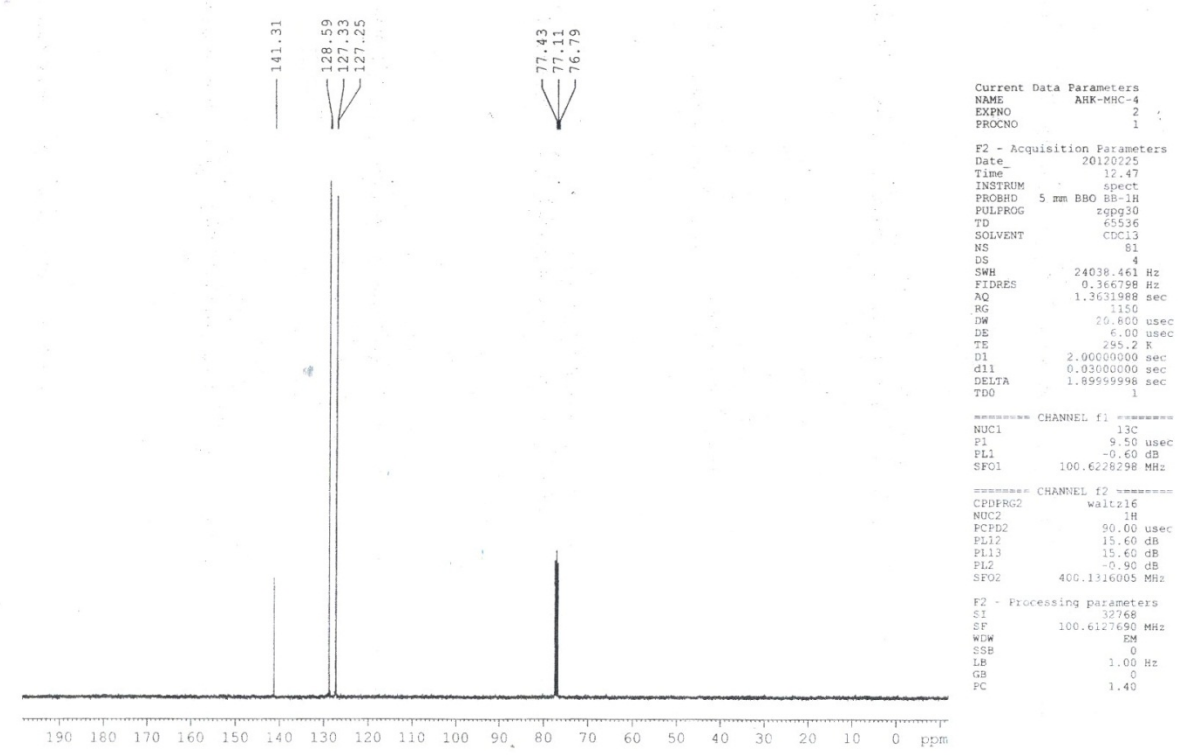


Fig. 17 100 MHz ^{13}C NMR Spectrum of Biphenyl in $CDCl_3$

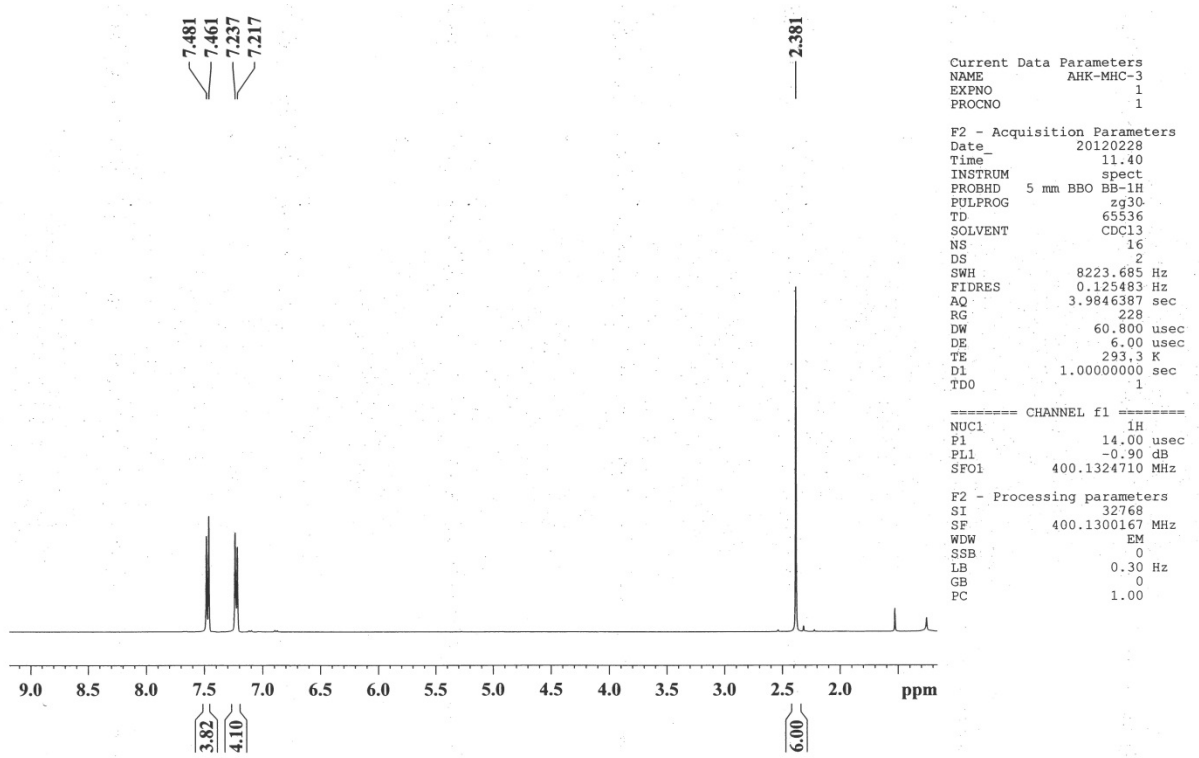


Fig. 18 400 MHz ^{1}H NMR Spectrum of 4,4'-dimethyl biphenyl in $CDCl_3$

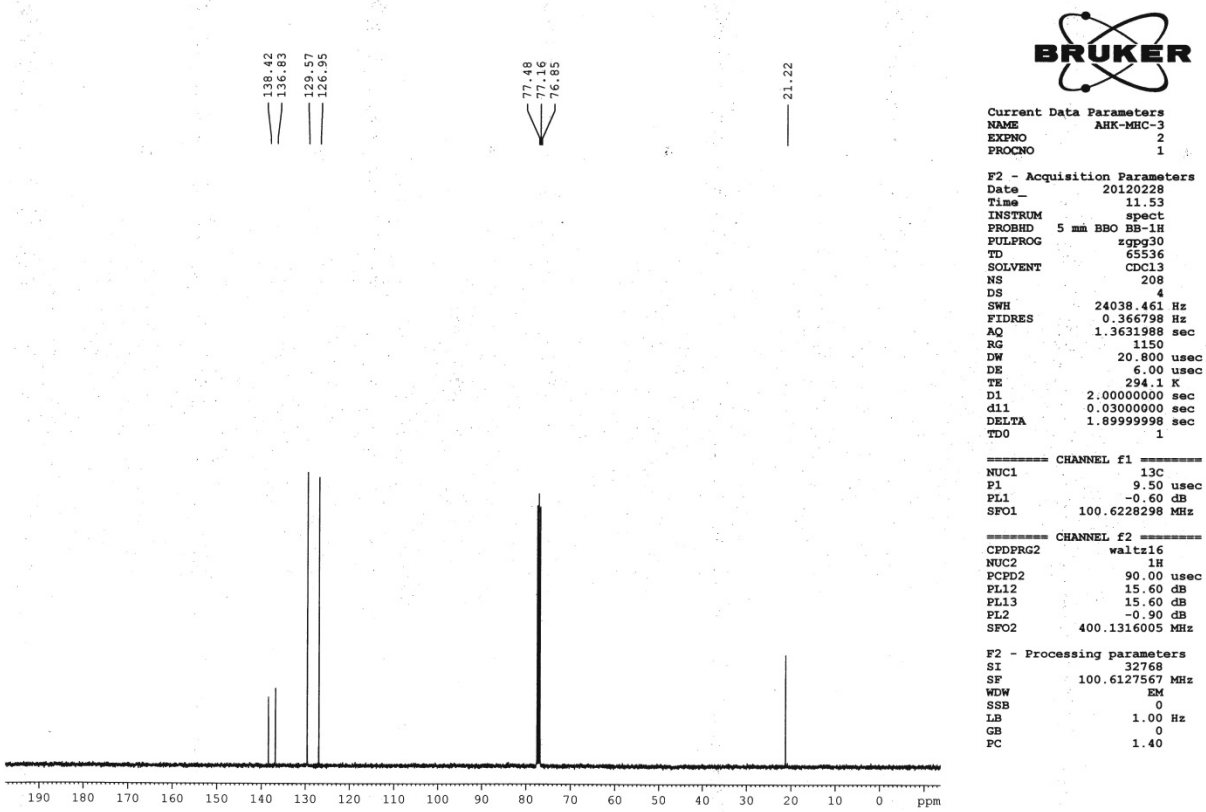


Fig. 19 100 MHz ^{13}C NMR Spectrum of 4,4'-dimethyl biphenyl in $CDCl_3$

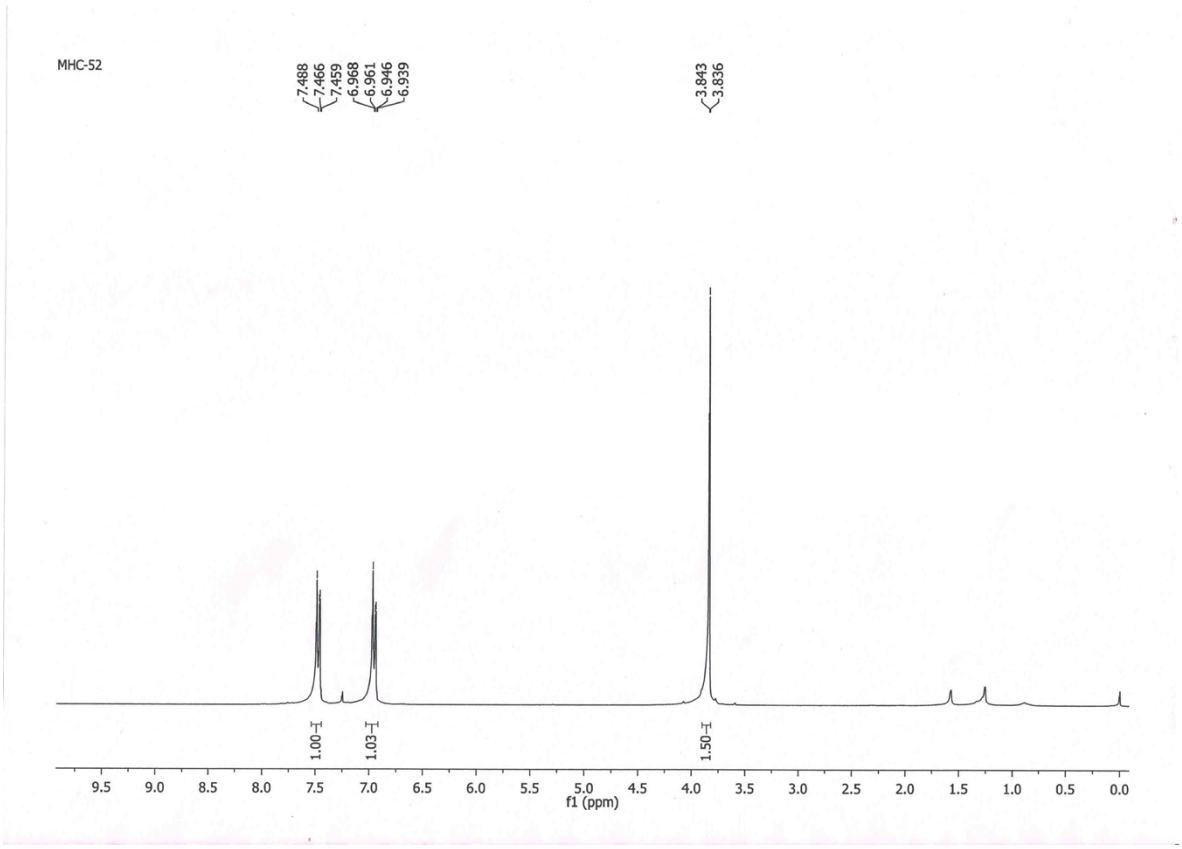


Fig. 20 400 MHz ^{1}H NMR Spectrum of 4,4'-dimethoxy biphenyl in $CDCl_3$

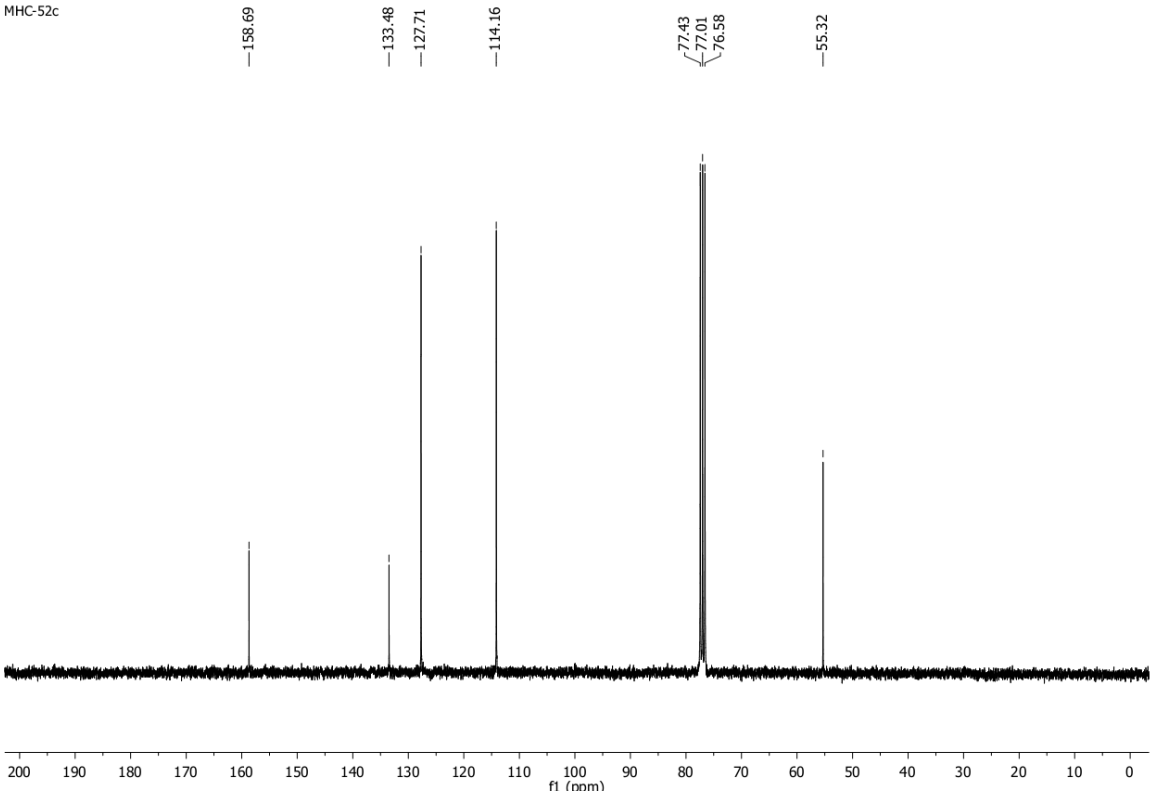


Fig. 21 75 MHz ^{13}C NMR Spectrum of 4,4'-dimethoxy biphenyl in $CDCl_3$

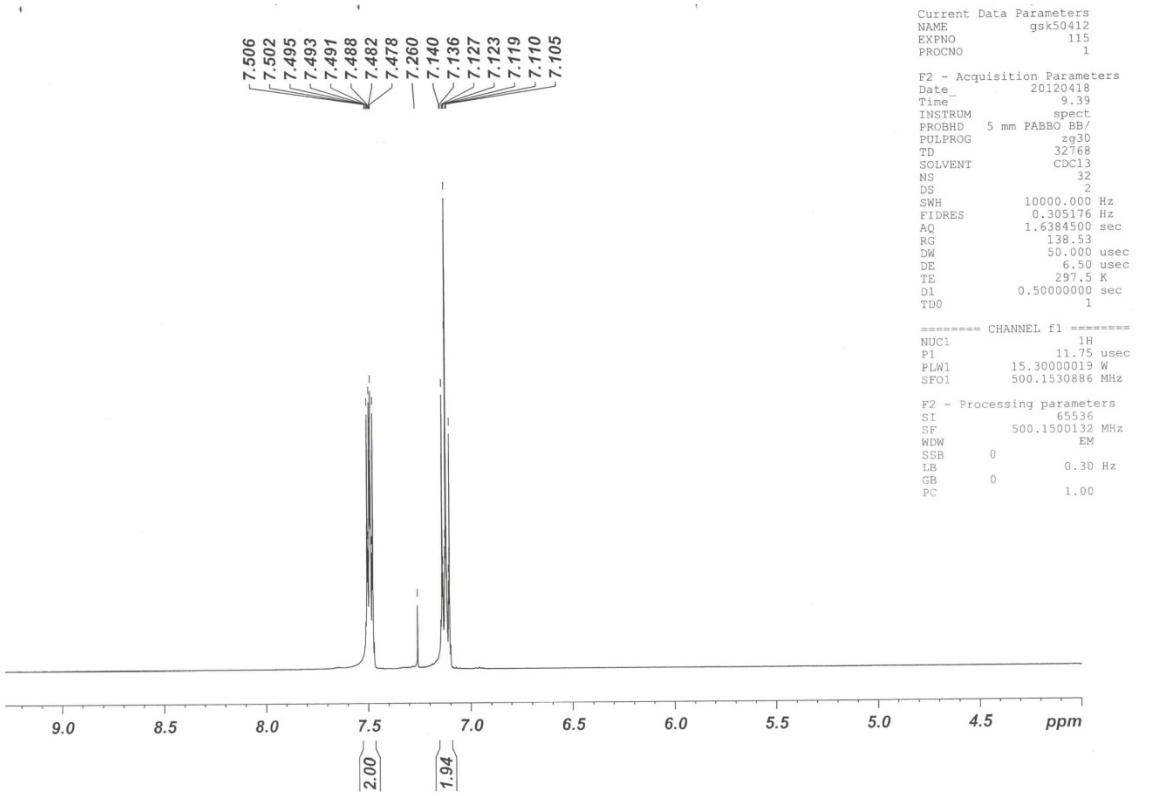


Fig. 22 500 MHz ^{1}H NMR Spectrum of 4,4'-difluoro biphenyl in $CDCl_3$

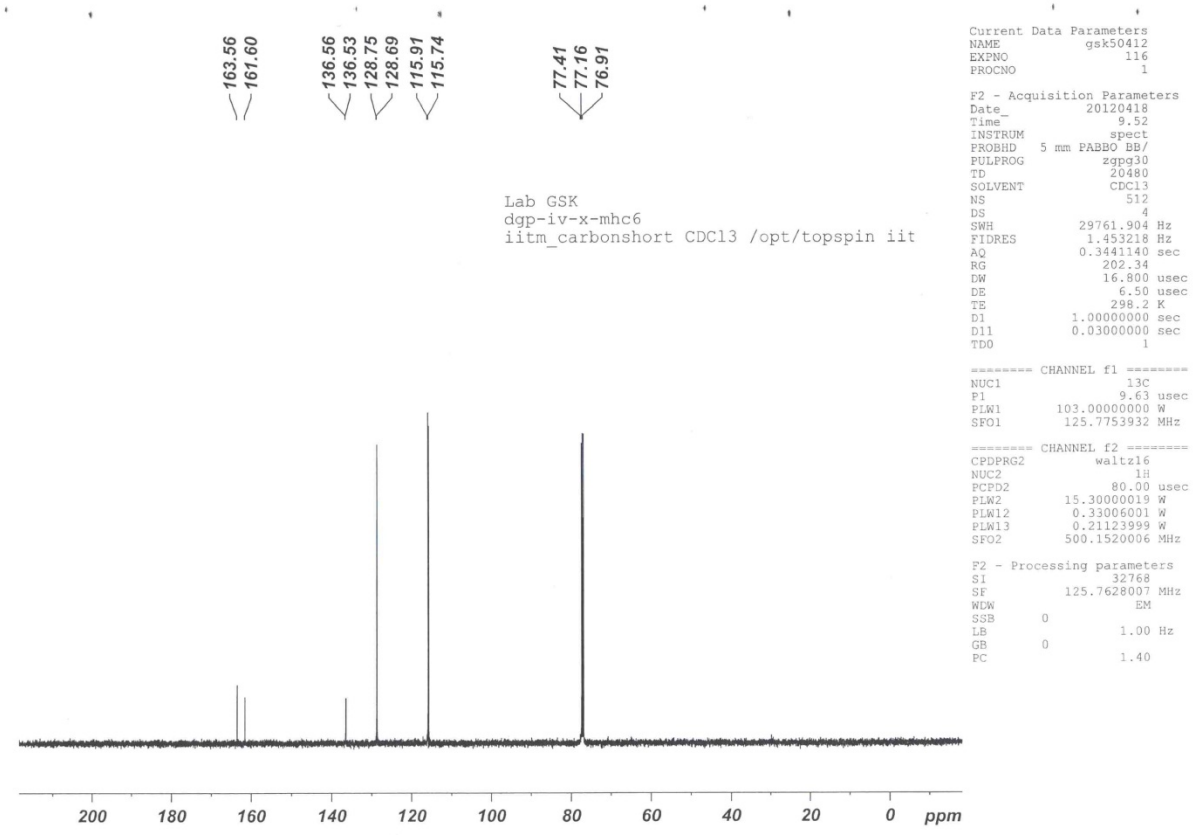


Fig. 23 125 MHz ^{13}C NMR Spectrum of 4,4'-difluoro biphenyl in $CDCl_3$

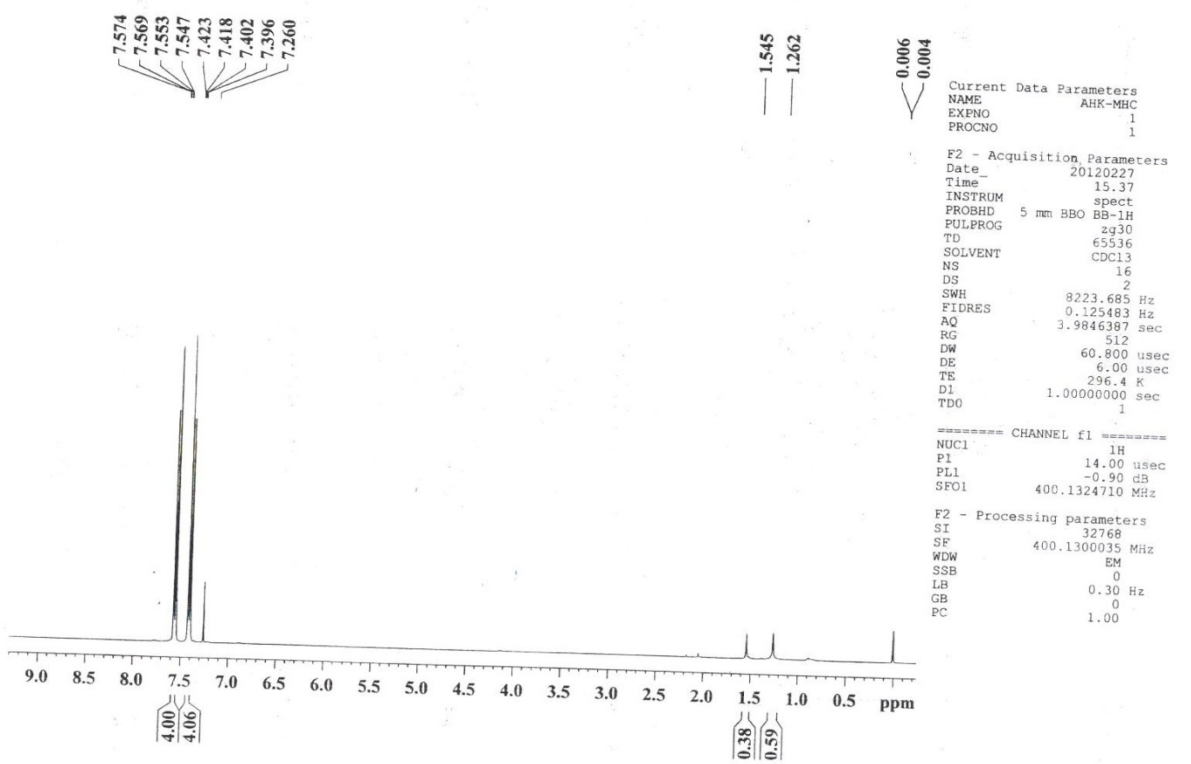


Fig. 24 400 MHz ^{1}H NMR Spectrum of 4,4'-dibromo biphenyl in $CDCl_3$

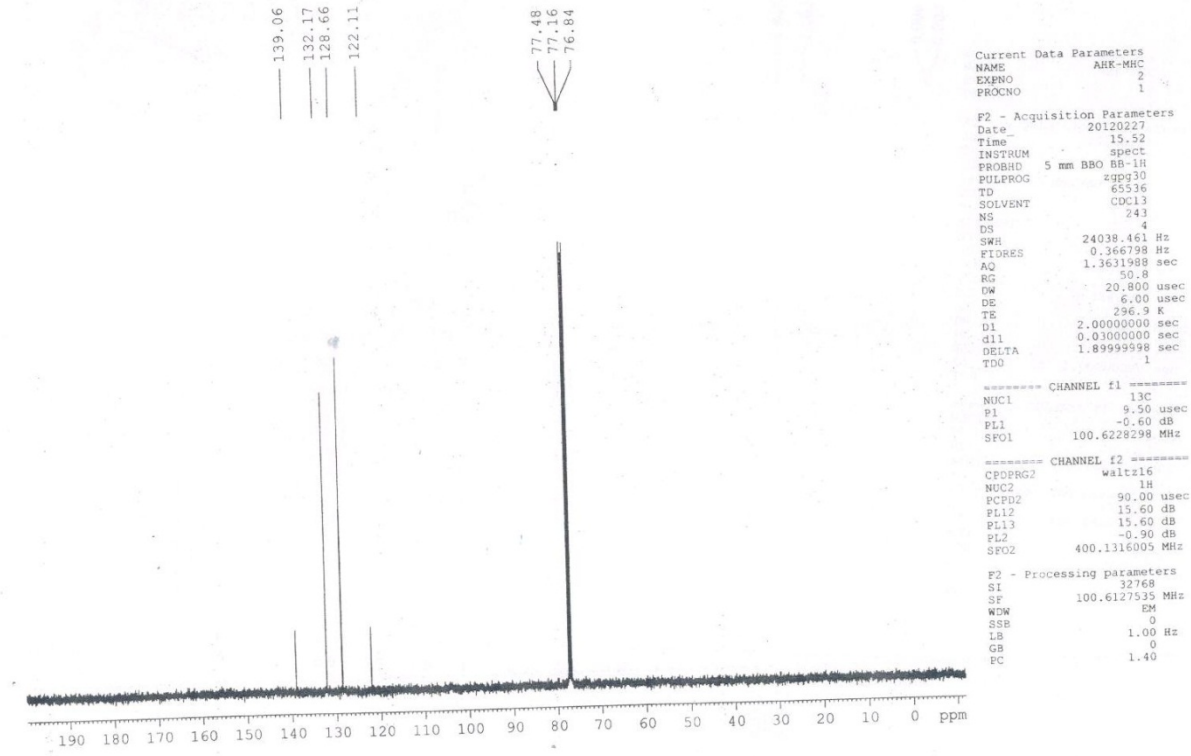


Fig. 25 100 MHz ^{13}C NMR Spectrum of 4,4'-dibromo biphenyl in $CDCl_3$

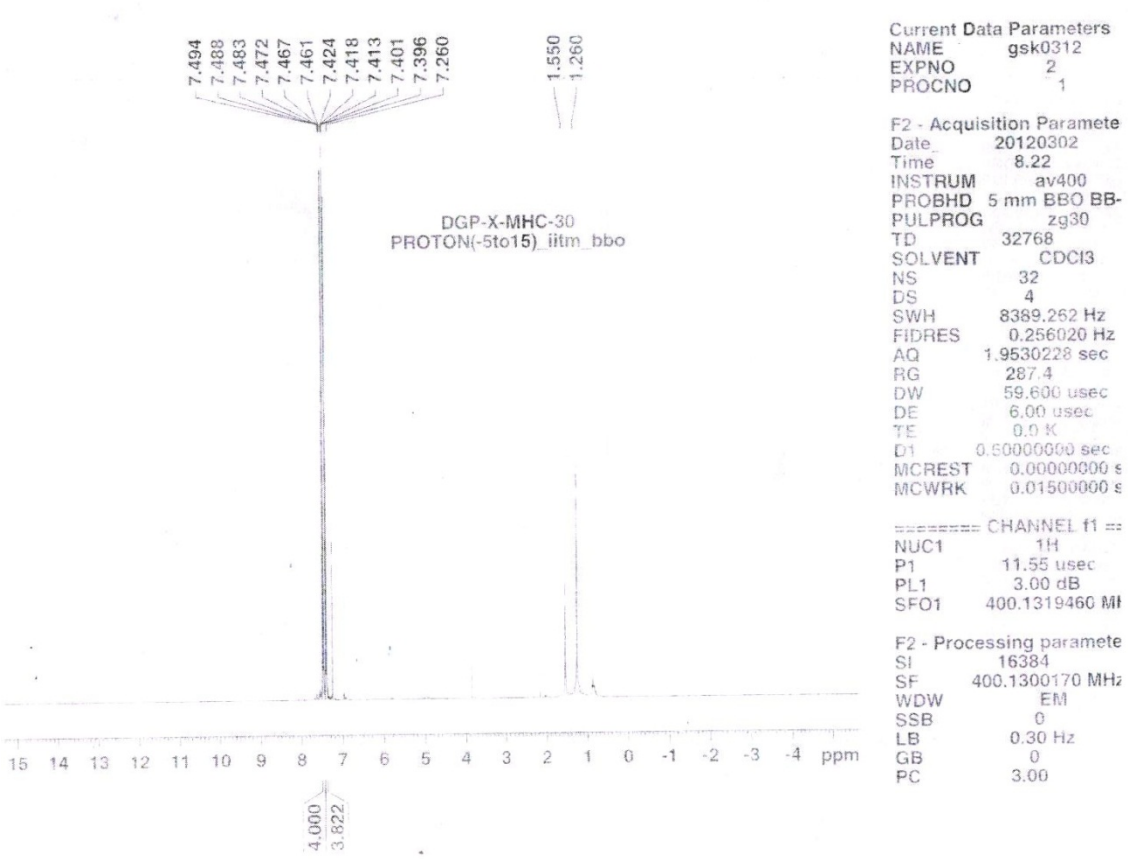


Fig. 26 400 MHz ^{1}H NMR Spectrum of 4,4'-dichloro biphenyl in $CDCl_3$

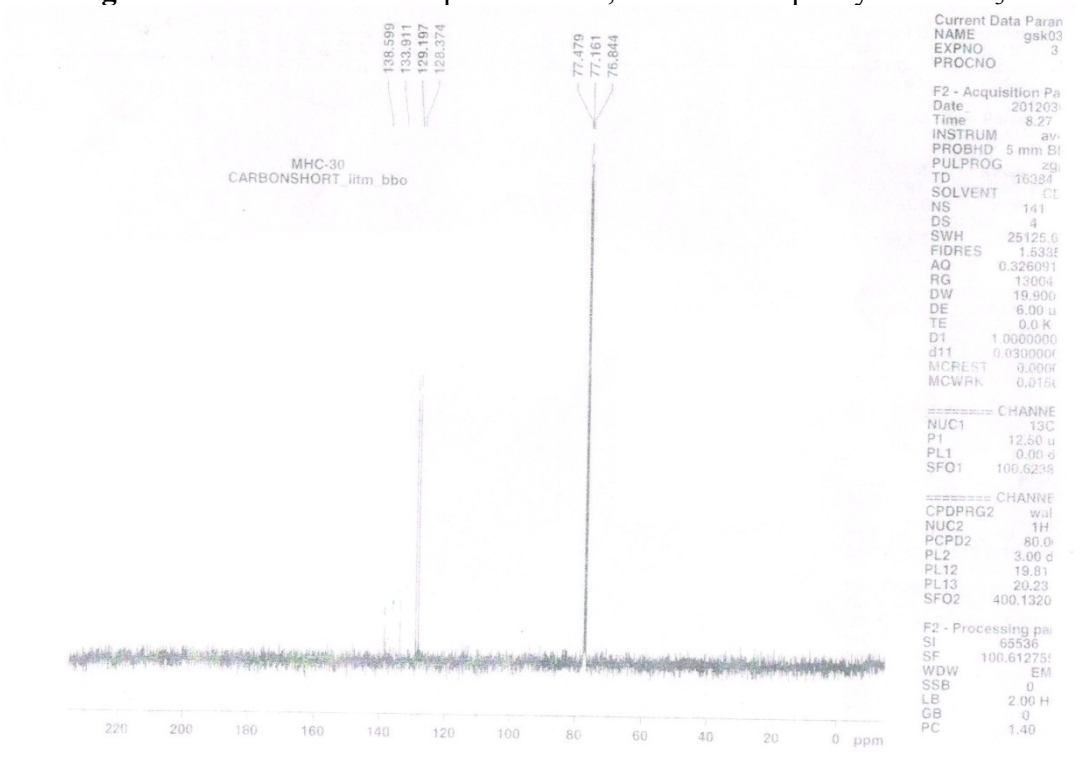


Fig. 27 100 MHz ^{13}C NMR Spectrum of 4,4'-dichloro biphenyl in $CDCl_3$

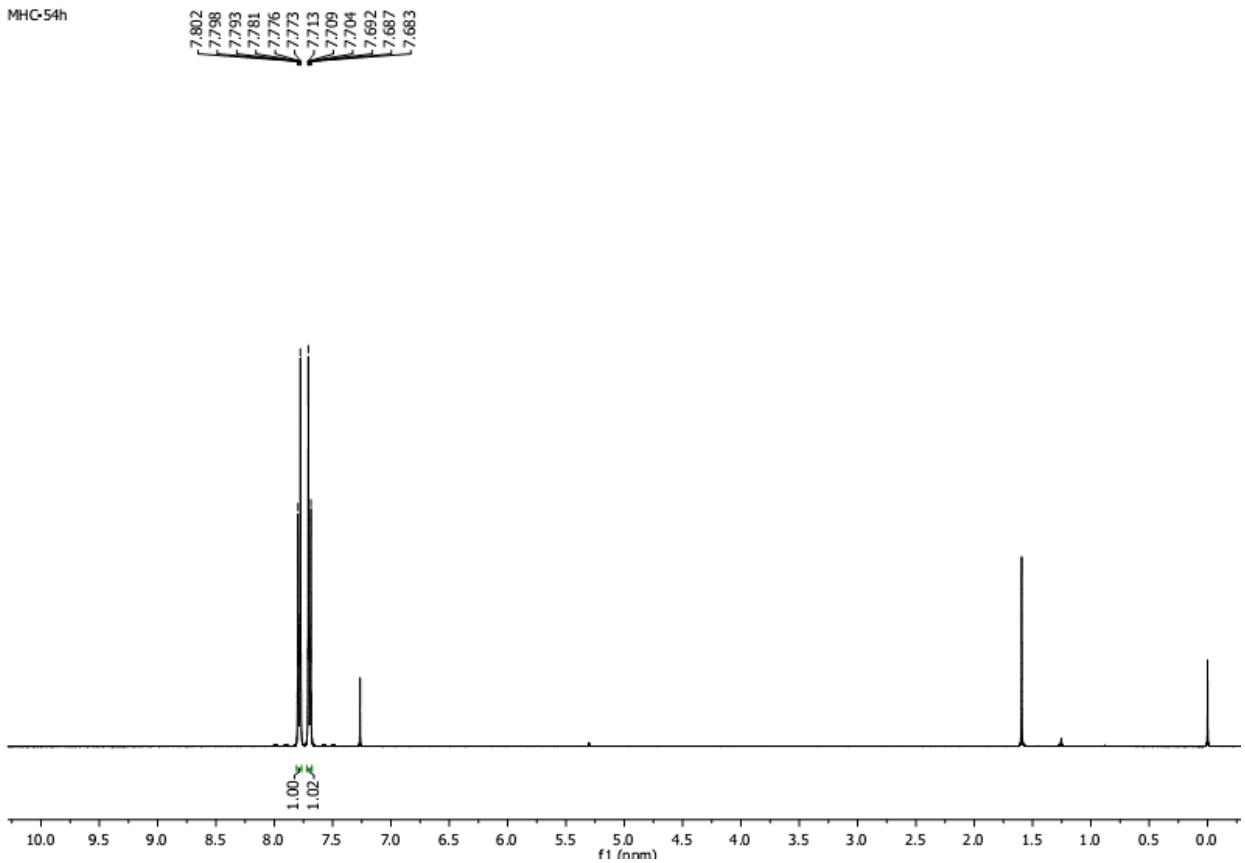


Fig. 28 400 MHz ^{1}H NMR Spectrum of 4,4'-dicyano biphenyl in $CDCl_3$

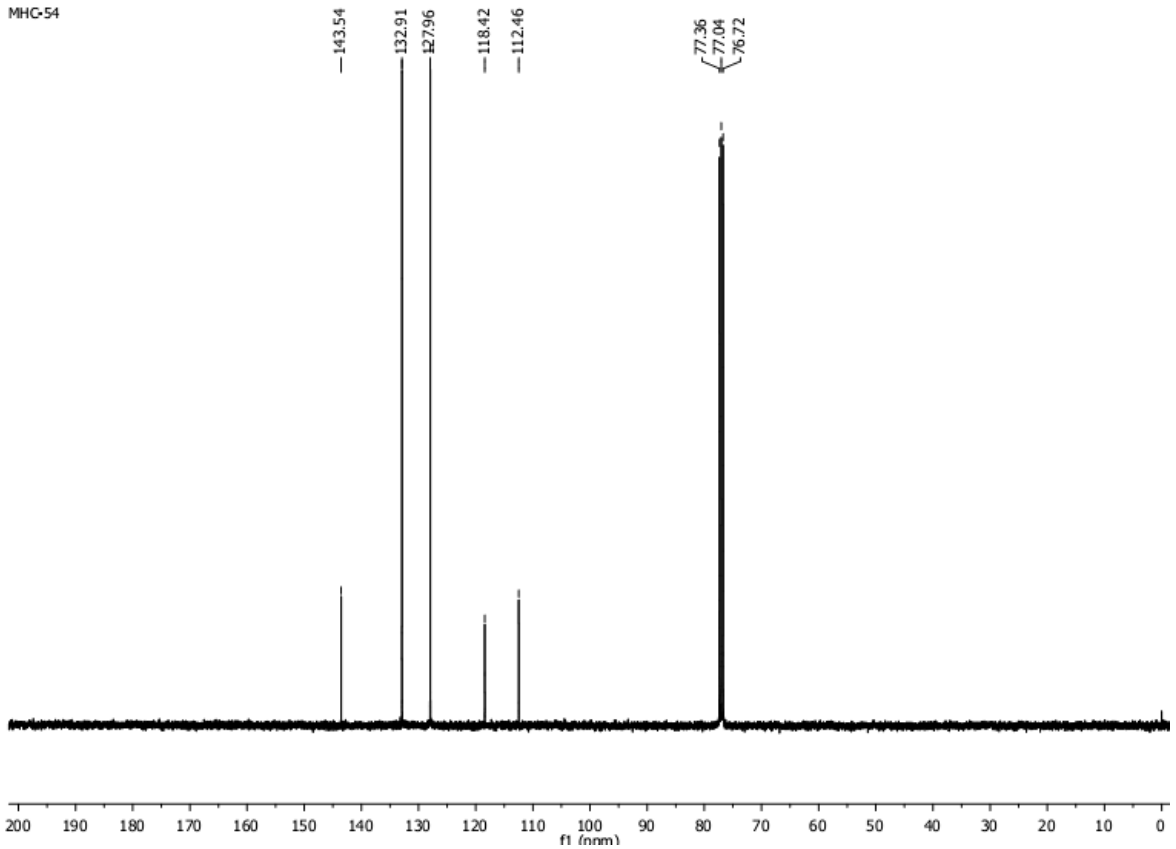


Fig. 29 100 MHz ^{13}C NMR Spectrum of 4,4'-dicyano biphenyl in $CDCl_3$

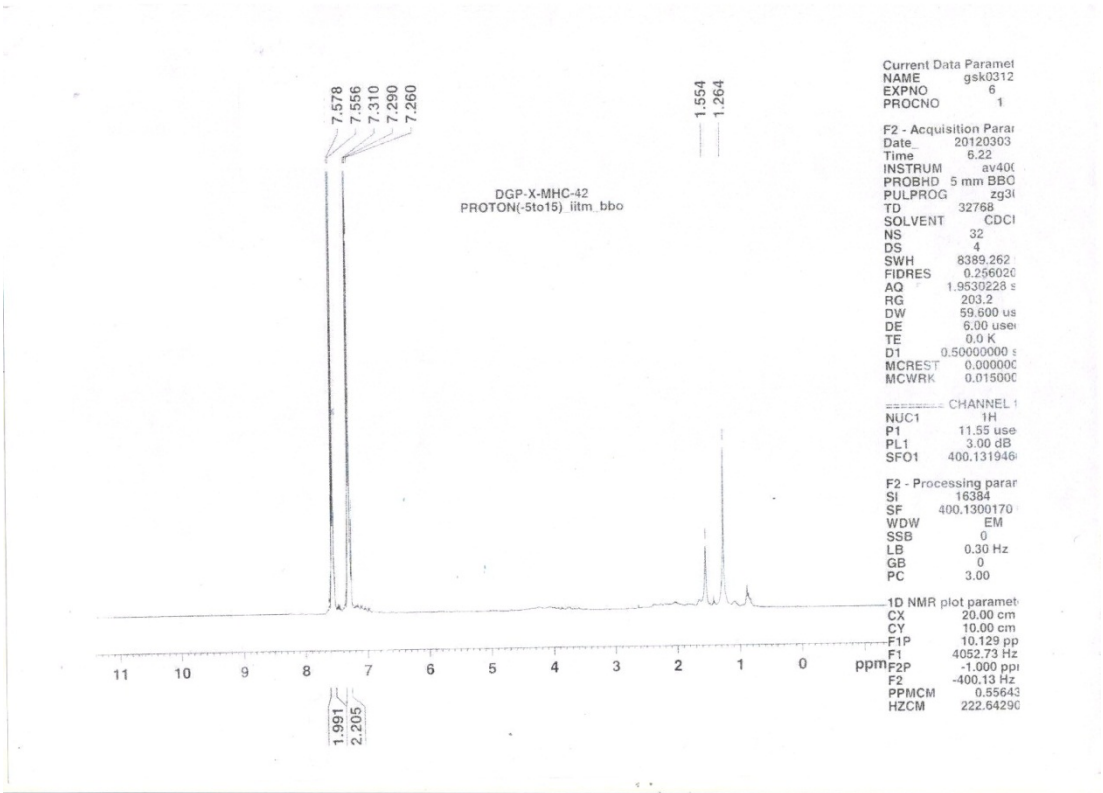


Fig. 30 400 MHz ^{1}H NMR Spectrum of 4,4'-di-(trifluoromethoxy) biphenyl in $CDCl_3$

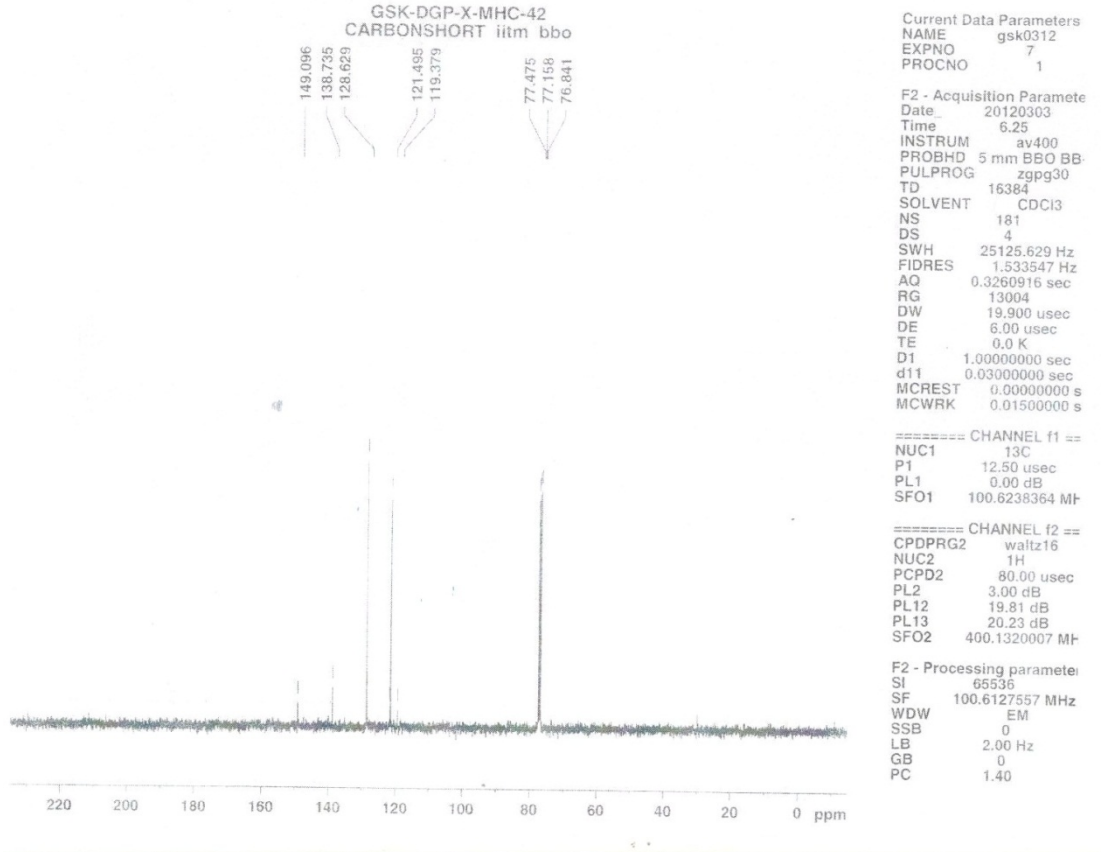


Fig. 31 100 MHz ^{13}C NMR Spectrum of 4,4'-di-(trifluoromethoxy) biphenyl in $CDCl_3$

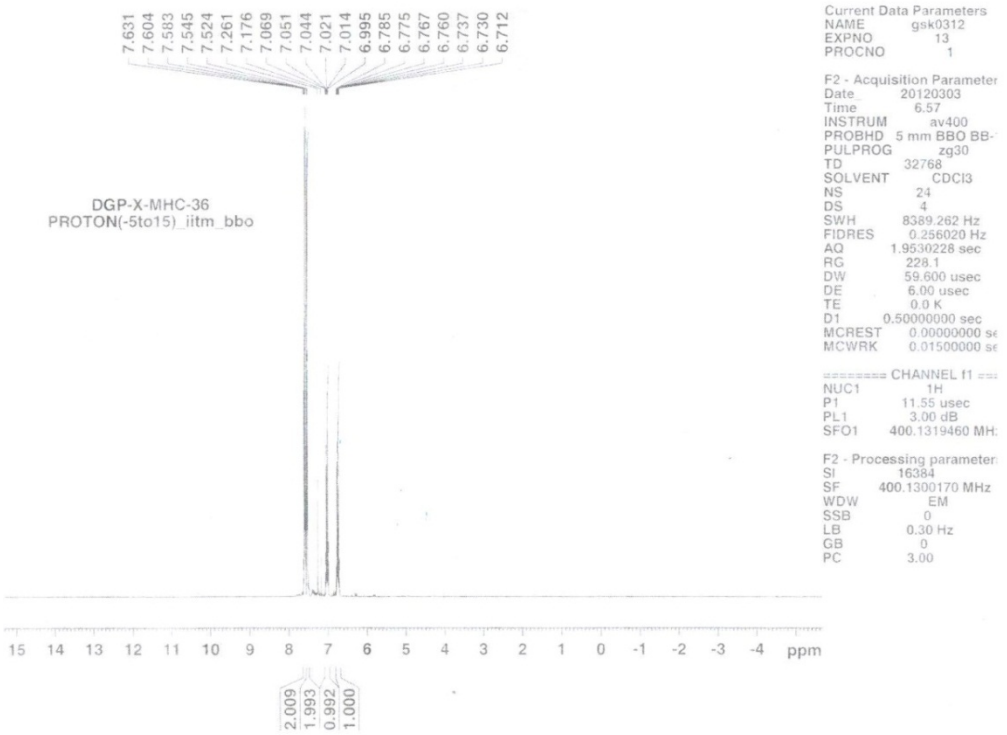


Fig. 32 400 MHz ^{1}H NMR Spectrum of 1,1'-(1*E*,3*E*)-1,3-butadiene-1,4-diylbis[4-(trifluoromethyl)- Benzene in $CDCl_3$

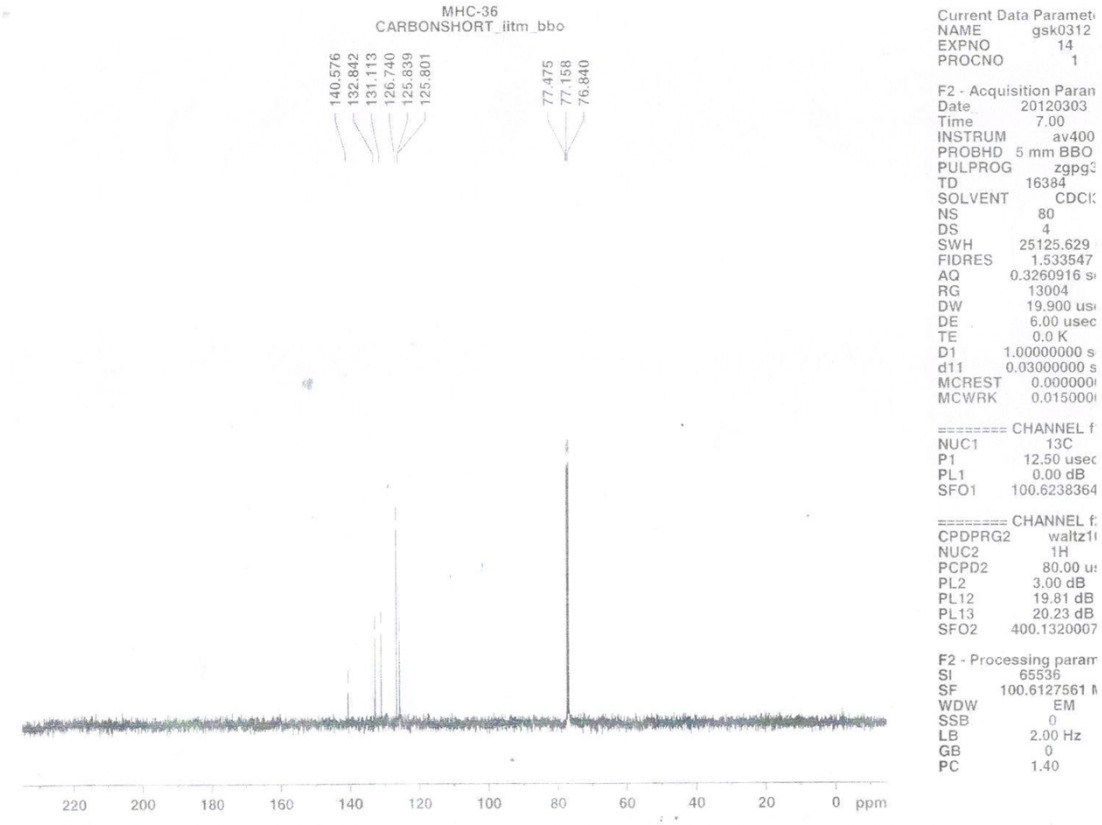


Fig. 33 100 MHz ^{13}C NMR Spectrum of 1,1'-(1*E*,3*E*)-1,3-butadiene-1,4-diylbis[4-(trifluoromethyl)- Benzene in $CDCl_3$

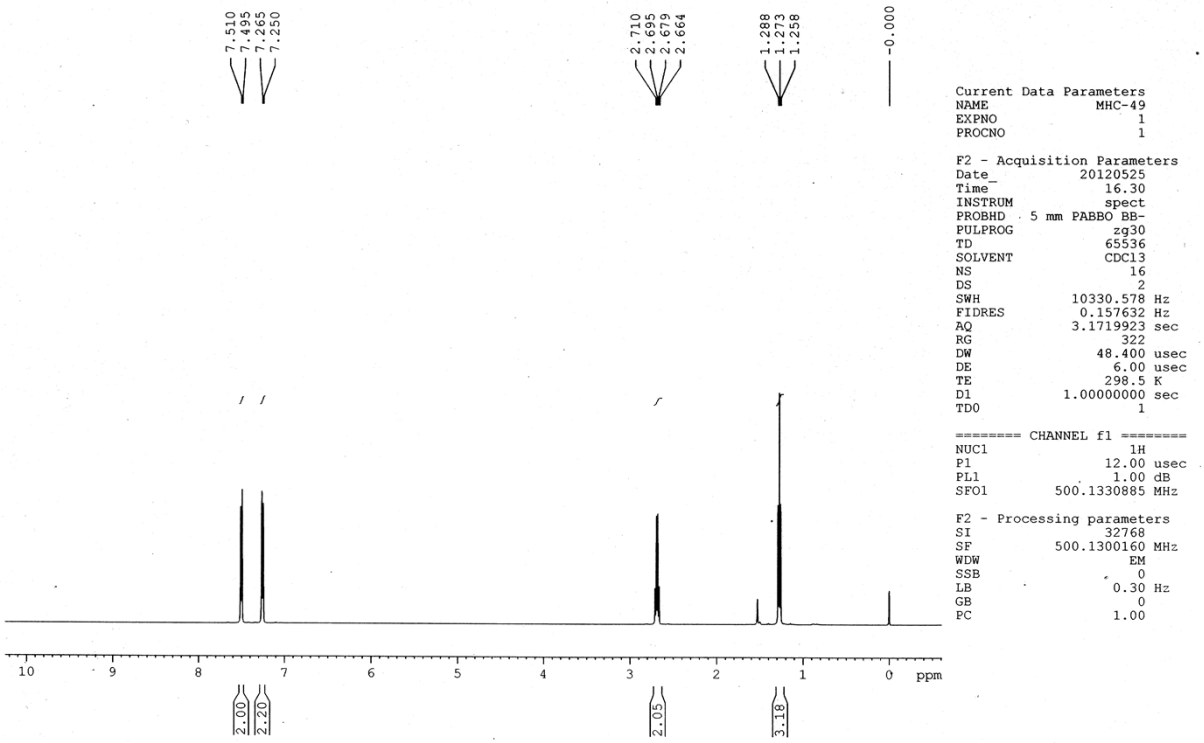


Fig. 34 500 MHz ^{1}H NMR Spectrum of 4,4'-diethyl biphenyl

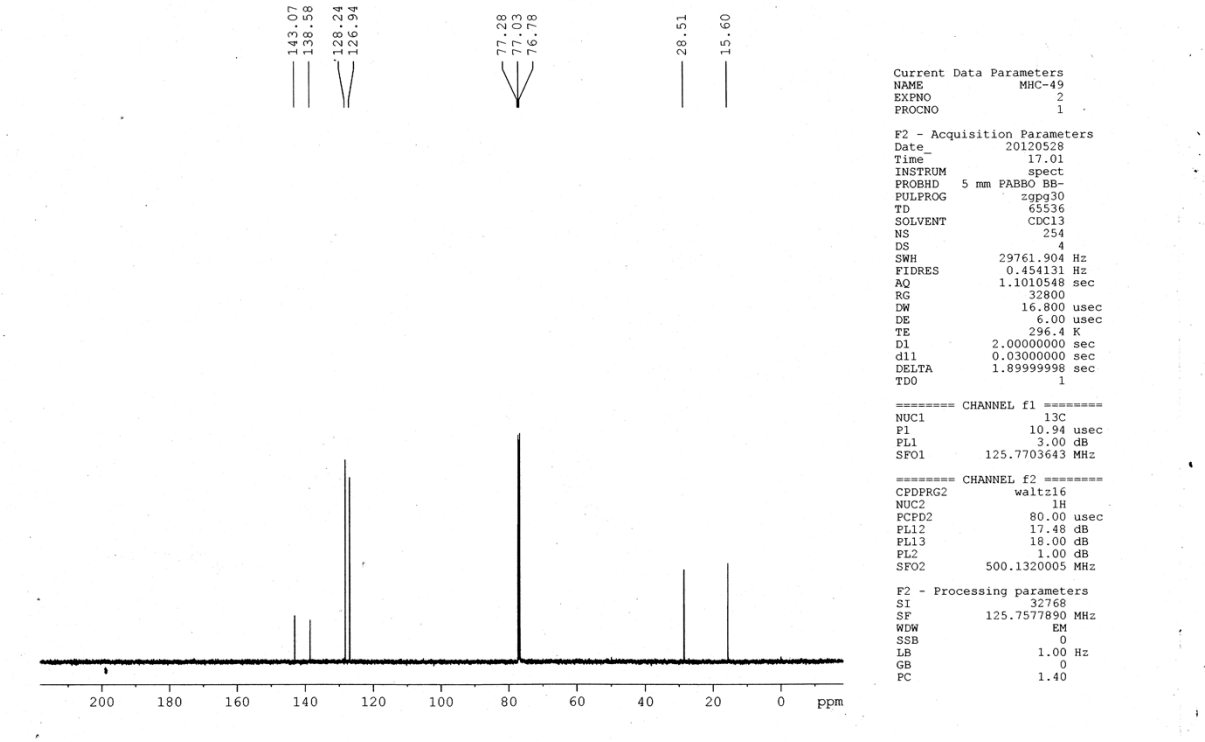


Fig. 35 125 MHz ^{13}C NMR Spectrum of 4,4'-diethyl biphenyl in $CDCl_3$

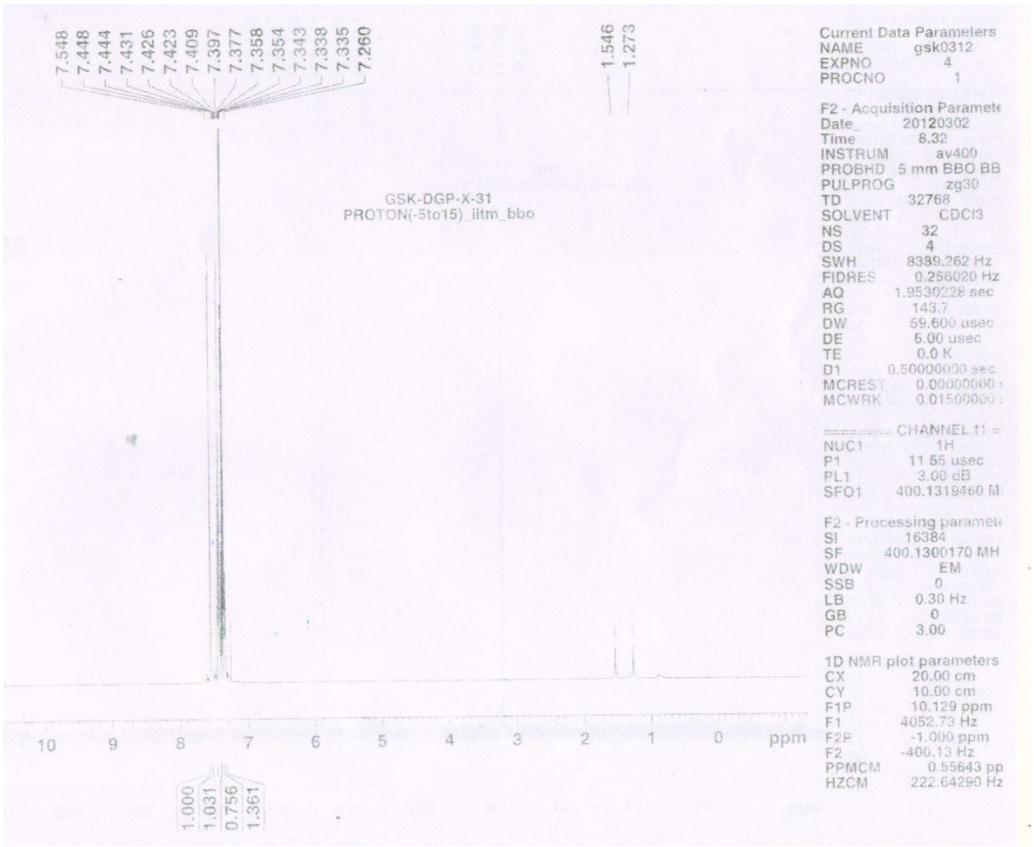


Fig. 36 400 MHz ^{1}H NMR Spectrum of 3,3'-dichloro biphenyl in $CDCl_3$

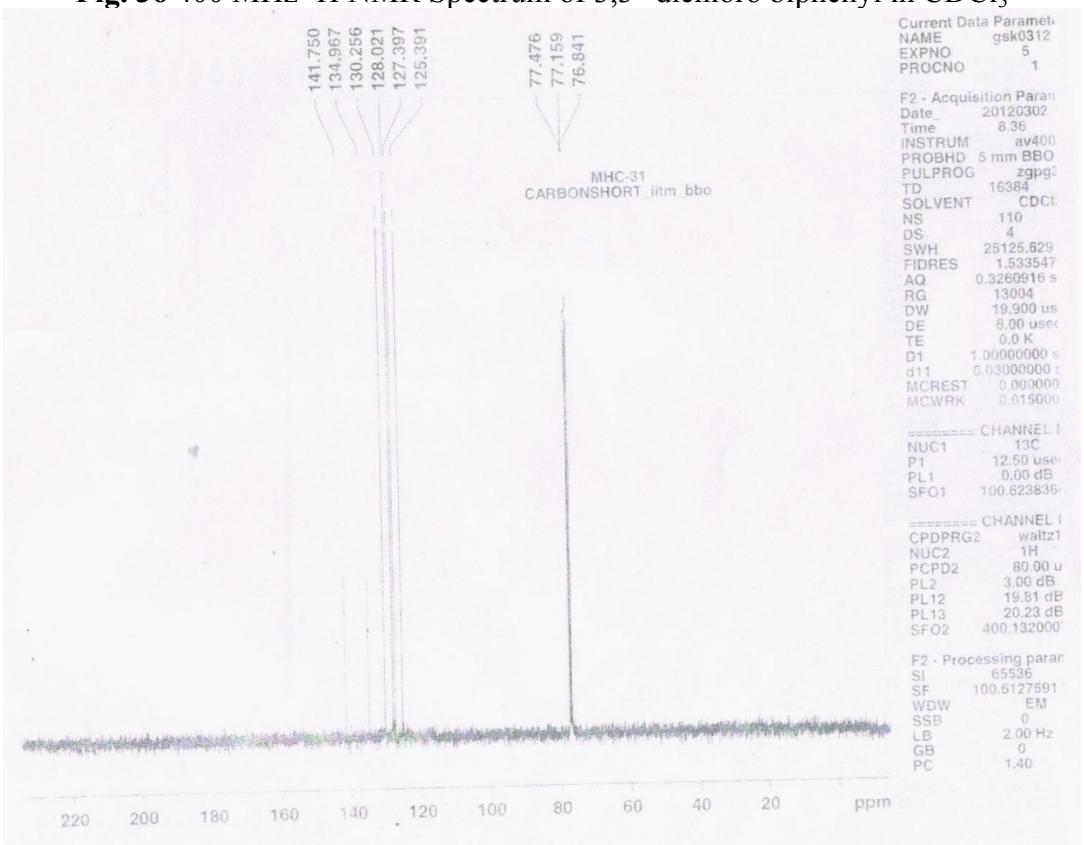


Fig. 37 100 MHz ^{13}C NMR Spectrum of 3,3'-dichloro biphenyl in $CDCl_3$

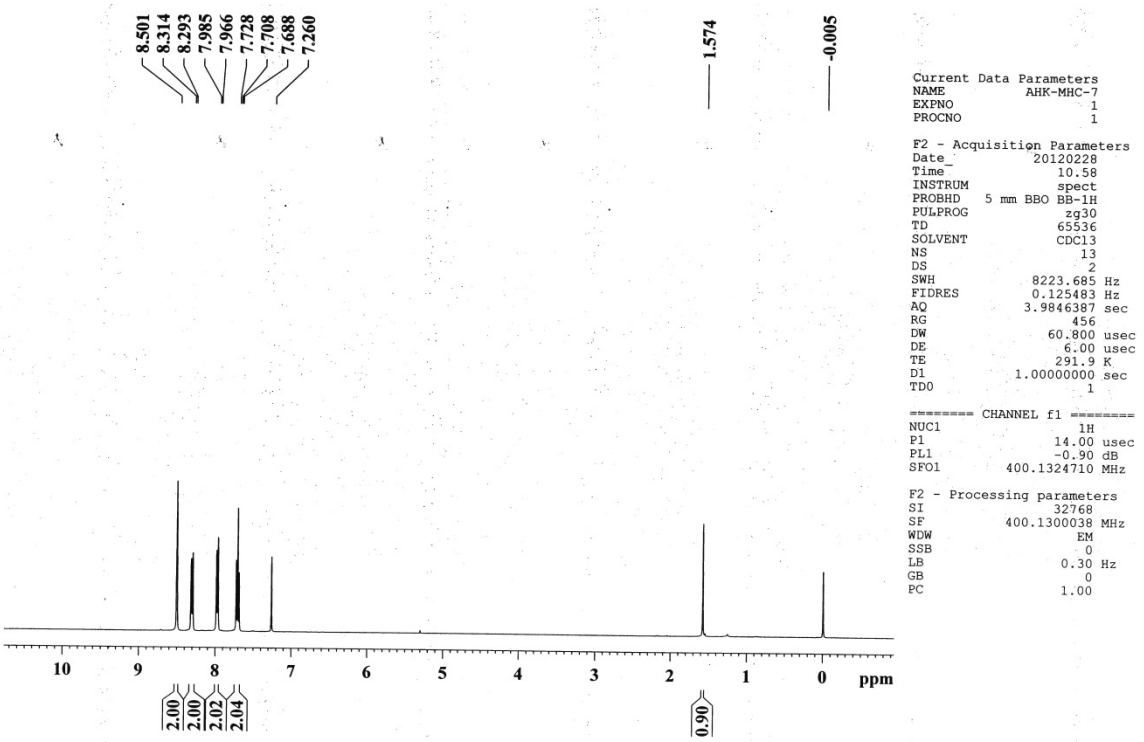


Fig. 38 400 MHz ^{1}H NMR Spectrum of 3,3'-dinitro biphenyl in $CDCl_3$

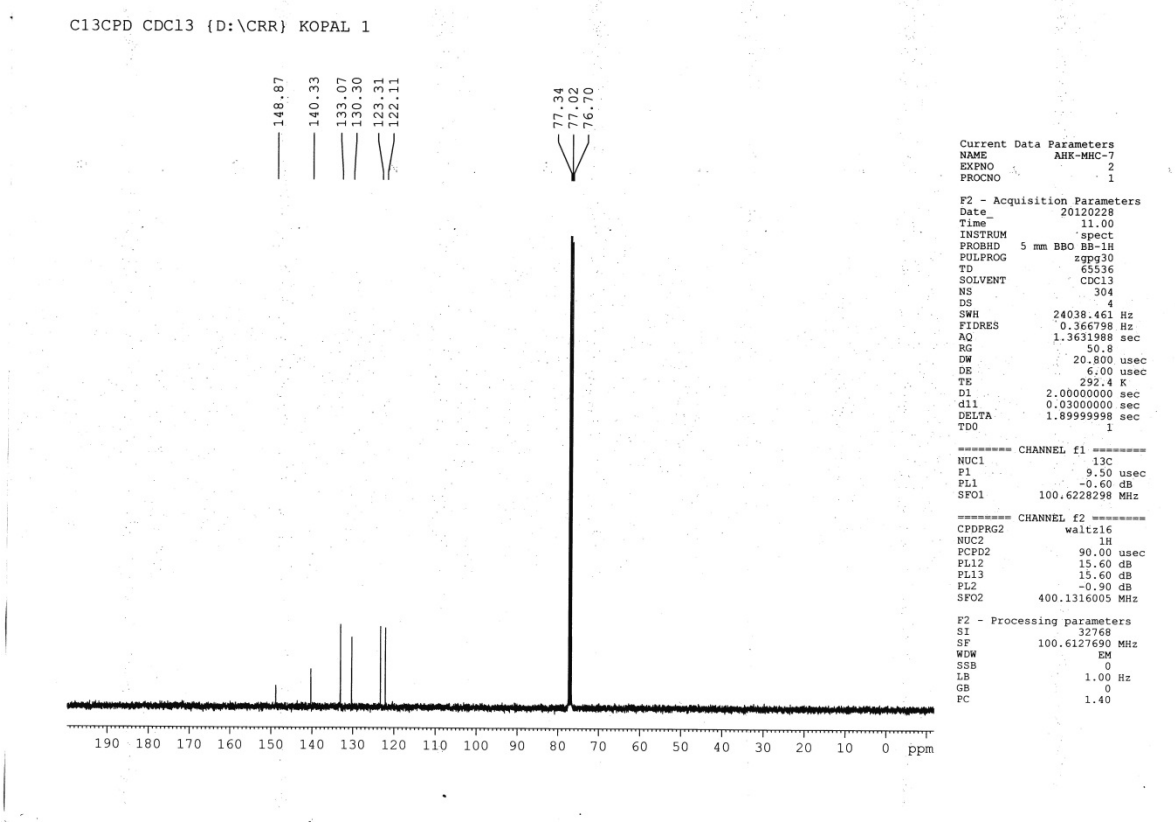


Fig. 39 100 MHz ^{13}C NMR Spectrum of 3,3'-dinitro biphenyl in $CDCl_3$

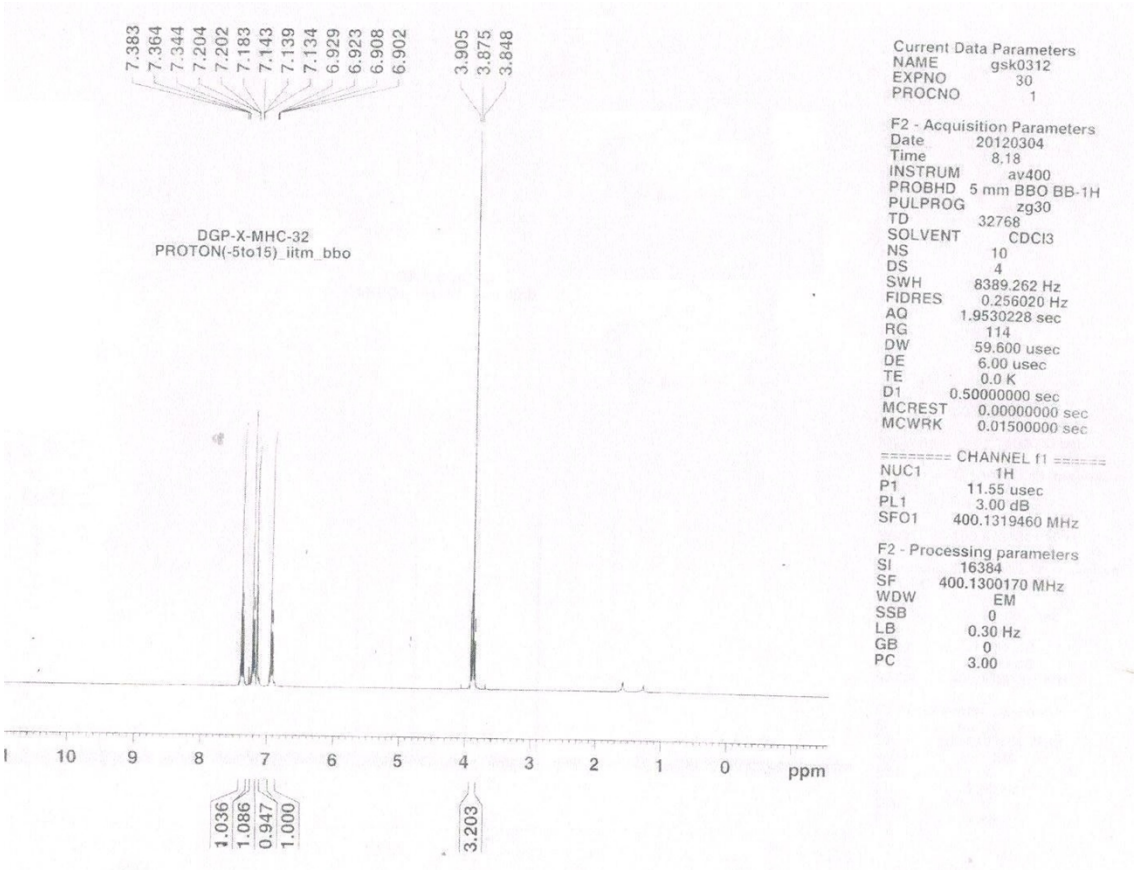


Fig. 40 400 MHz ^{1}H NMR Spectrum of 3,3'-dimethoxy biphenyl in $CDCl_3$

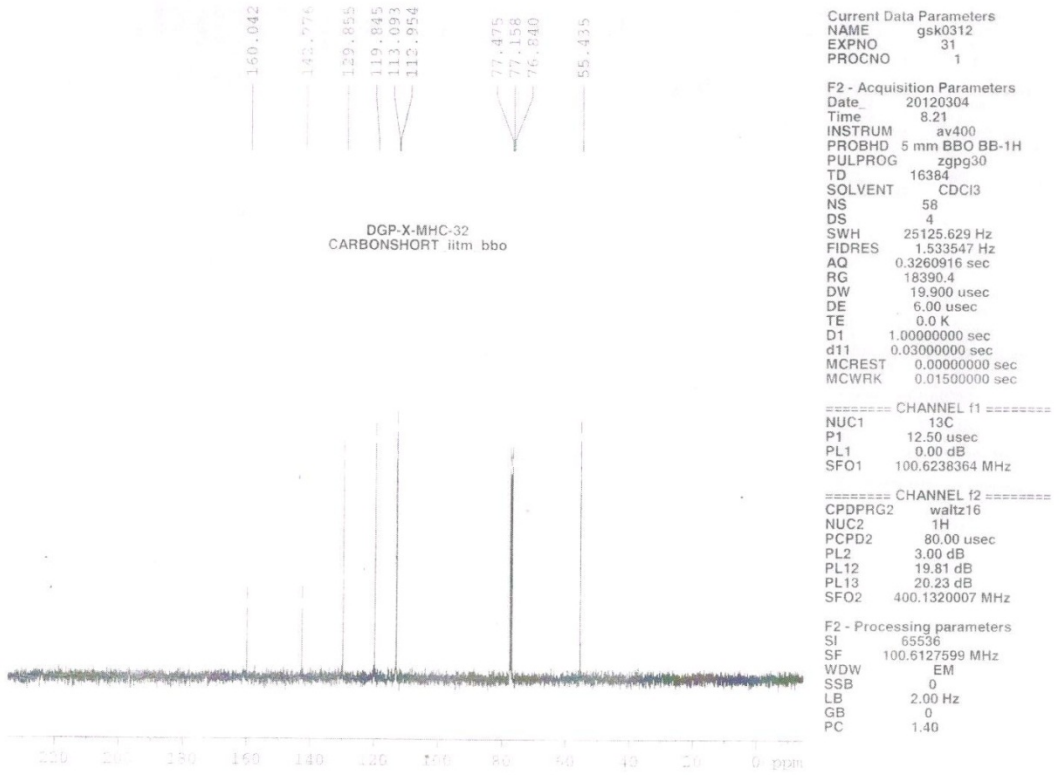


Fig. 41 100 MHz ^{13}C NMR Spectrum of 3,3'-dimethoxy biphenyl in $CDCl_3$

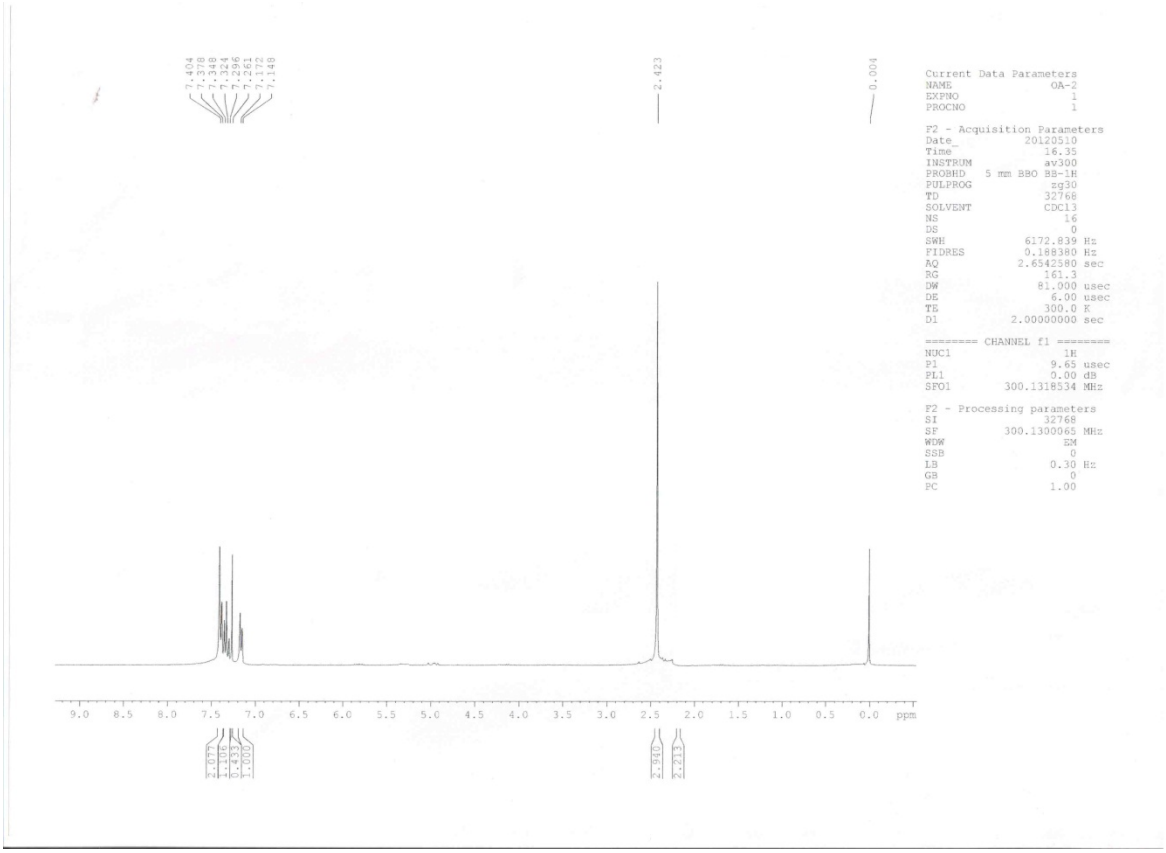


Fig. 42 300 MHz ^{1}H NMR Spectrum of 3,3'-dimethyl biphenyl in $CDCl_3$

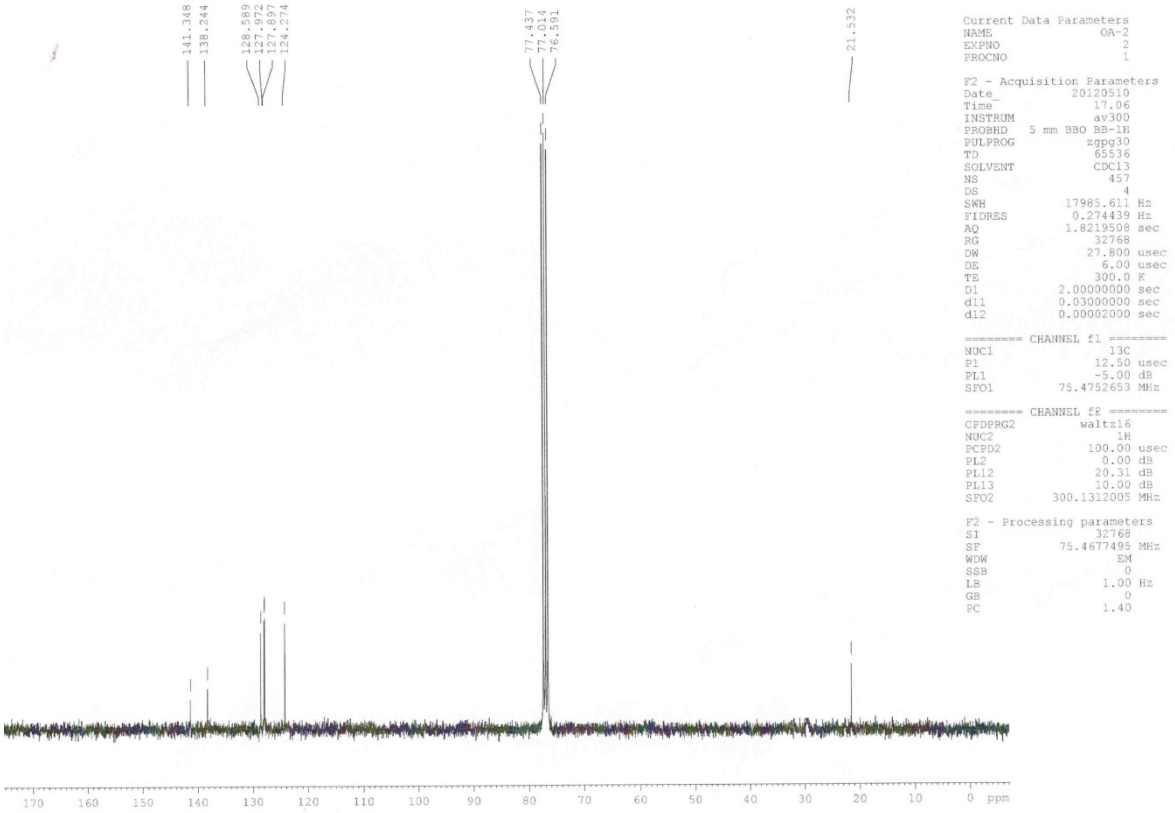


Fig. 43 75 MHz ^{13}C NMR Spectrum of 3,3'-dimethyl biphenyl in $CDCl_3$

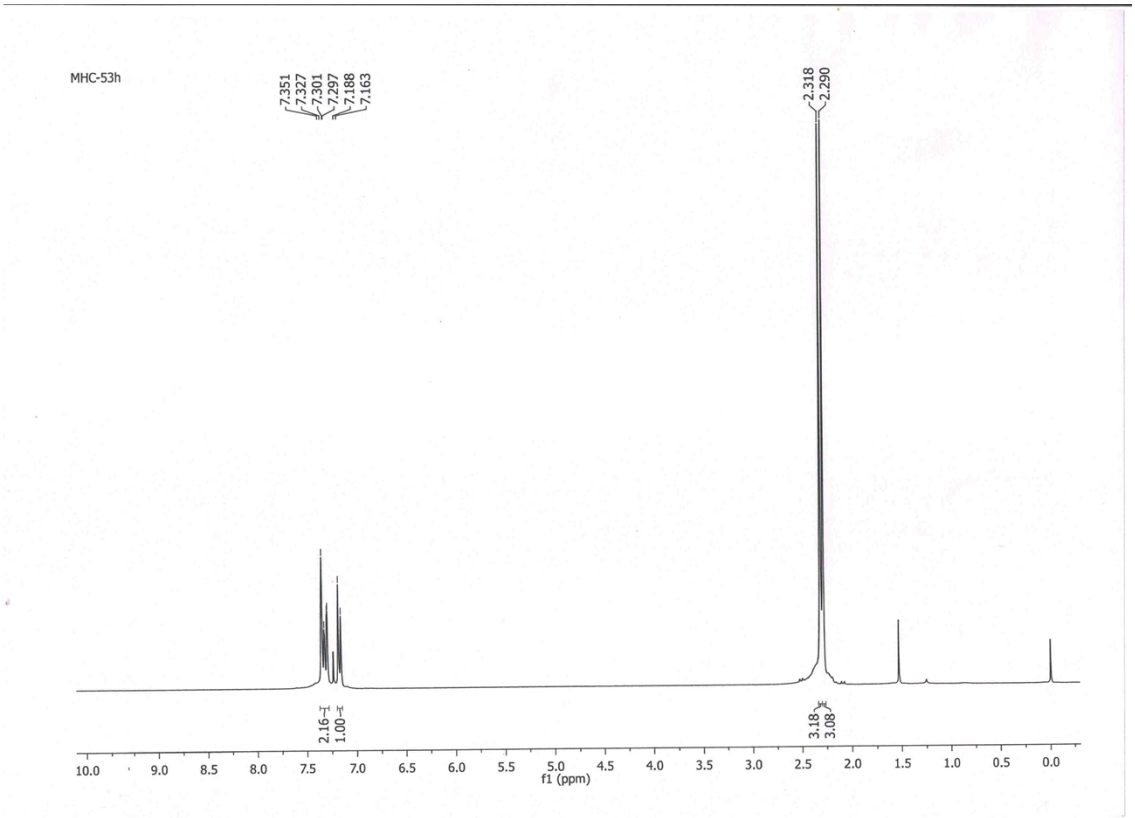


Fig. 44 300 MHz ^{1}H NMR Spectrum of 3,3',4,4'-tetramethyl biphenyl in $CDCl_3$

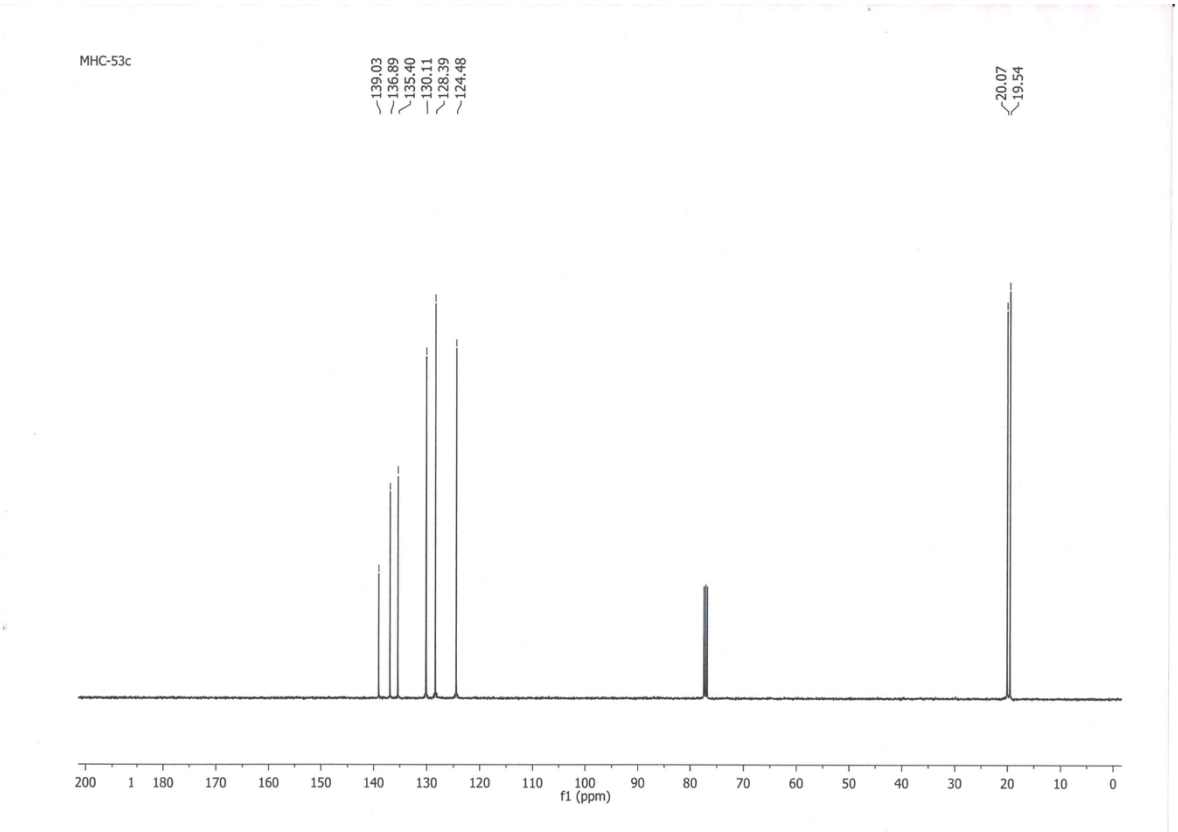


Fig. 45 100 MHz ^{13}C NMR Spectrum of 3,3',4,4'-tetramethyl biphenyl in $CDCl_3$

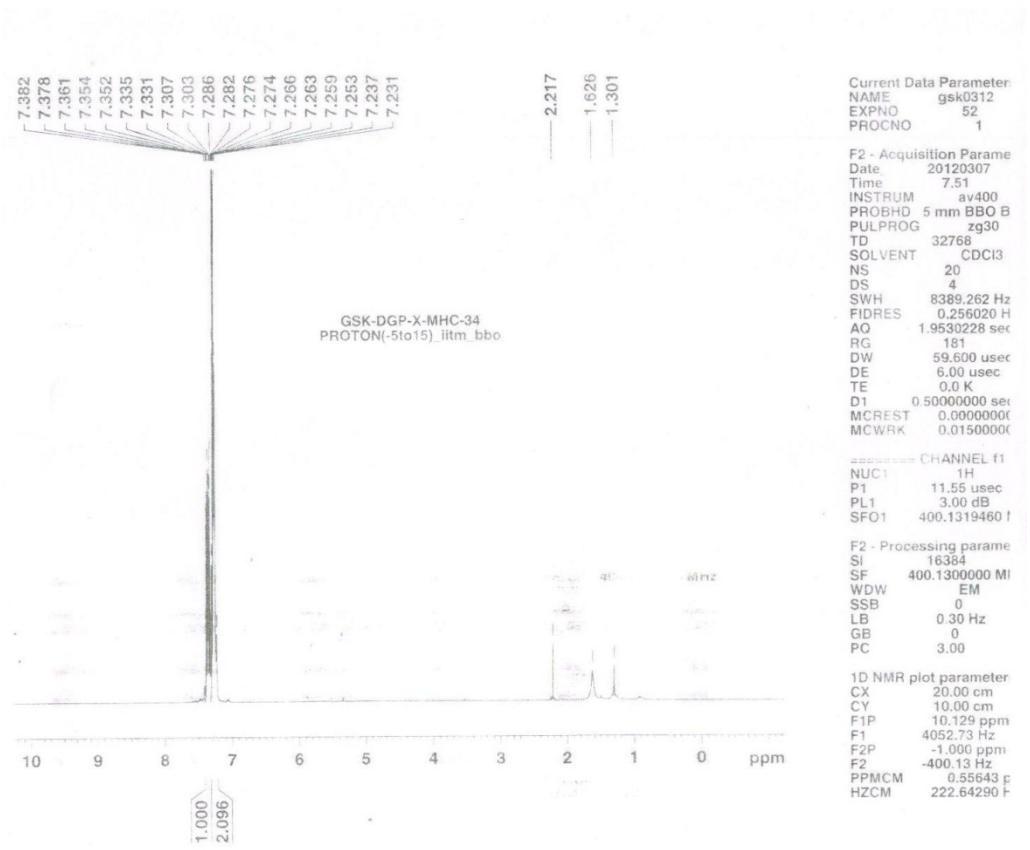


Fig. 46 400 MHz ^{1}H NMR Spectrum of 3,3',4,4'-tetrafluoro biphenyl in $CDCl_3$

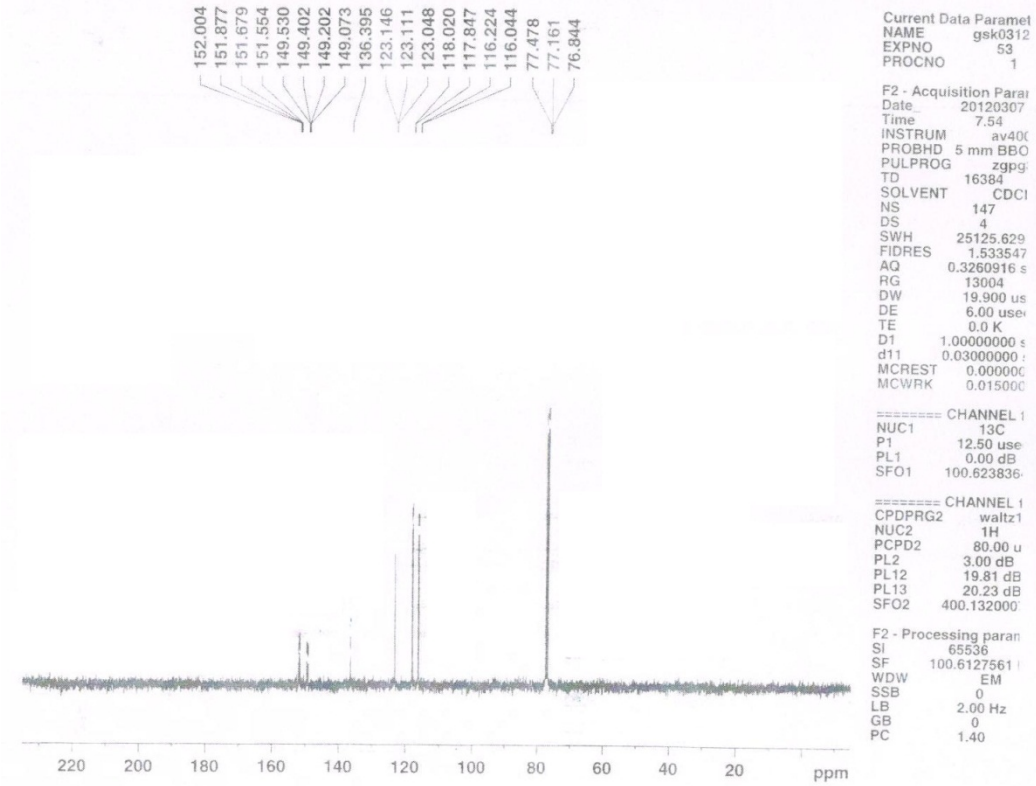


Fig. 47 100 MHz ^{13}C NMR Spectrum of 3,3',4,4'-tetrafluoro biphenyl in $CDCl_3$

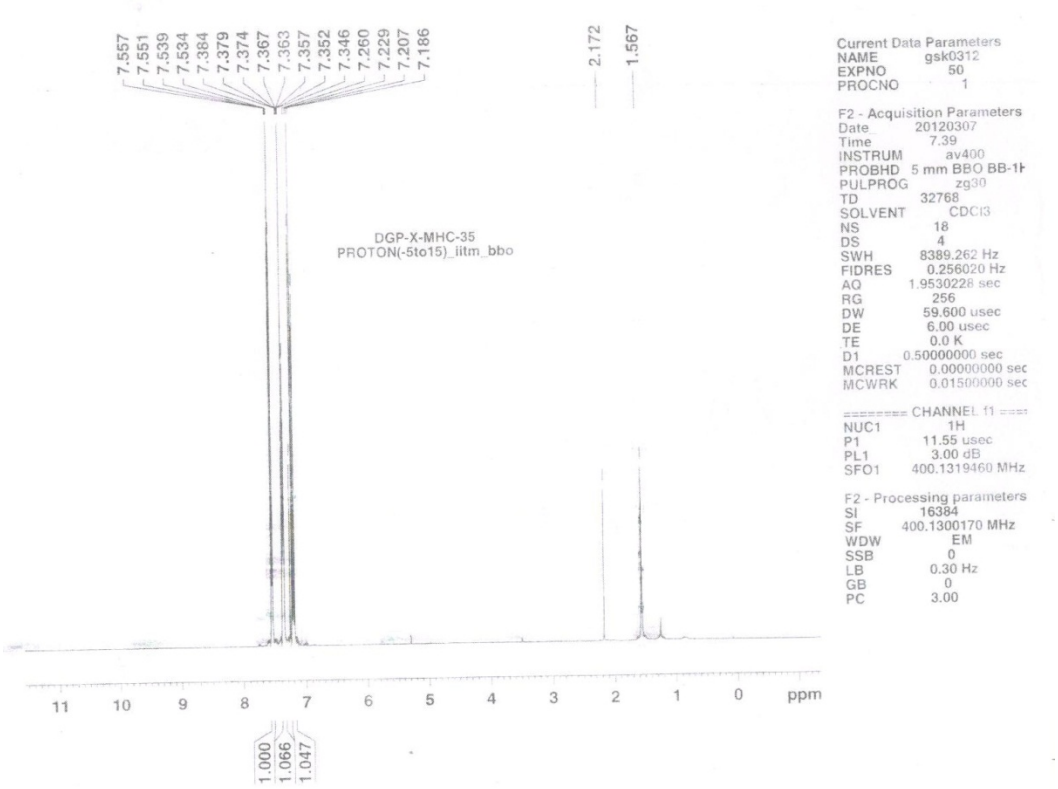


Fig. 48 400 MHz ^{1}H NMR Spectrum of 3,3'-dichloro-4,4'-difluoro biphenyl in $CDCl_3$

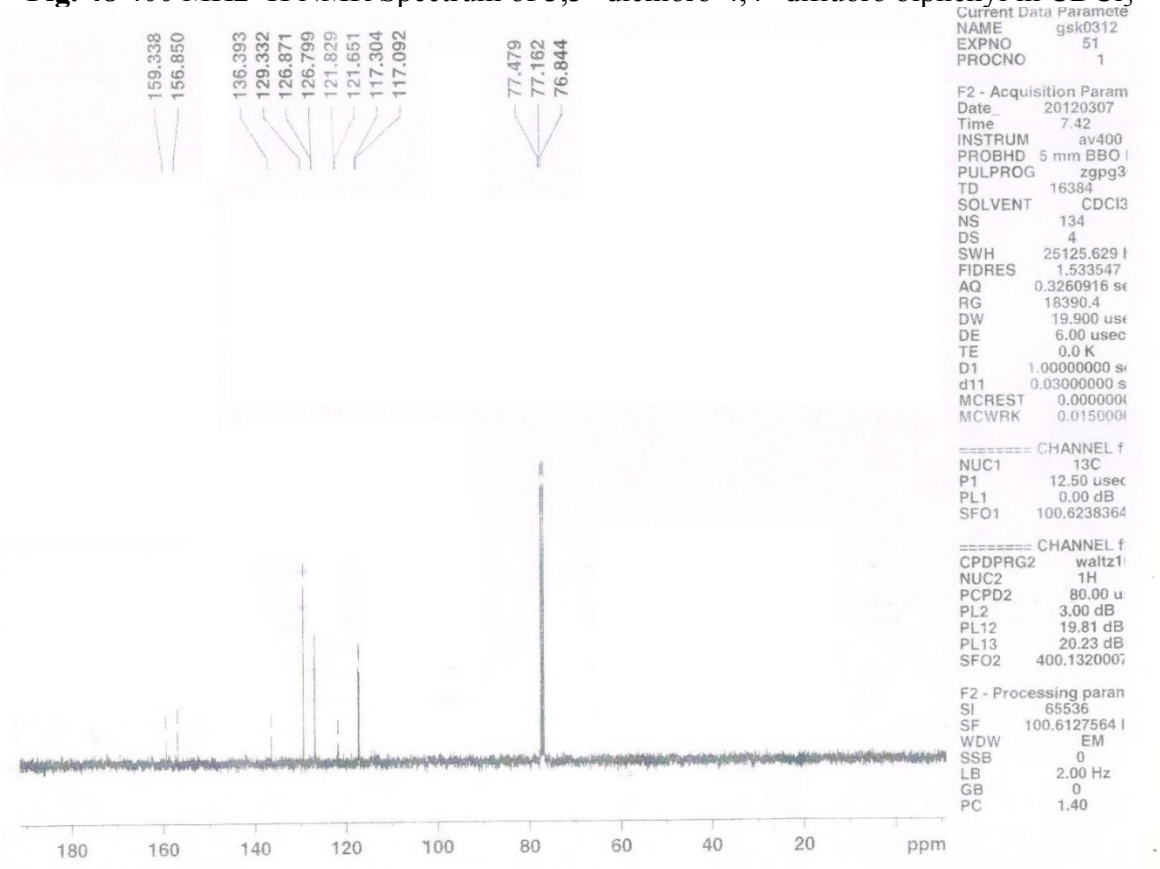


Fig. 49 100 MHz ^{13}C NMR Spectrum of 3,3'-dichloro-4,4'-difluoro biphenyl in $CDCl_3$

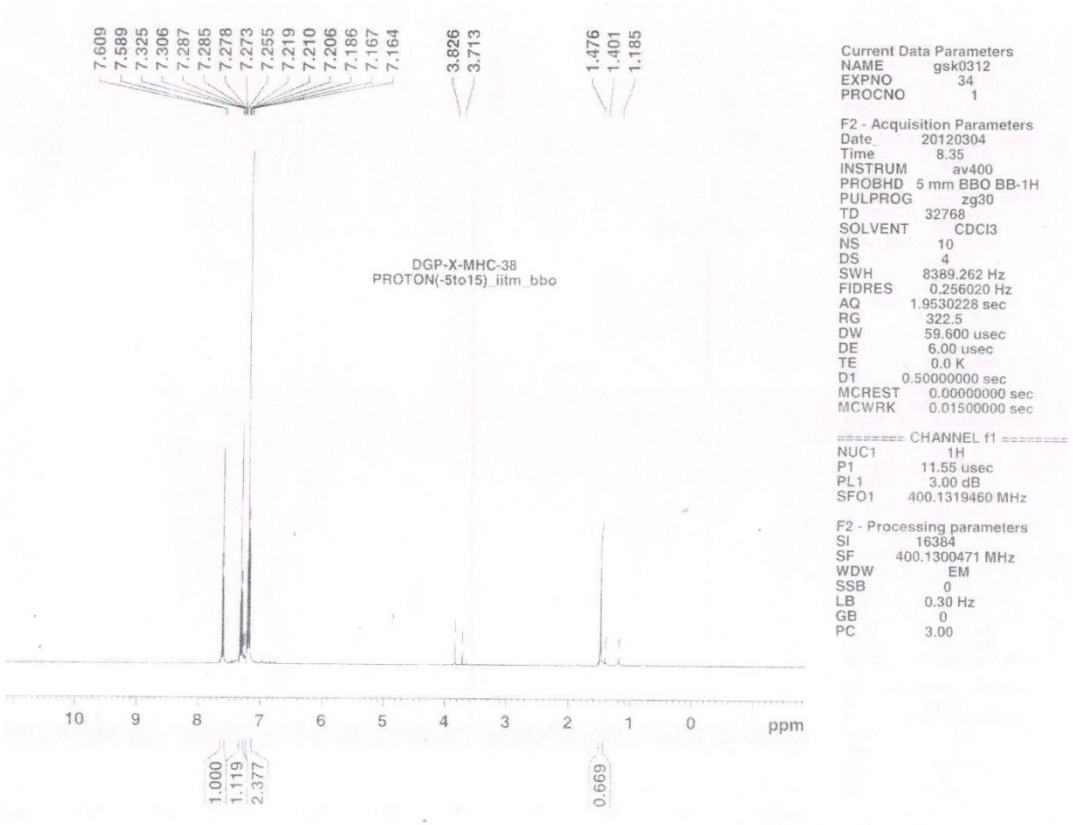


Fig. 50 400 MHz ^{1}H NMR Spectrum of 2,2'-dibromo biphenyl in $CDCl_3$

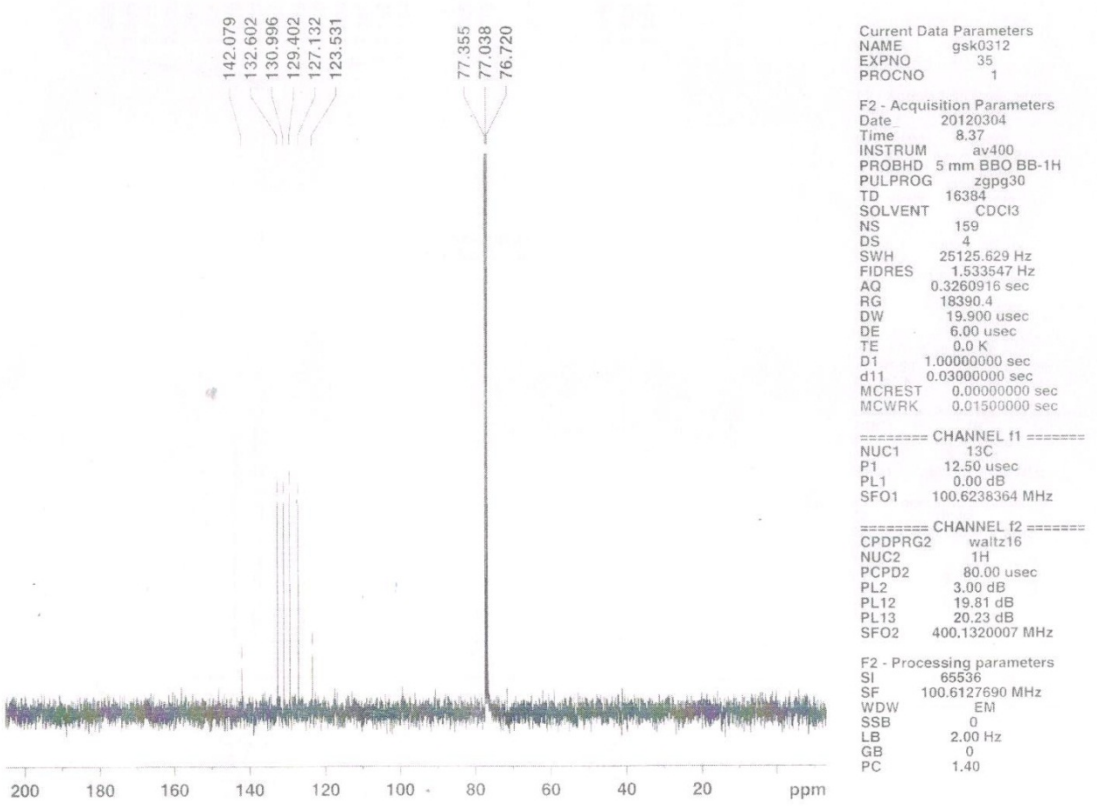


Fig. 51 100 MHz ^{13}C NMR Spectrum of 2,2'-dibromo biphenyl in $CDCl_3$

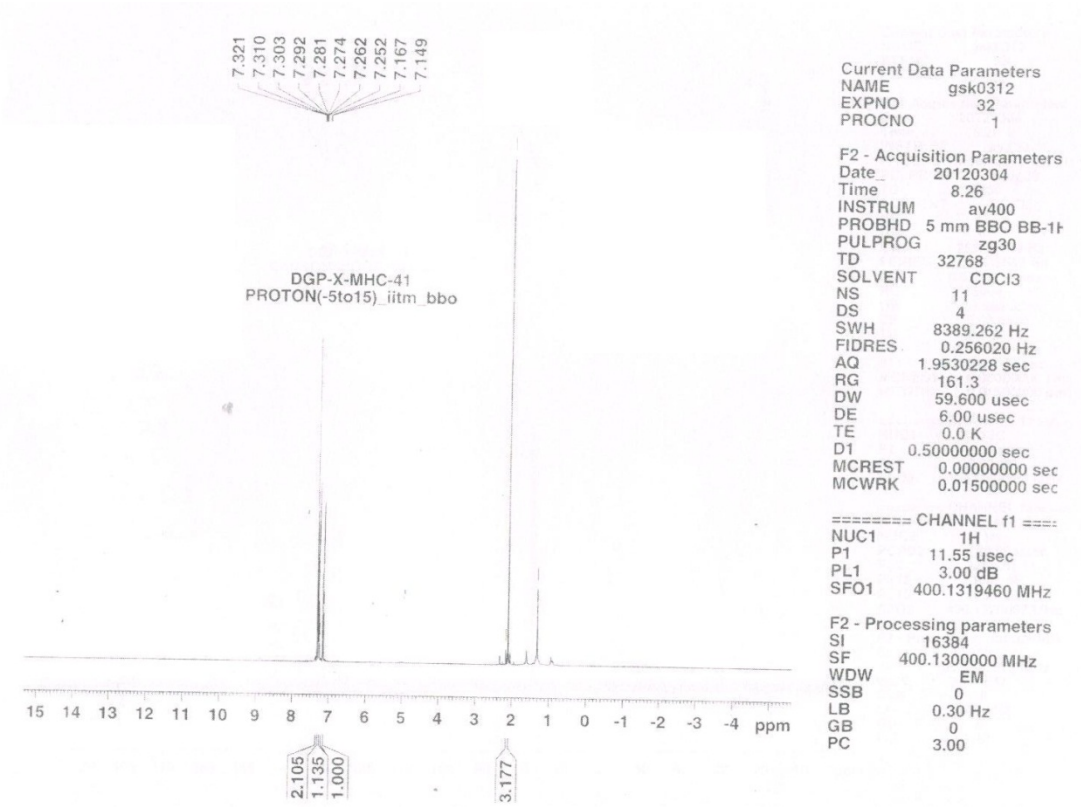


Fig. 52 400 MHz ^{1}H NMR Spectrum of 2,2'-dimethyl biphenyl in $CDCl_3$

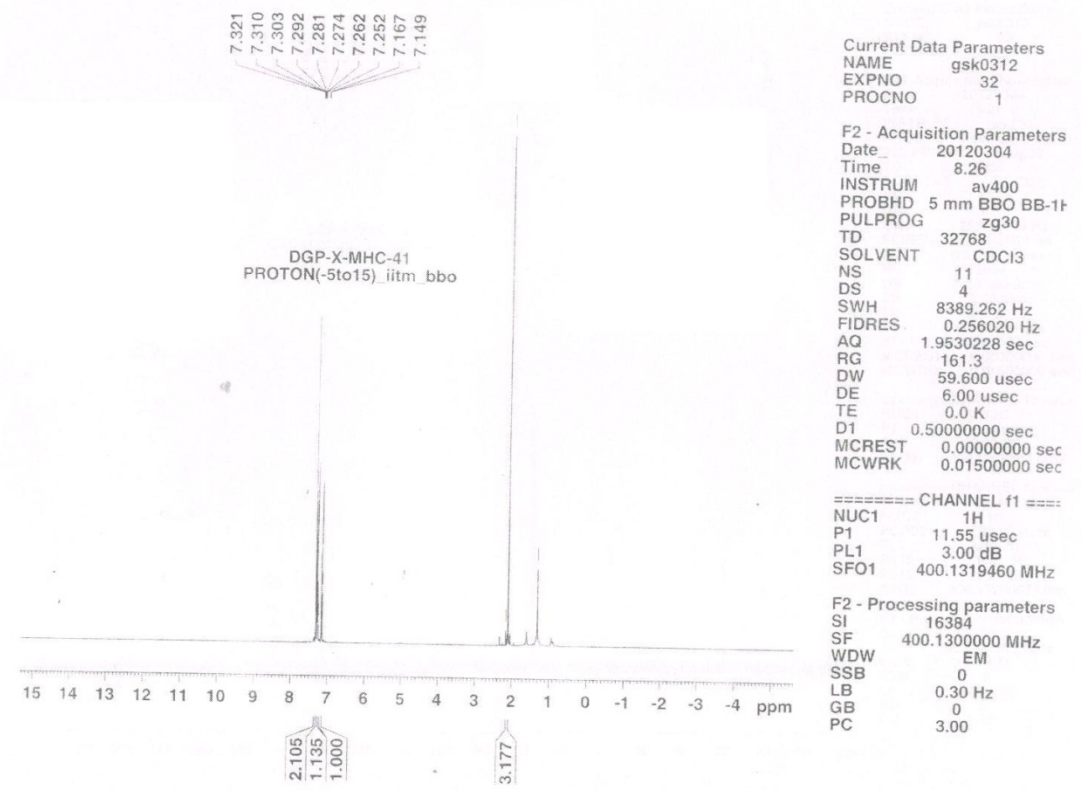


Fig. 53 100 MHz ^{13}C NMR Spectrum of 2,2'-dimethyl biphenyl in $CDCl_3$

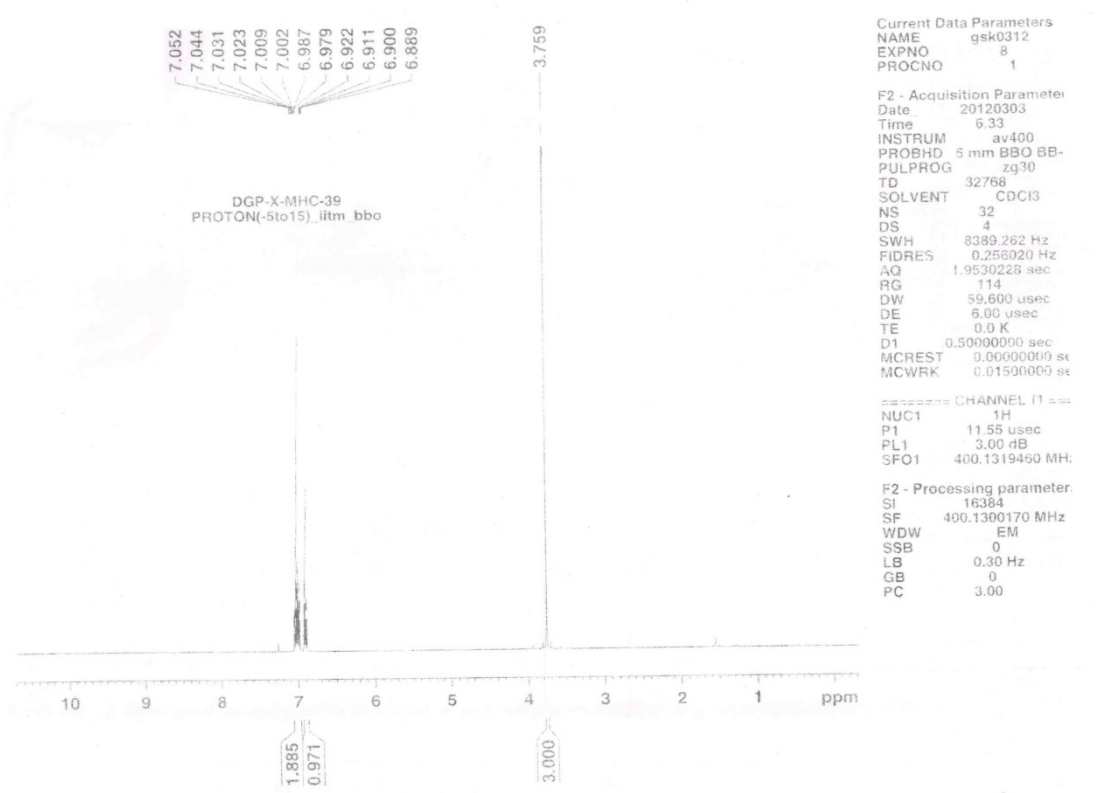


Fig. 54 400 MHz ^{1}H NMR Spectrum of 5,5'-difluoro-2,2'-dimethoxy biphenyl in $CDCl_3$

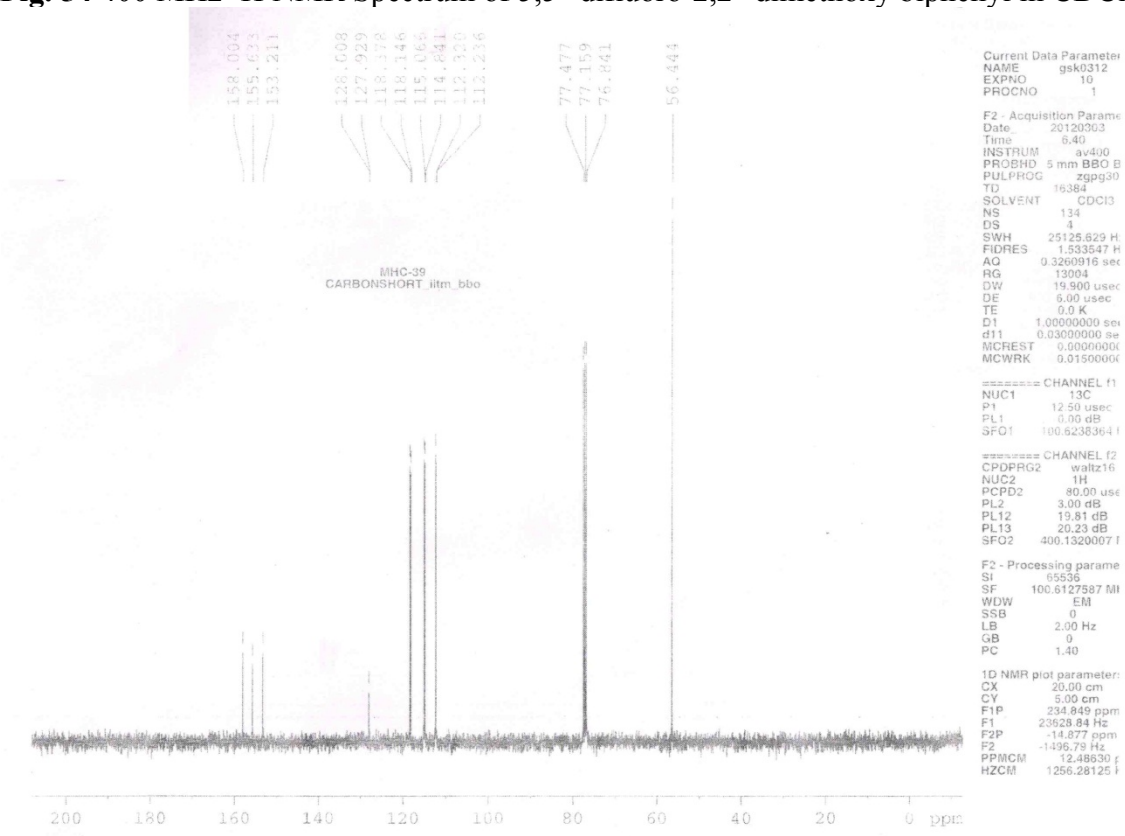


Fig. 55 100 MHz ^{13}C NMR Spectrum of 5,5'-difluoro-2,2'-dimethoxy biphenyl in $CDCl_3$

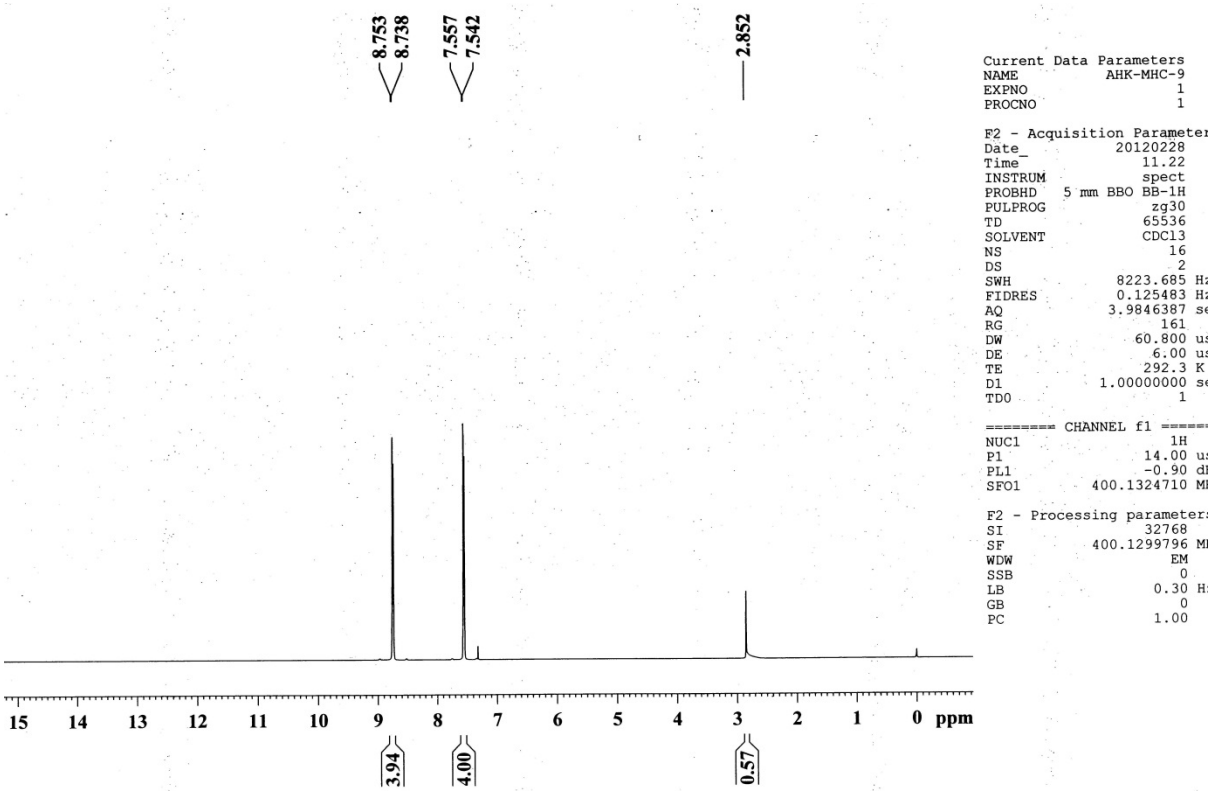


Fig. 56 400 MHz ^{1}H NMR Spectrum of 4,4'-bipyridyl in $CDCl_3$

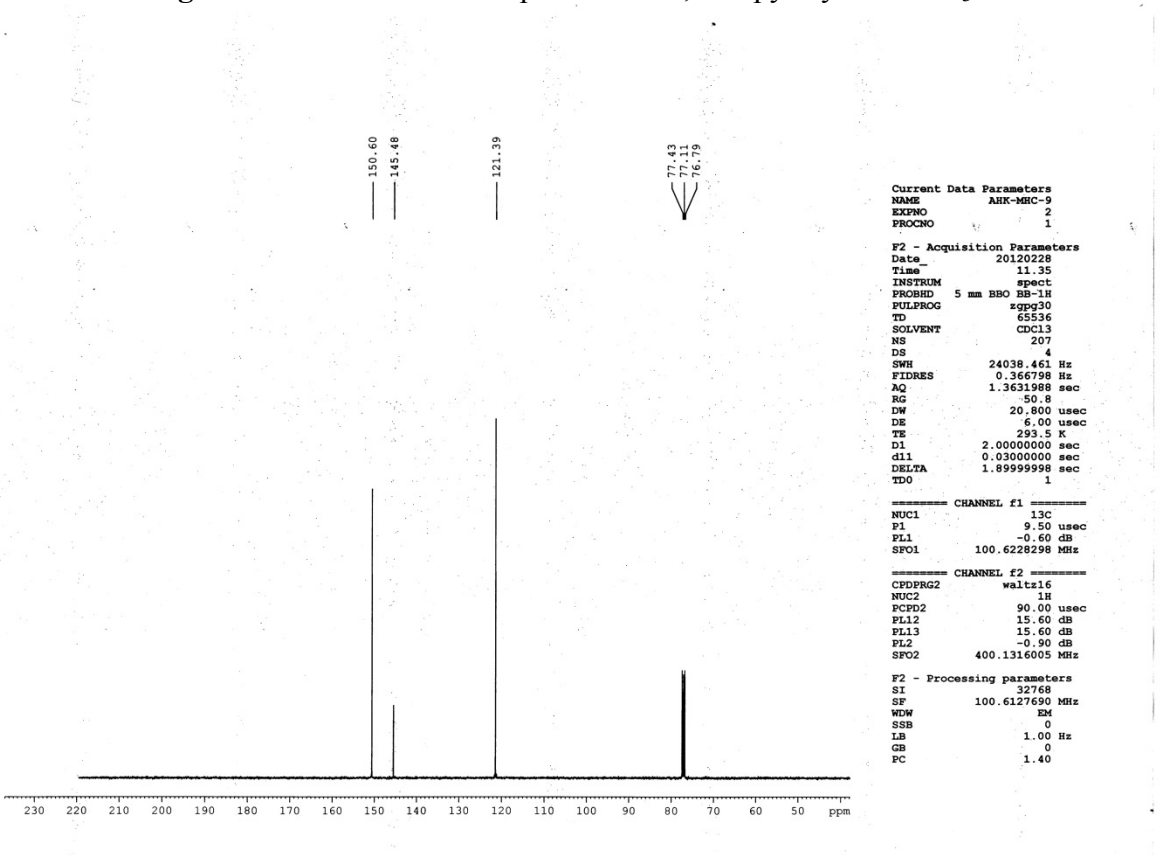


Fig. 57 100 MHz ^{13}C NMR Spectrum of 4,4'-bipyridyl in $CDCl_3$

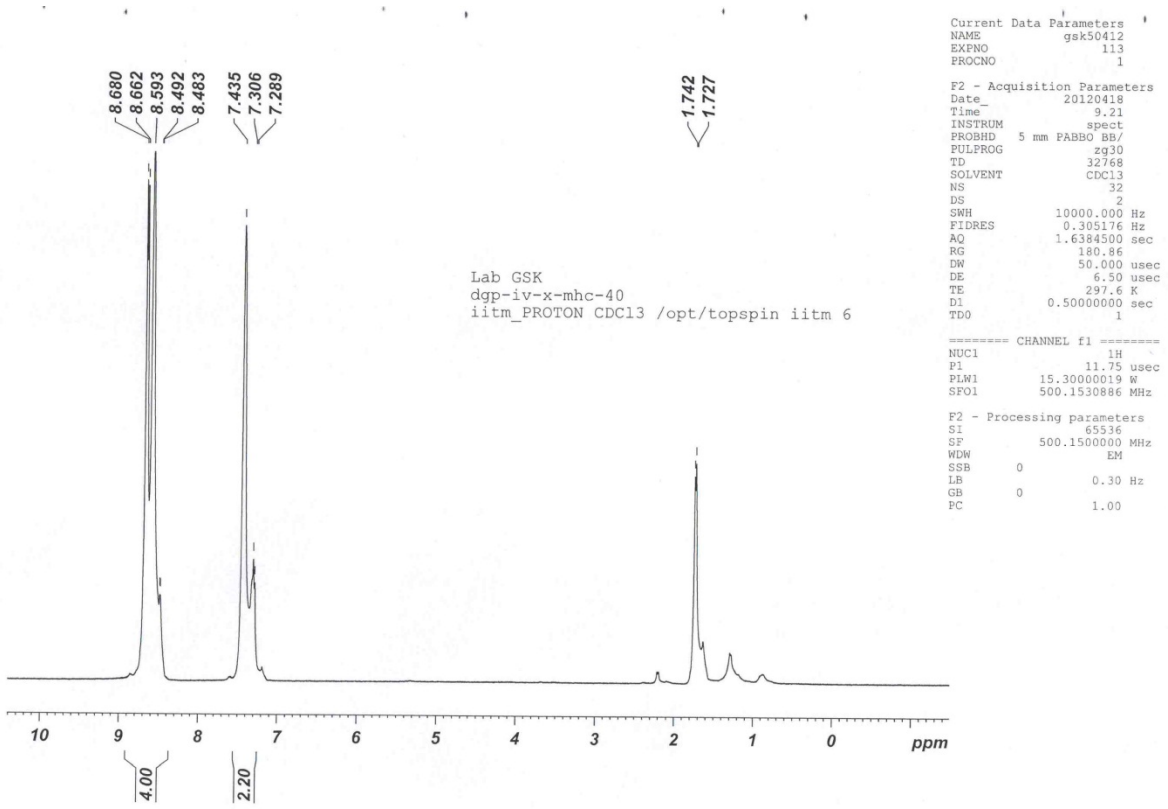


Fig. 58 500 MHz ^{1}H NMR Spectrum of 3,3'-difluoro-4,4'-bipyridyl in $CDCl_3$

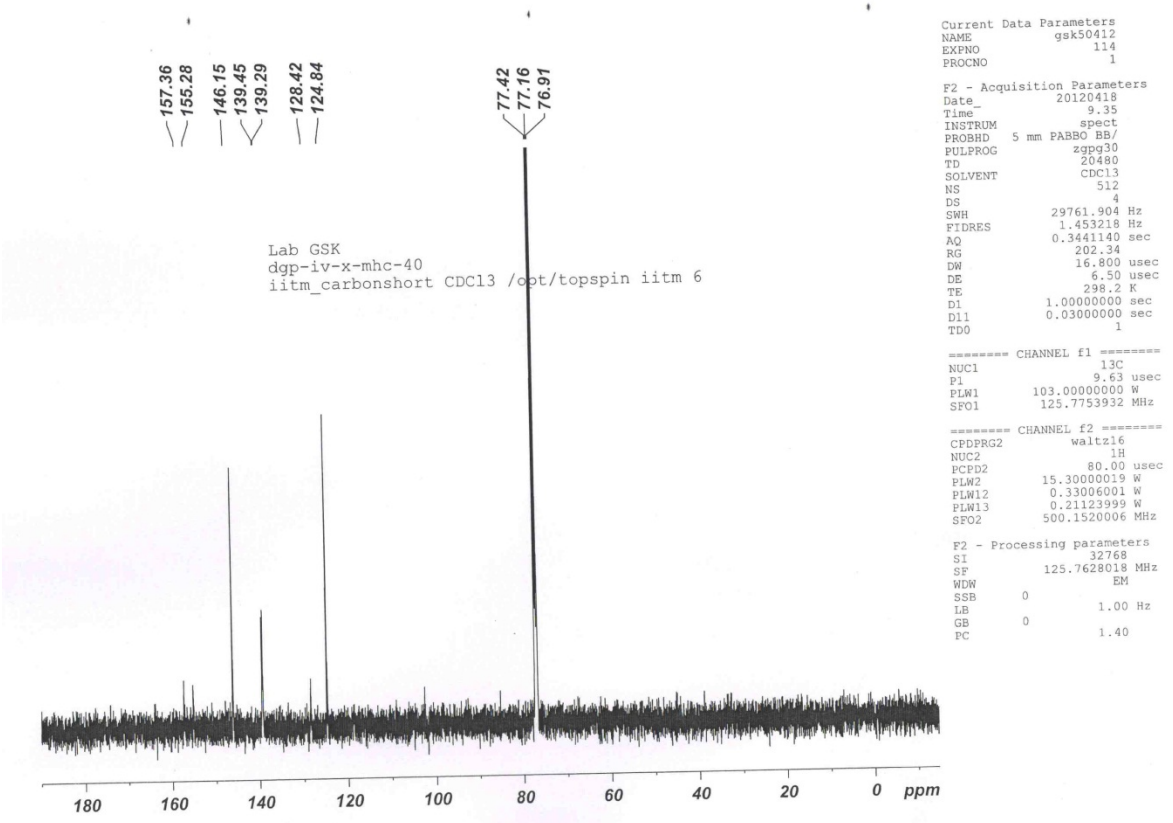


Fig. 59 125 MHz ^{13}C NMR Spectrum of 3,3'-difluoro-4,4'-bipyridyl in $CDCl_3$

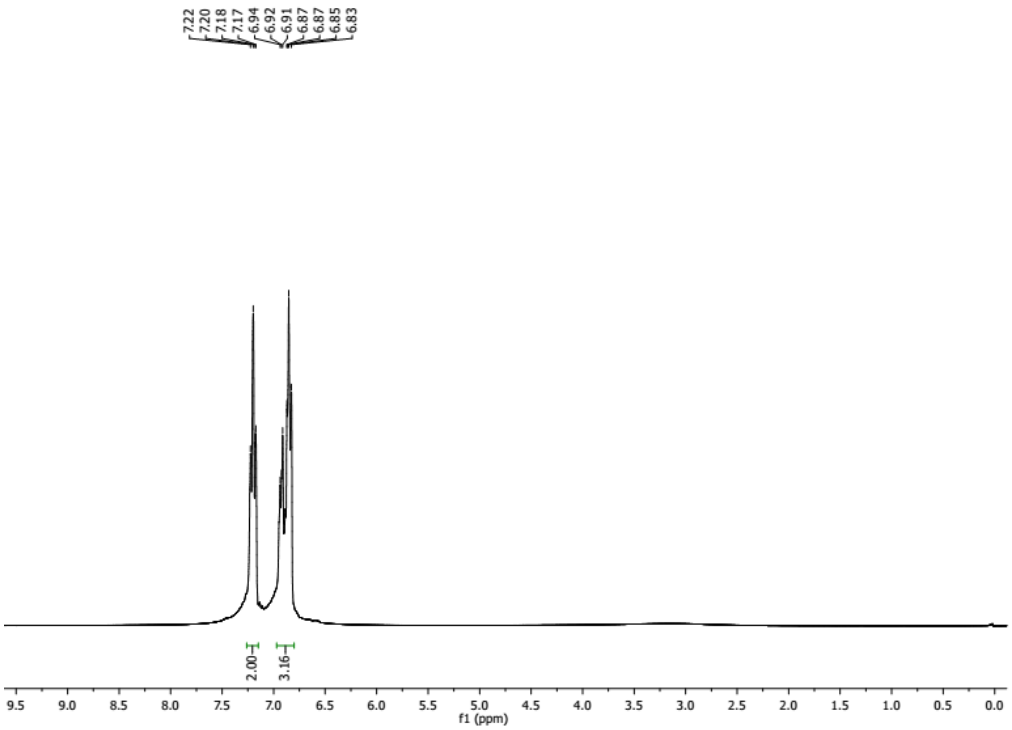


Fig. 60 300 MHz ^{1}H NMR Spectrum of phenol in $CDCl_3$

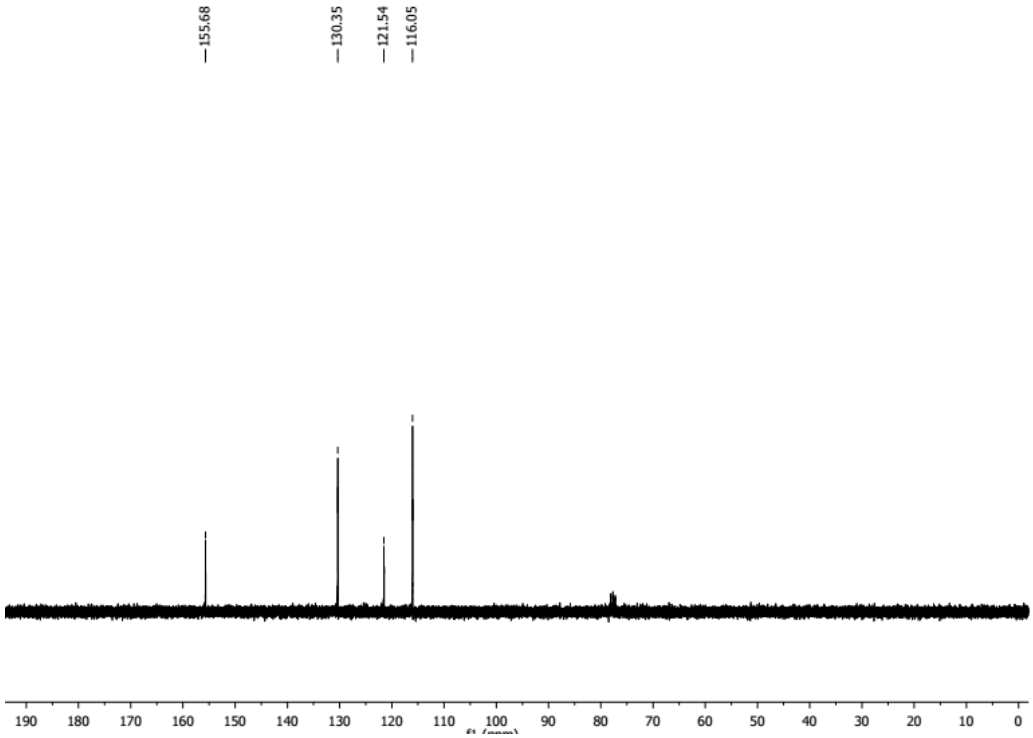


Fig. 61 75 MHz ^{13}C NMR Spectrum of phenol in $CDCl_3$

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