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Supporting Information

Synthesis of 1,3,5-Triazines via $Cu(OAc)_2$-Catalyzed Aerobic Oxidative Coupling of Alcohols and Amidine hydrochlorides

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Content

Typical Experimental Procedure

(A) Remarks

All starting materials and reagents were commercially available and used directly without further purification. All known products gave satisfactory analytical data by NMR spectra, which corresponding to the reported literature values. Unknown compounds were confirmed by HRMS additionally. NMR spectra were determined at room temperature on Bruker Avance-300 or Bruker Avance-500 at 300 MHz or 500 MHz with tetramethylsilane (TMS) as an internal standard. Chemical shifts are given in δ relative to TMS, the coupling constants J are given in Hz. High-resolution mass spectral (HRMS) were obtained using APCI, ESI or EI in positive mode.

(B) Typical experimental procedure for the synthesis of 3

A mixture of alcohol **1** (0.6 mmol), amidine hydrochloride **2** (1.0 mmol), $NaCO_3$ (1.0 mmol, 1.0 equiv) and $Cu(OAc)_2$ (10 mol %) was stirred in toluene (2.5 mL) under reflux in air for 24 h. The resulting mixture was cooled to room temperature and then extracted it for several times with EtOAc (10 mL) and brine (5 mL). The organic phases were combined and dried with anhydrous Na_2SO_4 and evaporated under vacuum. The crude product was purified by column chromatography on silica gel using petroleum ether/EtOAc (100:1) as an eluent to give the corresponding products **3aa**–**3rb**.

Characterization data for the products

2,4,6-triphenyl-1,3,5-triazine[1] (3aa)

White solid; yield 88%; m.p.237-239 °C; Lit.m.p:233-234 °C; ^{1}H NMR (300MHz, $CDCl_3$) δ 8.80-8.78(m, 6H), 7.65-7.56(m, 9H); ^{13}C NMR (75 MHz, d^6-DMSO) δ 166.6, 134.6, 129.8, 128.9.

2-(4-chlorophenyl)-4,6-diphenyl-1,3,5-triazine[1] (3ba)

White solid; yield 88%; m.p.198-199 °C; Lit.m.p:199-200 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.74-8.66(m, 6H), 7.59-7.50(m, 8H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.0, 171.0, 139.1, 136.4, 135.1, 133.0, 130.6, 129.3, 129.3, 129.0.

2-(2-chlorophenyl)-4,6-diphenyl-1,3,5-triazine[2] (3ca)

White solid; yield 85%; m.p.135-136 °C; Lit.m.p:130-133 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.76(d, *J* = 6.6 Hz, 4H), 8.18-8.15(m, 1H), 7.65-7.54(m, 7H), 7.51-7.44(m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.2, 172.0, 136.4, 136.3, 134.2, 133.1, 132.8, 132.0, 131.7, 129.5, 129.1, 127.3.

2-(3-chlorophenyl)-4,6-diphenyl-1,3,5-triazine[3] (3da)

White solid; yield 55%; m.p.195-197 °C; Lit.m.p:194-195 °C; ^{1}H NMR (300MHz, $CDCl_3$) δ 8.79-8.74(m, 5H), 8.67(d, *J* = 7.8 Hz, 1H), 7.66-7.49(m, 8H); ^{13}C NMR (75MHz, $CDCl_3$) δ 172.2, 171.0, 138.5, 136.3, 135.2, 133.1, 132.8, 130.3, 129.4, 129.3, 129.1, 127.4.

2,4-diphenyl-6-(p-tolyl)-1,3,5-triazine[4] (3ea)

Yellow solid; yield 88%; m.p.196-197 °C; Lit.m.p:197-199 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.72(d, *J* = 6.0 Hz, 4H), 8.60(d, *J* = 7.8 Hz, 2H), 7.53 (d, *J* = 6.6 Hz, 6H), 7.3(d, *J* = 7.8 Hz, 2H), 2.40(s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.9, 171.8, 143.5, 136.7, 133.9, 132.8, 129.8, 129.3, 129.0, 22.2.

2,4-diphenyl-6-(o-tolyl)-1,3,5-triazine[5] (3fa)

White solid; yield 47%; m.p.122-123 °C; Lit.m.p:121-122 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.76(d, *J* = 6.3Hz, 4H), 8.35(d, *J* = 7.2Hz, 1H), 7.64-7.56(m, 6H), 7.50-7.38(m, 3H), 2.87(s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 174.9, 171.7, 139.5, 136.6, 136.5, 132.9, 132.3, 131.7, 131.4, 129.4, 129.1, 126.5, 22.8.

2,4-diphenyl-6-(m-tolyl)-1,3,5-triazine (3ga)

White solid; yield 85%; m.p.167-168 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.80-8.77(m, 4H), 8.60-8.58(m, 2H), 7.65-7.56(m, 6H), 7.50-7.42(m, 2H), 2.53(s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.0, 169.4, 138.7, 136.6, 136.5, 133.7, 132.9, 129.8, 129.3, 129.0, 128.9, 126.6, 22.0. HRMS (EI) calcd for $C_{22}H_{17}N_3$ ($[M]^+$) 323.1422, found 323.1430.

2,4-diphenyl-6-(4-(trifluoromethyl)phenyl)-1,3,5-triazine (3ha)

White solid; yield 87%; m.p.183-184 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.84(d, *J*=8.1 Hz, 2H), 8.76-8.73 (m, 4H), 7.81(d, *J* = 8.1 Hz, 2H), 7.66-7.55(m, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.3, 170.8, 140.0, 136.3, 134.2(q, *J* = 32.3 Hz), 133.2, 129.6, 129.4, 129.1, 125.9(q, *J* = 3.5 Hz), 124.4(q, *J* = 270.8 Hz). HRMS (EI) calcd for $C_{22}H_{14}F_3N_3$ ($[M]^+$) 377.1140, found 377.1135.

2-(4-methoxyphenyl)-4,6-diphenyl-1,3,5-triazine[1] (3ia)

White solid; yield 90%; m.p.159-161 °C; Lit.m.p:158-160 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.78-8.73(m , 6H), 7.64-7.54(m, 6H), 7.07(d, *J* = 8.7 Hz, 2H), 3.92(s, 3H); ^{13}C NMR (75 MHz, d^6-DMSO) δ 171.5, 164.1, 136.3, 133.8, 131.5, 129.8, 129.4, 128.4, 115.2, 56.4.

2-(4-bromophenyl)-4,6-diphenyl-1,3,5-triazine[5] (3ja)

White solid; yield 52%; m.p.200-201 °C; Lit.m.p:204-205 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68(d, *J* = 8.1Hz, 2H), 8.60(d, *J* = 6.9Hz, 4H), 7.70(d, *J*=7.8Hz, 2H), 7.54-7.45(m, 6H); ^{13}C NMR (75MHz, $CDCl_3$) δ 172.1, 171.2, 136.4, 135.5, 133.0, 132.3, 130.8,129.3, 129.0, 127.8.

2-(4-nitrophenyl)-4,6-diphenyl-1,3,5-triazine[1] (3ka)

Yellow solid; yield 46%; m.p.217-218 °C; Lit.m.p:216-218 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.93(d, *J* = 8.7Hz, 2H), 8.78-8.75(m, 4H), 8.41(d, *J* = 9.0Hz, 2H), 7.68-7.57(m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.4, 170.3, 136.0, 133.4, 130.2, 129.4, 129.2, 124.1.

2-(4-isopropylphenyl)-4,6-diphenyl-1,3,5-triazine[6] (3la)

White solid; yield 92%; m.p.153-154 °C; Lit.m.p:149-150 °C; ^{1}H NMR (300MHz,

$CDCl_3$) δ 8.80-8.77 (m, 4H), 8.70(d, *J* = 8.1Hz, 2H), 7.65-7.55(m, 6H), 7.44(d, *J* = 8.1Hz, 2H), 3.11-2.98(m, 1H), 1.34(d, *J* = 6.9Hz, 2H); ^{13}C NMR(75MHz, $CDCl_3$) δ 172.0, 171.9, 154.3, 136.7, 134.3, 132.8, 129.5, 129.3, 129.0, 127.2.

2-(4-fluorophenyl)-4,6-diphenyl-1,3,5-triazine (3ma)

White solid; yield 95%; m.p.248-249 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 8.82-8.75 (m, 6H), 7.64-7.56(m, 6H), 7.28-7.22(m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.1, 171.1, 166.2(d, *J* = 251.4 Hz), 136.5, 132.9, 132.8, 131.7(d, *J* = 9.0 Hz), 129.4, 129.0, 116.1(d, *J* = 21.6 Hz). HRMS (ESI) calcd for $C_{21}H_{14}FN_3$ ($[M+H]^+$) 328.1250, found 328.1237.

2-(2,4-dichlorophenyl)-4,6-diphenyl-1,3,5-triazine (3na)

White solid; yield 90%; m.p.161-162 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 8.65(d, *J* = 6 Hz, 4H), 8.09(d, *J* = 8.1 Hz, 1H), 7.50(d, *J* = 7.2 Hz, 7H), 7.36(d, *J* = 8.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.0, 137.6, 136.1, 135.2, 133.7, 133.2, 131.5, 129.5, 129.1, 127.6. HRMS (EI) calcd for $C_{21}H_{13}Cl_2N_3$ ($[M]^+$) 377.0486, found 377.0494.

2,4-di-phenyl-6-(pyridin-2-yl)-1,3,5-triazine[1] (3oa)

White solid; yield 97%; m.p.237-238 °C; Lit.m.p:230-231 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 8.97(d, *J* = 4.5 Hz, 1H), 8.81(d, *J* = 6.6Hz, 5H), 8.00-7.94(m, 1H), 7.66-7.51(m, 7H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.7, 171.3, 154.2, 150.7, 137.6, 136.1, 133.2, 129.6, 129.0, 126.5, 125.2.

2,4-di-phenyl-6-(pyridin-3-yl)-1,3,5-triazine[1] (3pa)

White solid; yield 97%; m.p.268-269 °C; Lit.m.p:254-256 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 9.96(s, 1H), 9.03(d, *J* = 8.1Hz, 1H), 8.85-8.69(m, 5H), 7.65-7.56(m, 7H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.3, 170.6, 152.7, 150.5, 137.0, 136.1, 133.3, 132.6, 129.4, 129.1, 124.1.

2-phenyl-4,6-di-p-tolyl-1,3,5-triazine[1] (3ab)

White solid; yield 87%; m.p.233-234 °C; Lit.m.p:213-216 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 8.77(d, *J* = 6.0 Hz, 2H), 8.66(d, *J* = 8.1Hz, 4H), 7.63-7.55(m, 3H), 7.37(d, *J* = 7.8 Hz, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.9, 171.8, 143.4, 136.8, 134.0, 132.7, 129.7, 129.3, 129.3, 128.9, 22.1.

2-(4-chlorophenyl)-4,6-di-p-tolyl-1,3,5-triazine[1] (3bb)

White solid; yield 96%; m.p.298-299 °C; Lit.m.p:282-285 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.69(d, *J* = 8.4 Hz, 2H), 8.63(d, *J* = 7.8 Hz, 4H), 7.52(d, *J* = 8.7 Hz, 2H), 7.36(d, *J* = 8.1 Hz, 4H), 2.48(s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.9, 171.0, 143.5, 138.9, 135.3, 133.8, 130.6, 129.8, 129.3, 129.2, 22.1.

2,4,6-tri-p-tolyl-1,3,5-triazine[7] (3eb)

White solid; yield 86%; m.p.297-298 °C; Lit.m.p:283-285 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65(d, *J* = 6.3 Hz, 6H), 7.36(d, *J* = 6.3Hz, 6H), 2.47(s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.7, 143.2, 134.1, 129.7, 129.3, 22.1.

2-(o-tolyl)-4,6-di-p-tolyl-1,3,5-triazine (3fb)

White solid; yield 66%; m.p.152-153 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63(d, *J* = 8.1Hz, 4H), 8.30(d, *J* = 6.9Hz, 1H), 7.48-7.35(m, 7H), 2.84(s, 3H), 2.48(s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 174.7, 171.5, 143.4, 139.3, 136.7, 134.0, 132.2, 131.5, 131.2, 129.8, 129.3, 126.4, 22.7, 22.1. HRMS (APCI) calcd for $C_{24}H_{21}N_3$ ($[M+H]^+$) 352.1814, found 352.1800.

2,4-di-p-tolyl-6-(4-(trifluoromethyl)phenyl)-1,3,5-triazine (3hb)

White solid; yield 87%; m.p.233-234 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.78(d, *J* = 7.8Hz, 2H), 8.58(d, *J* = 7.8Hz, 4H), 7.77(d, *J* = 8.1Hz, 2H), 7.33(d, *J* = 7.8Hz, 4H), 2.46(s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.2, 170.6, 143.7, 140.2, 134.1(q, *J* = 32.1Hz), 133.7, 129.8, 129.6, 129.4, 125.9(q, *J* = 3.5Hz), 124.4(q, *J* = 270.8Hz), 22.1. HRMS (APCI) calcd for $C_{24}H_{18}F_3N_3$ ($[M+H]^+$) 406.1531, found 406.1517.

2-(4-fluorophenyl)-4,6-di-p-tolyl-1,3,5-triazine (3mb)

White solid; yield 94%; m.p.248-249 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.79-8.74(m, 2H), 8.63(d, *J* = 8.1Hz, 4H), 7.36(d, *J* = 7.8Hz, 4H), 7.22(d, *J* = 8.7Hz, 2H), 2.48(s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.9, 170.8, 166.1(d, *J* = 250.9Hz), 143.4, 134.0, 133.0, 131.6(d, *J* = 8.5Hz), 129.7, 129.3, 116.0(d, *J* = 21.6Hz), 22.1. HRMS (APCI) calcd for $C_{23}H_{18}FN_3$ ($[M+H]^+$) 356.1563, found 356.1548.

2,4-bis(4-bromophenyl)-6-(4-methoxyphenyl)-1,3,5-triazine (3ic)

White solid; yield 50%; m.p.294-295 °C; ^{1}H NMR (300MHz, $CDCl_3$) δ 8.65(d, *J* =

8.4Hz, 2H), 8.55(d, *J* = 8.1Hz, 4H), 7.67(d, *J* = 8.4Hz, 4H), 7.04(d, *J* = 8.7Hz, 2H), 3.92(s, 3H); ^{13}C NMR (75MHz, $CDCl_3$) δ 170.9, 163.9, 135.5, 132.2, 131.3, 130.8, 130.7, 128.6, 127.8, 114.4, 55.9. HRMS (ESI) calcd for $C_{22}H_{15}Br_2N_3O$ ($[M+H]^+$) 495.9660, found 495.9642.

2,4-bis(4-bromophenyl)-6-(4-isopropylphenyl)-1,3,5-triazine (3lc)

White solid; yield 66%; m.p.181-182 °C; ^{1}H NMR (300MHz, $CDCl_3$) δ 8.59-8.52(m, 6H), 7.65(d, *J* = 8.1Hz, 4H), 7.40(d, *J* = 8.4Hz, 2H), 3.10-2.97(m, 1H),1.34(d, *J* = 6.9Hz, 6H); ^{13}C NMR (75MHz, $CDCl_3$) δ 172.1, 171.0, 154.6, 135.4, 133.8, 132.2, 130.7, 129.5, 127.9, 127.2, 34.7, 24.2. HRMS (APCI) calcd for $C_{24}H_{19}Br_2N_3$ ($[M+H]^+$) 508.0024, found 508.0008.

2-phenyl-4,6-bis(4-(trifluoromethyl)phenyl)-1,3,5-triazine (3ad)

White solid; yield 98%; m.p.168-169 °C; ^{1}H NMR (300MHz, $CDCl_3$) δ 8.85(d, *J* = 8.1Hz, 4H), 8.76-8.73(m, 2H), 7.83(d, *J* = 8.1Hz, 4H), 7.68-7.56(m, 3H); ^{13}C NMR (125MHz, $CDCl_3$) δ 172.6, 171.1, 139.6, 135.9, 134.5(q, *J* = 32.3Hz), 133.5, 129.7, 129.5, 129.2, 126.0(q, *J* = 3.5Hz), 124.3(q, *J* = 270.9Hz). HRMS (ESI) calcd for $C_{23}H_{13}F_6N_3$ ($[M+H]^+$) 446.1092, found 446.1086.

2-(4-chlorophenyl)-4,6-bis(4-(trifluoromethyl)phenyl)-1,3,5-triazine (3bd)

White solid; yield 88%; m.p.244-246 °C; ^{1}H NMR (300MHz, $CDCl_3$) δ 8.83(d, *J* = 8.1Hz, 4H), 8.68(d, *J* = 8.4Hz, 2H), 7.83(d, *J* = 8.1Hz, 4H), 7.55(d, *J* = 8.7Hz, 2H); ^{13}C NMR (125MHz, $CDCl_3$) δ 171.7, 171.2, 139.9, 139.4, 134.7(q, *J* = 32.4Hz), 134.4, 130.8, 129.7, 129.5, 126.1(q, *J* = 3.4Hz), 124.3(q, *J* = 271.0Hz).

2-(4-methoxyphenyl)-4,6-bis(4-(trifluoromethyl)phenyl)-1,3,5-triazine (3id)

White solid; yield 75%; m.p.190-192 °C; ^{1}H NMR (300MHz, $CDCl_3$) δ 8.85(d, *J* = 8.1Hz, 4H), 8.73(d, *J* = 9.0Hz, 2H), 7.83(d, *J* = 8.1Hz, 4H), 7.09(d, *J* = 9.0Hz, 2H), 3.95(s, 3H); ^{13}C NMR (125MHz, $CDCl_3$) δ 172.2, 170.9, 164.2, 139.8, 134.4(q, *J* = 32.4Hz), 131.5, 129.6, 128.4, 125.98(q, *J* = 3.4Hz), 124.3(q, *J* = 270.7Hz), 114.6, 55.9. HRMS (ESI) calcd for $C_{24}H_{15}F_6N_3O$ ($[M+H]^+$) 476.1197, found 476.1192.

2,4-diphenyl-1,3,5-triazine[1] (3qa)

Light yellow solid; yield 75%; m.p.81-82 °C; Lit.m.p:76-78 °C; ^{1}H NMR (300MHz,

$CDCl_3$) δ 9.27(s, 1H), 8.67-8.64(m, 4H), 7.64-7.53(m, 6H); ^{13}C NMR (75MHz, $CDCl_3$) δ 171.7, 167.1, 135.9, 133.2, 129.3, 129.1.

2-methyl-4,6-diphenyl-1,3,5-triazine[8] (3ra)

Light yellow solid; yield 86%; m.p.97-98 °C; Lit.m.p:109-110 °C; ^1H NMR (300MHz, $CDCl_3$) δ 8.67-8.64(m, 4H), 7.62-7.52(m, 6H), 2.80(s, 3H); ^{13}C NMR (75MHz, $CDCl_3$) δ 177.4, 171.6, 136.3, 132.9, 129.3, 129.0, 26.5. HRMS (ESI) calcd for $C_{16}H_{13}N_3$ ($[M+H]^+$) 248.1188, found 248.1176.

2,4-diphenyl-6-propyl-1,3,5-triazine[9] (3sa)

White solid; yield 75%; m.p.77-79 °C; Lit.m.p:79-80 °C; ^1H NMR (300MHz, $CDCl_3$) δ 8.67(d, *J* = 6.6Hz, 4H), 7.60-7.54(m, 6H), 3.00(t, *J* = 7.5Hz, 2H), 2.07-1.95(m, 2H), 1.09(t, *J* = 7.5Hz, 3H); ^{13}C NMR (75MHz, $CDCl_3$) δ 180.3, 171.5, 136.4, 132.8, 129.3, 129.0, 41.5, 21.5, 14.4. HRMS (ESI) calcd for $C_{18}H_{17}N_3$ ($[M+H]^+$) 276.1501, found 276.1497.

2-isopropyl-4,6-diphenyl-1,3,5-triazine (3ta)

White solid; yield 70%; m.p.45-47 °C; ^1H NMR (300MHz, $CDCl_3$) δ 8.69-8.67(m, 4H), 7.61-7.52(m, 6H), 3.30-3.21(m, 1H), 1.47(d, *J* = 6.6Hz, 6H); ^{13}C NMR(125MHz, $CDCl_3$) δ 184.4, 171.6, 136.7, 132.7, 129.3, 129.0, 37.9, 21.5. HRMS (ESI) calcd for $C_{18}H_{17}N_3$ ($[M+H]^+$) 276.1501, found 276.1491.

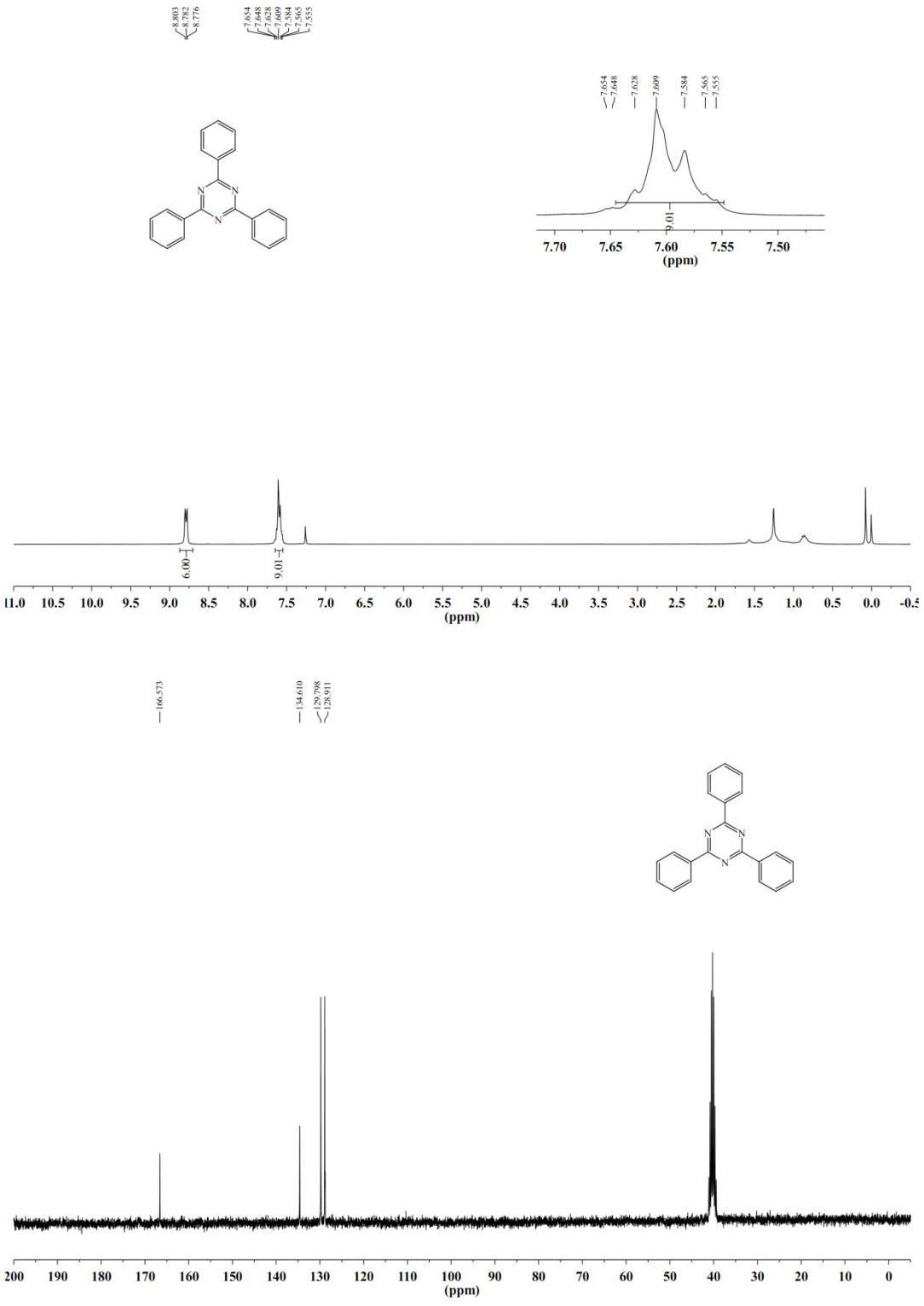
2,4-di-p-tolyl-1,3,5-triazine[1] (3qb)

White solid; yield 71%; m.p.150-151 °C; Lit.m.p:160-162 °C; ^1H NMR (300MHz, $CDCl_3$) δ 9.20(s, 1H), 8.53(d, *J* = 8.4Hz, 4H), 7.35(d, *J* = 8.1Hz, 4H), 2.47(s, 6H); ^{13}C NMR(75MHz, $CDCl_3$) δ 171.5, 166.8, 143.9, 133.2, 129.9, 129.3, 22.1.

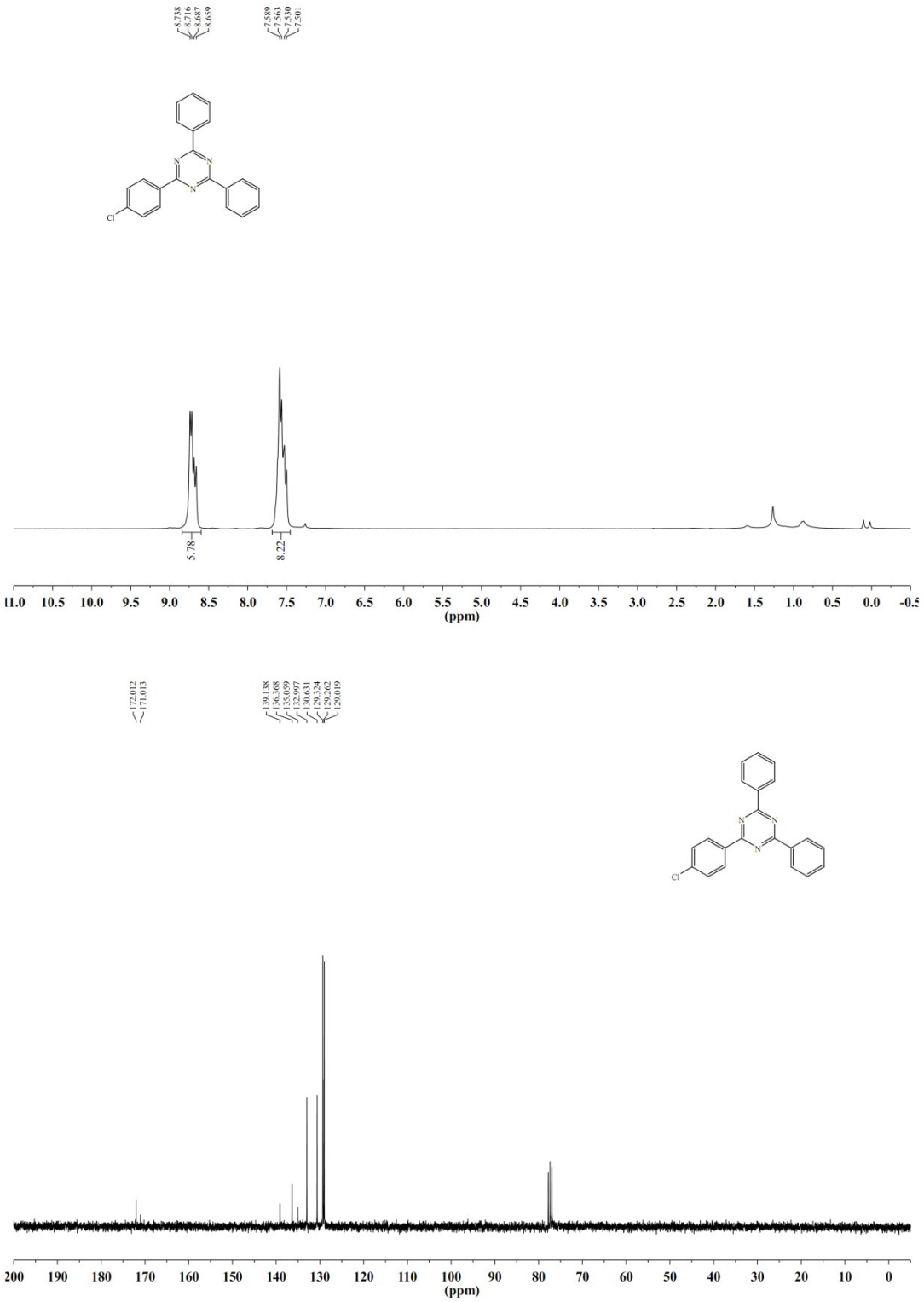
2-methyl-4,6-di-p-tolyl-1,3,5-triazine (3rb)

White solid; yield 80%; m.p.144-145 °C; Lit.m.p:152-153 °C; ^1H NMR (300MHz, $CDCl_3$) δ 8.53(d, *J* = 8.4Hz, 4H), 7.33(d, *J* = 7.8Hz, 4H), 2.76(s, 3H), 2.46(s, 6H); ^{13}C NMR (75MHz, $CDCl_3$) δ 177.1, 171.5, 143.4, 133.7, 129.8, 129.2, 26.5, 22.1. HRMS (ESI) calcd for $C_{18}H_{17}N_3$ ($[M+H]^+$) 276.1501, found 276.1490.

^{1}H and ^{13}C NMR spectra of the products.



3aa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132.997
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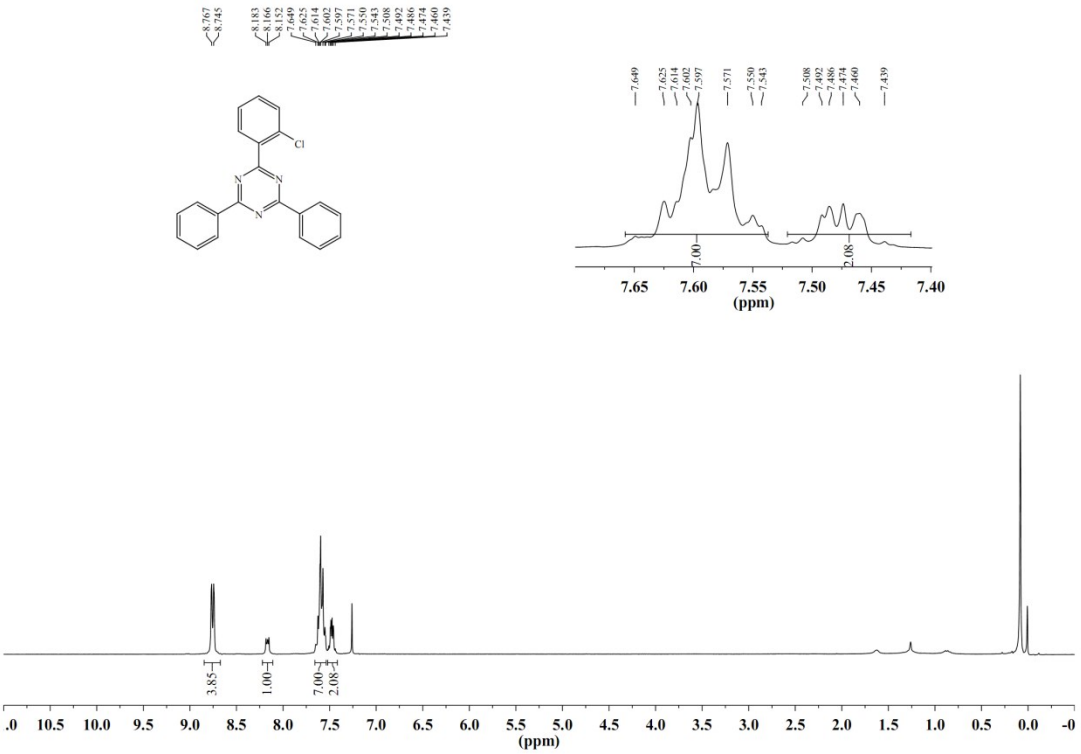
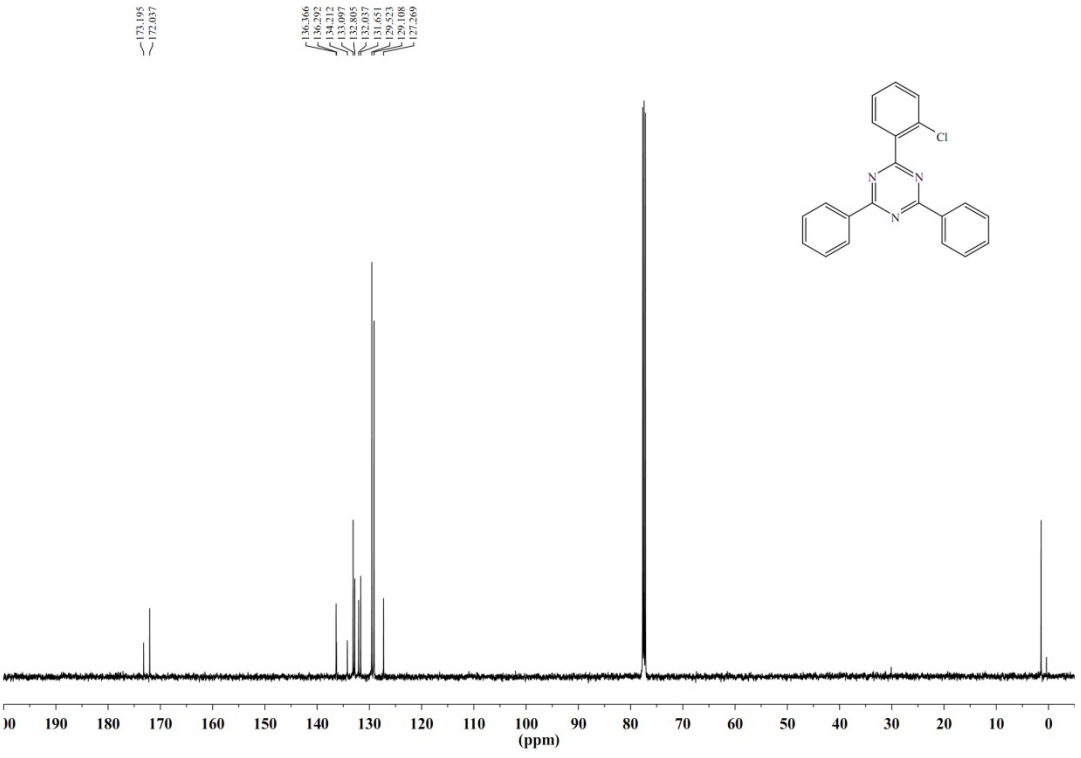
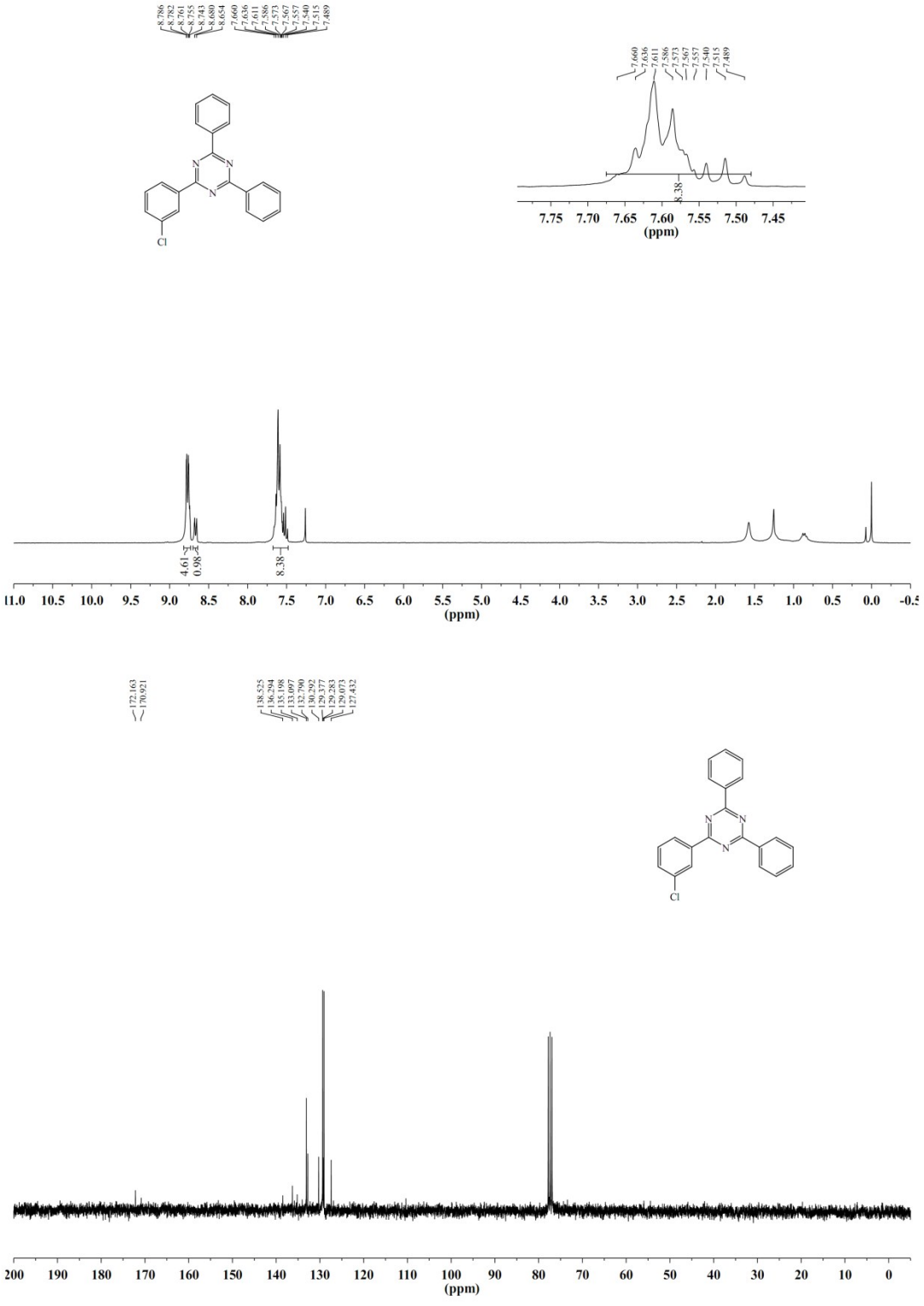
Cl
(ppm)

3ba

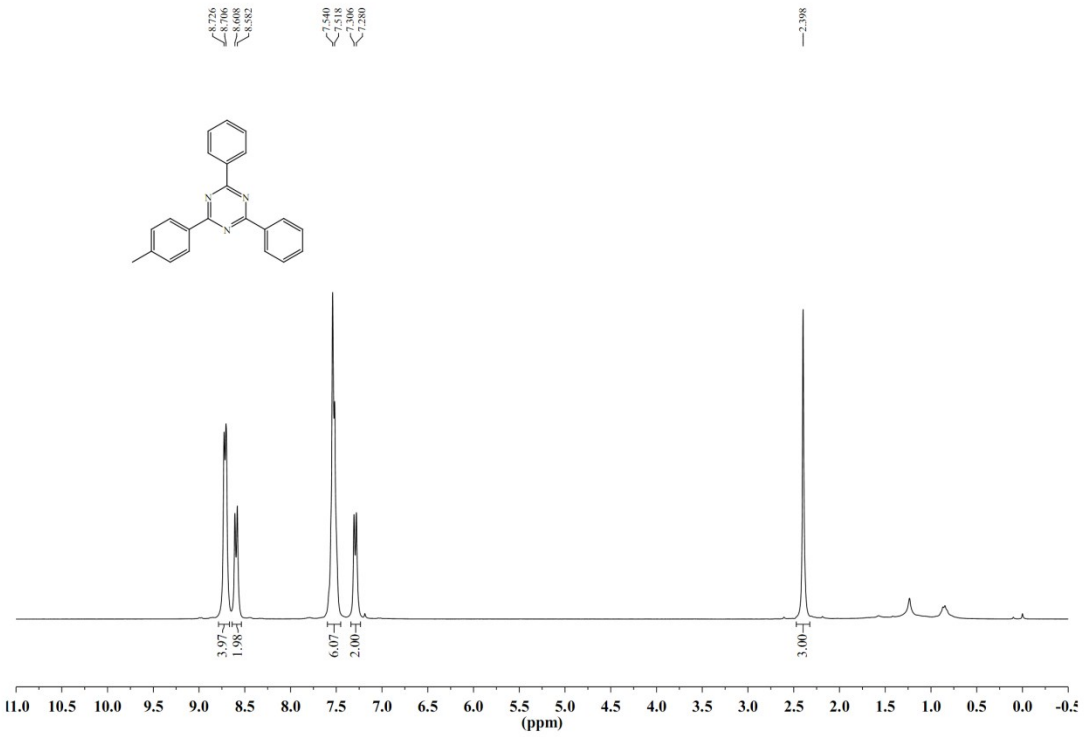

8.767
8.745
8.183
8.166
8.152
7.649
7.625
7.614
7.602
7.597
7.571
7.550
7.543
7.508
7.492
7.486
7.474
7.460
7.439
Cl
N
N
N
7.649
7.625
7.614
7.602
7.597
7.571
7.550
7.543
7.508
7.492
7.486
7.474
7.460
7.439
7.00
2.08
7.65
7.60
7.55
7.50
7.45
7.40
(ppm)
3.85
1.00
7.00
2.08
(ppm)

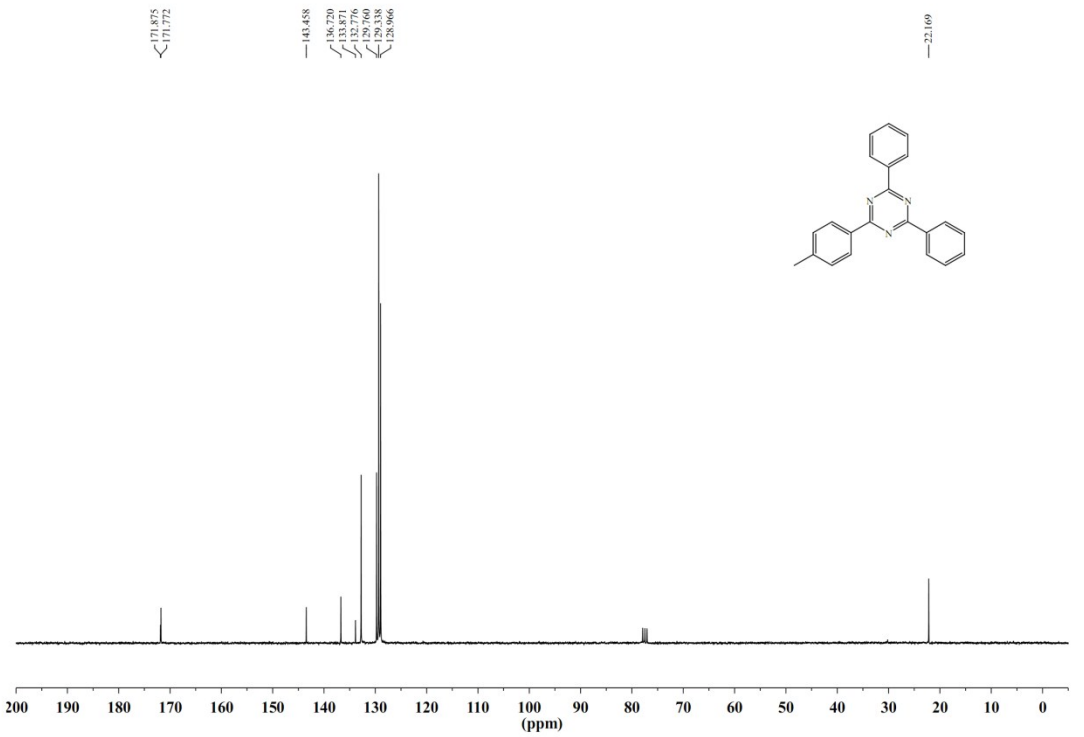

173.195
172.037
136.366
136.292
134.212
133.097
132.805
132.037
131.651
129.523
129.168
127.269
Cl
N
N
N
(ppm)

3ca

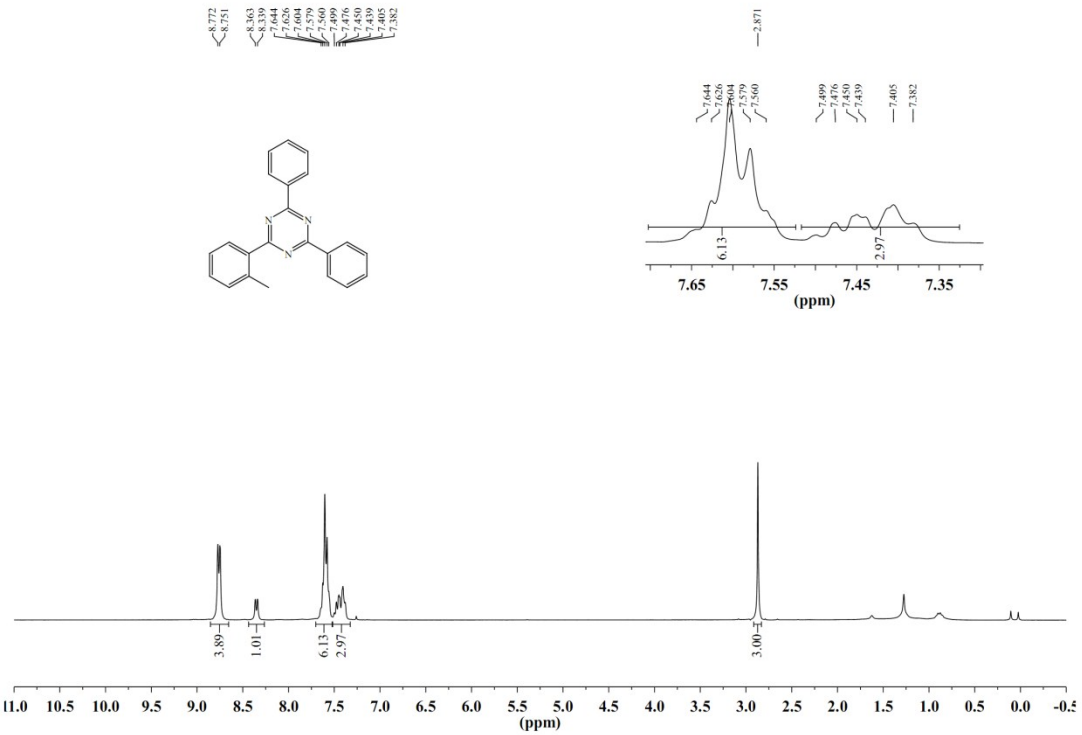

8.786
8.782
8.761
8.755
8.743
8.680
8.654
7.660
7.636
7.611
7.586
7.573
7.567
7.557
7.540
7.515
7.489
Cl
4.61
0.98
8.38
(ppm)
172.163
170.921
138.525
136.294
135.198
133.097
132.790
130.292
129.577
129.283
129.073
127.432
Cl
(ppm)

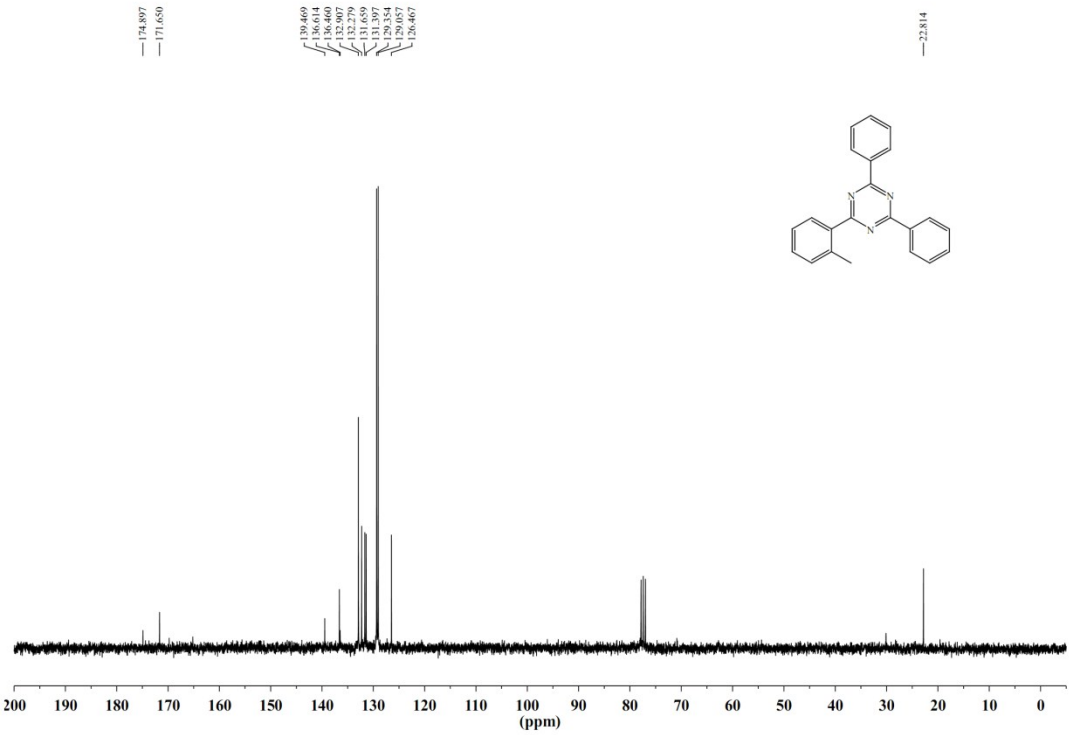
3da


8.726
8.706
8.608
8.582
7.540
7.518
7.306
7.280
2.398
3.97
1.98
6.07
2.00
3.00
(ppm)


171.875
171.772
143.458
136.720
133.871
132.776
129.760
129.338
128.966
22.169
(ppm)

3ea

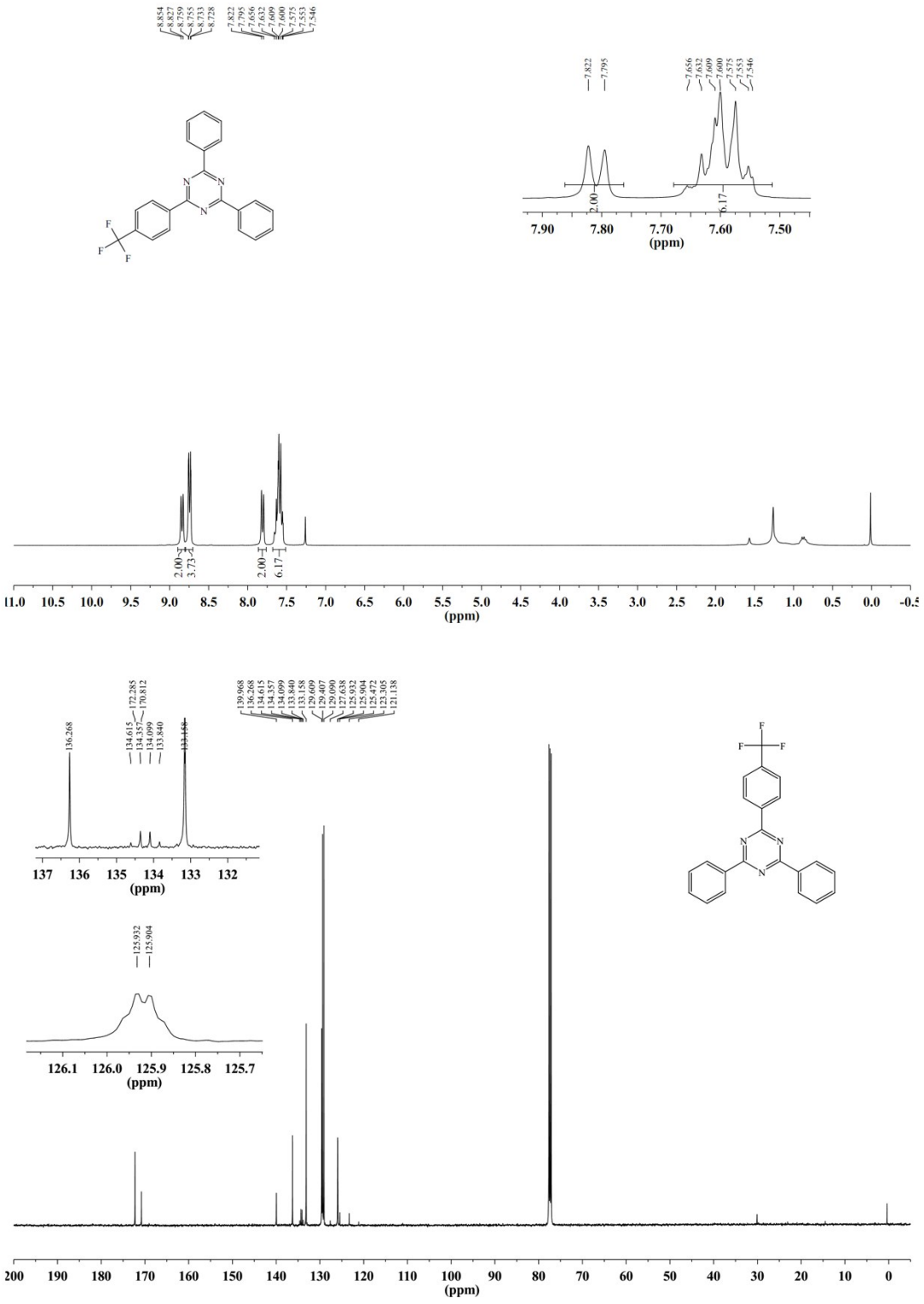

8.772
8.751
8.363
8.339
7.644
7.626
7.604
7.579
7.560
7.499
7.476
7.450
7.439
7.405
7.382
2.871
3.89
1.01
6.13
2.97
3.00
(ppm)


174.897
171.650
139.469
136.614
136.460
132.907
132.279
131.659
131.397
129.354
129.057
126.467
22.814
(ppm)

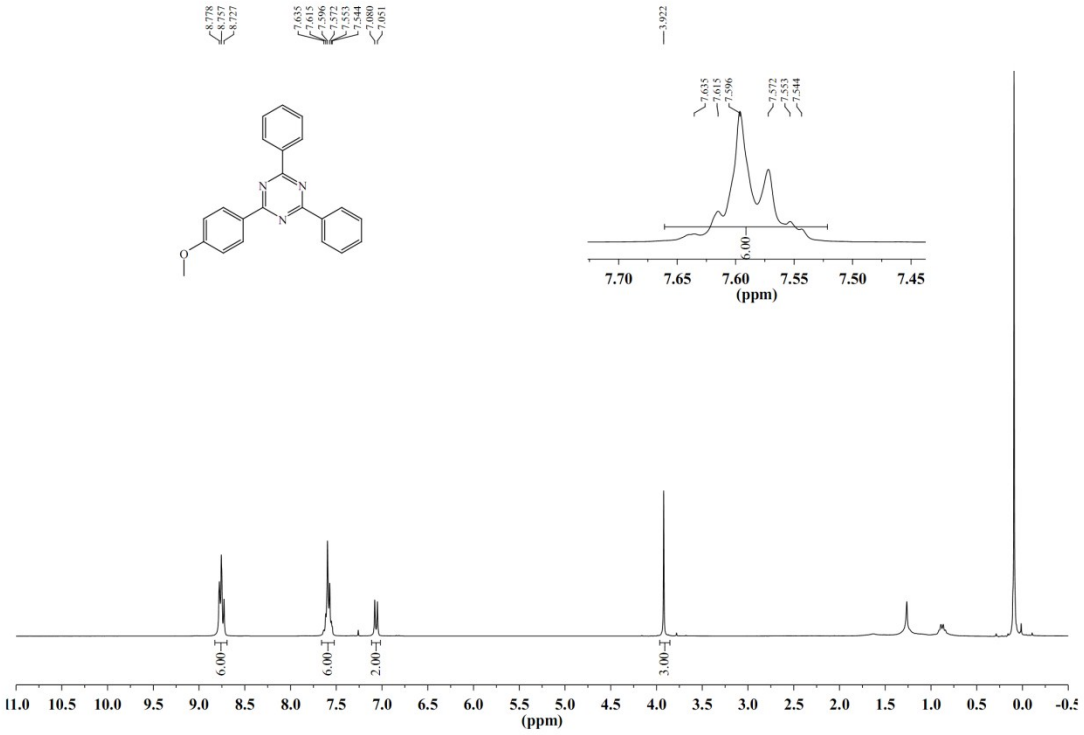
3fa

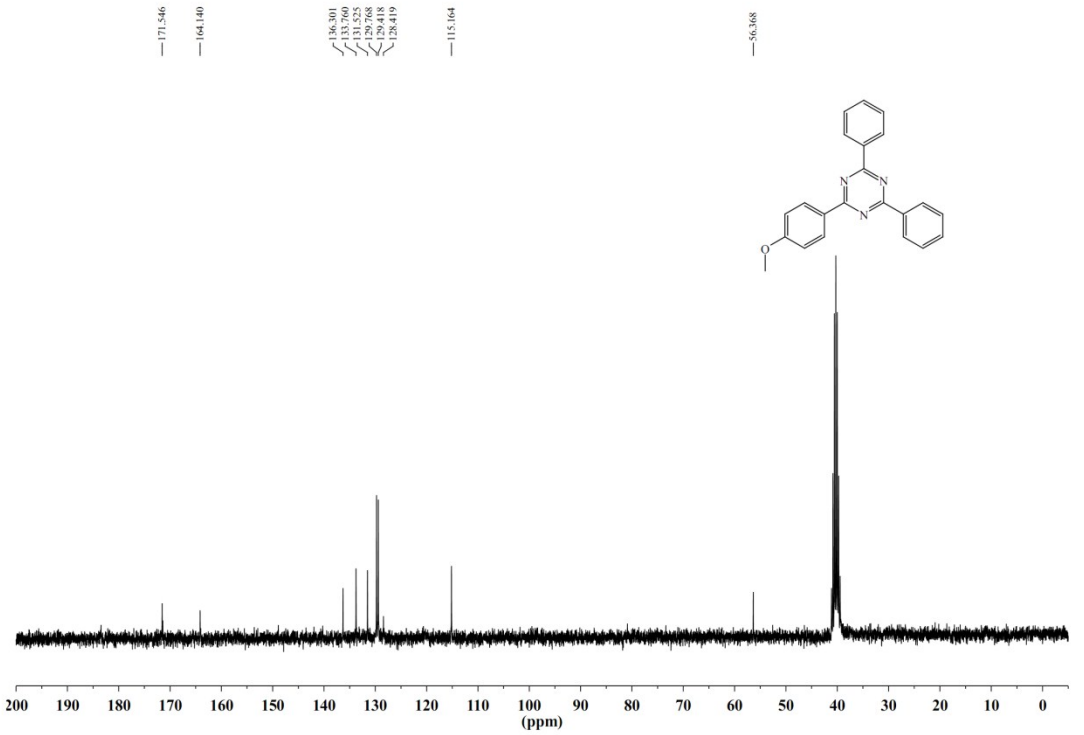

8.801
8.780
8.774
8.601
8.583
7.647
7.627
7.609
7.585
7.566
7.556
7.503
7.478
7.451
7.442
7.417
2.534
6.00
2.09
7.65
7.60
7.55
7.50
7.45
7.40
(ppm)
3.96
1.98
6.00
2.09
3.00
(ppm)
171.968
169.441
138.711
136.640
136.526
133.729
132.859
129.804
129.332
129.011
128.944
126.573
21.960
(ppm)

3ga

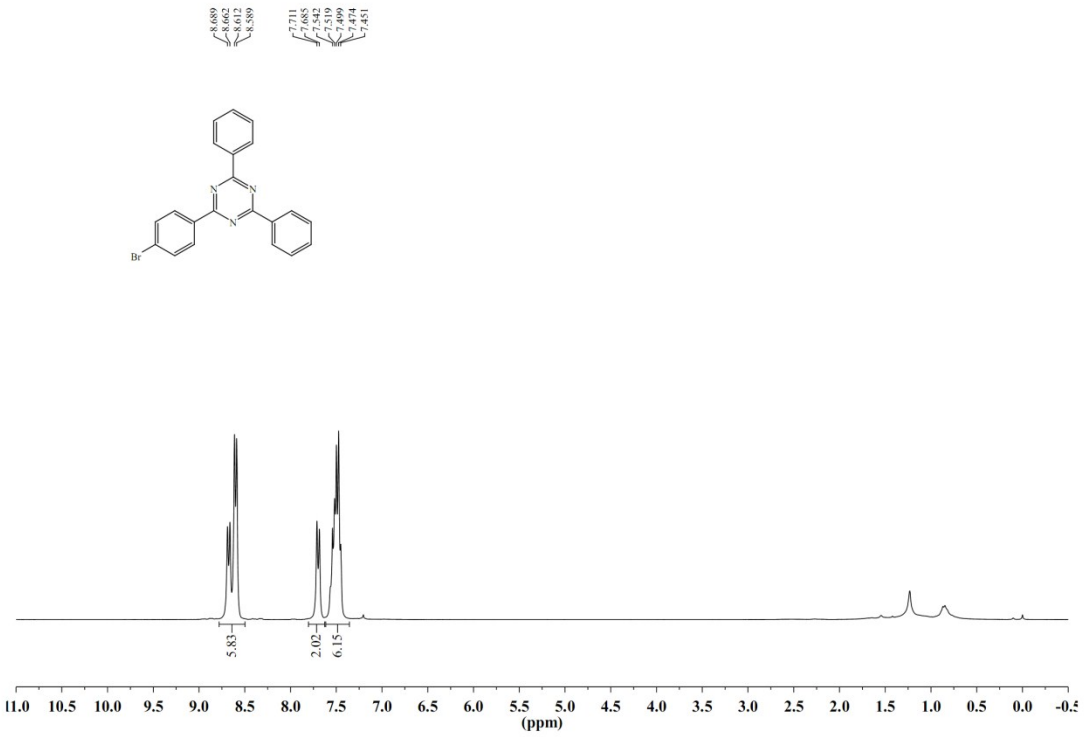

8.854
8.827
8.759
8.735
8.733
8.728
7.822
7.795
7.656
7.632
7.609
7.600
7.575
7.553
7.546
F
F
F
N
N
N
2.00
6.17
7.90
7.80
7.70
7.60
7.50
(ppm)
2.00
3.73
2.00
6.17
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
(ppm)
136.268
134.615
134.357
134.099
133.840
133.158
172.285
170.812
139.968
136.268
134.615
134.357
134.099
133.840
133.158
129.609
129.407
129.090
127.638
125.932
125.904
125.472
123.305
121.138
137
136
135
134
133
132
(ppm)
125.932
125.904
126.1
126.0
125.9
125.8
125.7
(ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

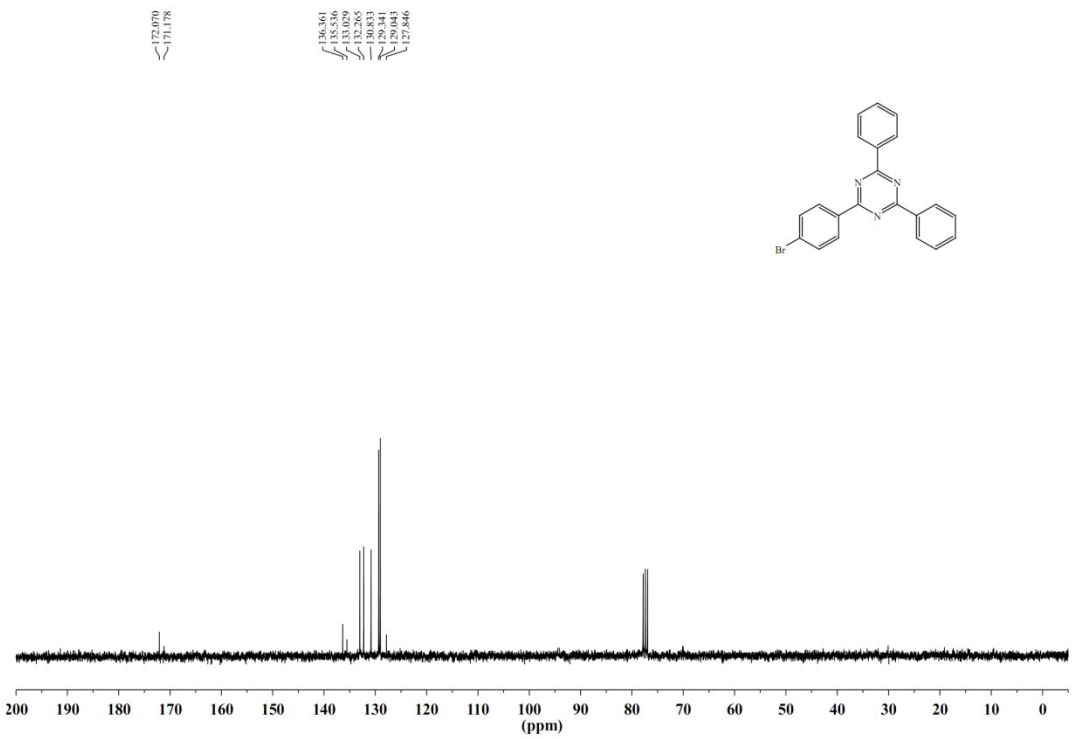
3ha


8.778
8.757
8.727
7.635
7.615
7.596
7.572
7.553
7.544
7.080
7.051
3.922
6.00
6.00
2.00
3.00
(ppm)

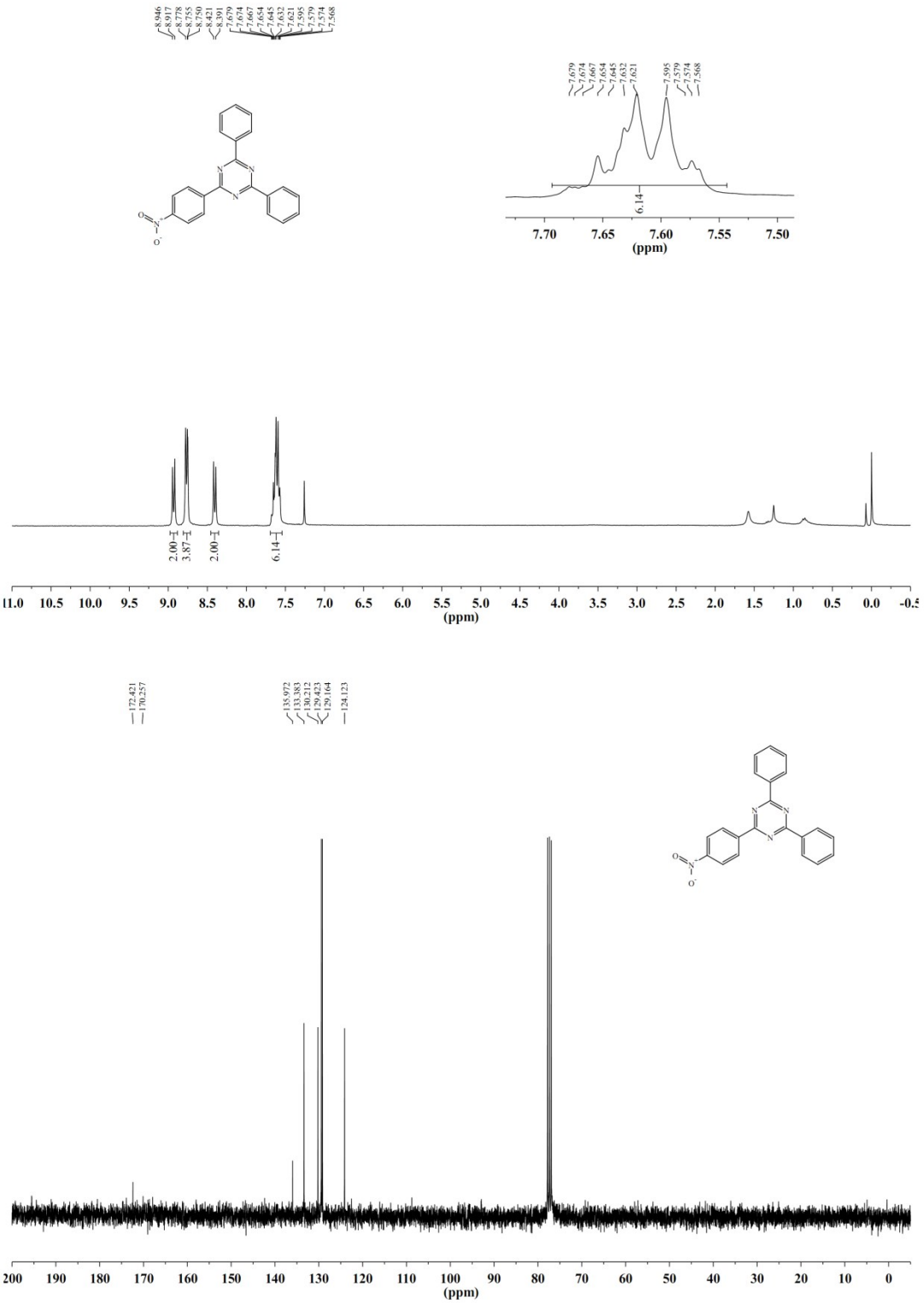

171.546
164.140
136.301
133.760
131.525
129.768
129.418
128.419
115.164
56.368
(ppm)

3ia

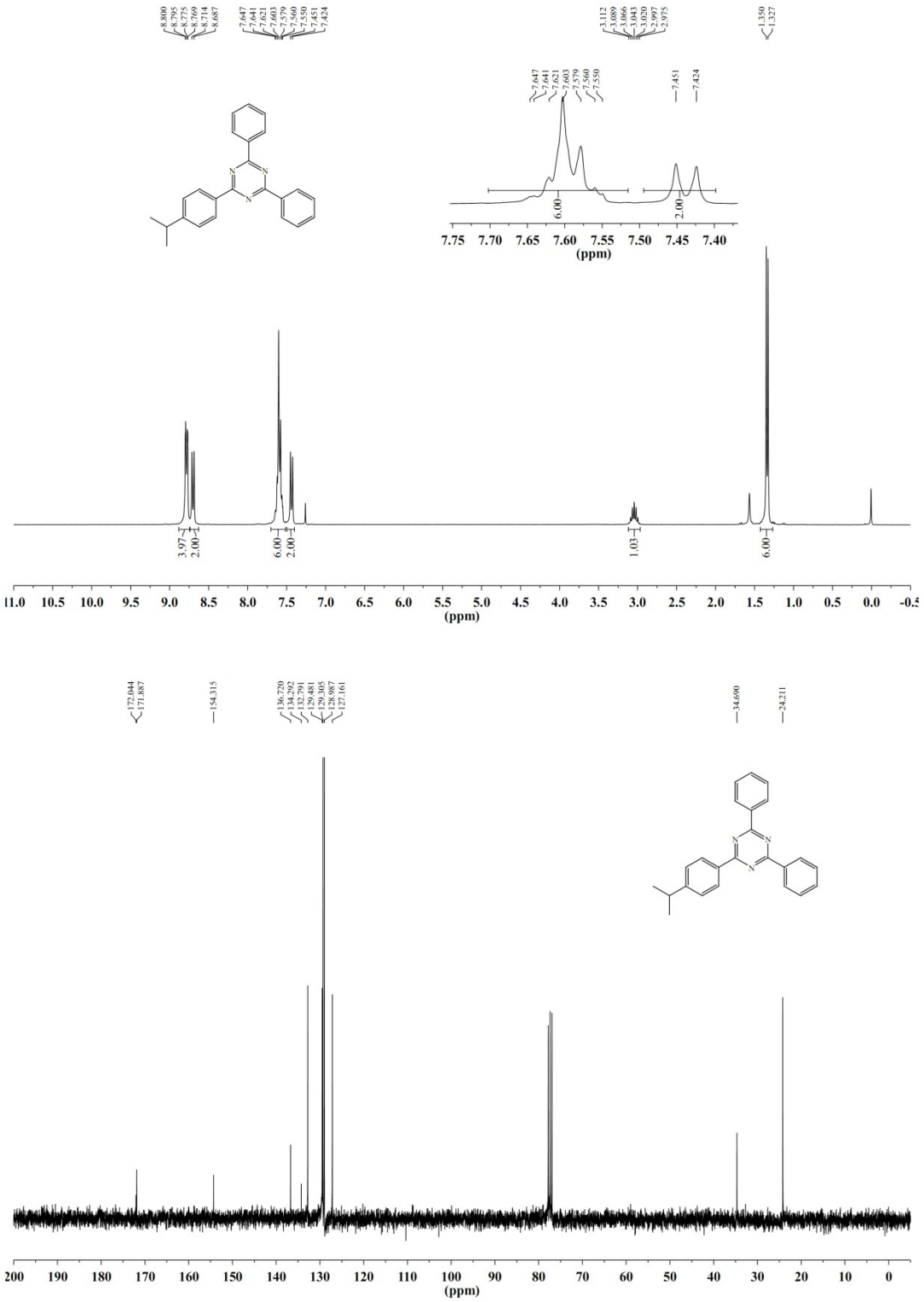

8.689
8.662
8.617
8.589
7.711
7.685
7.542
7.519
7.499
7.474
7.451
Br
5.83
2.02
6.15
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)


172.070
171.178
136.361
135.536
133.029
132.265
130.833
129.341
129.043
127.846
Br
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

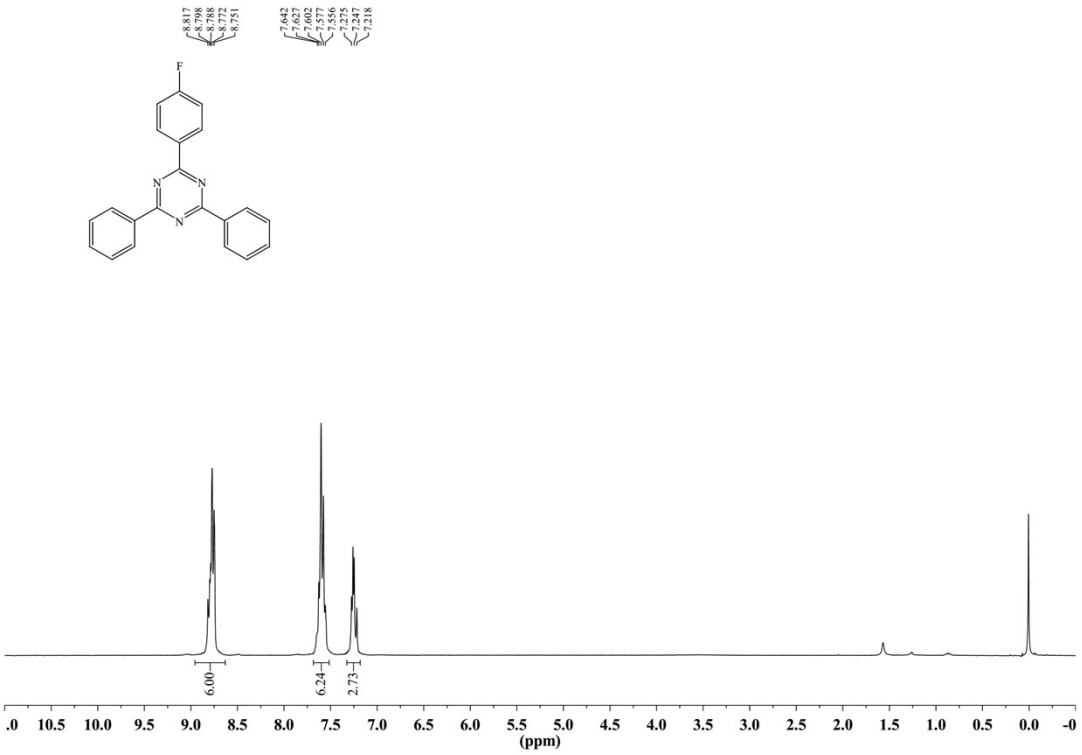
3ja

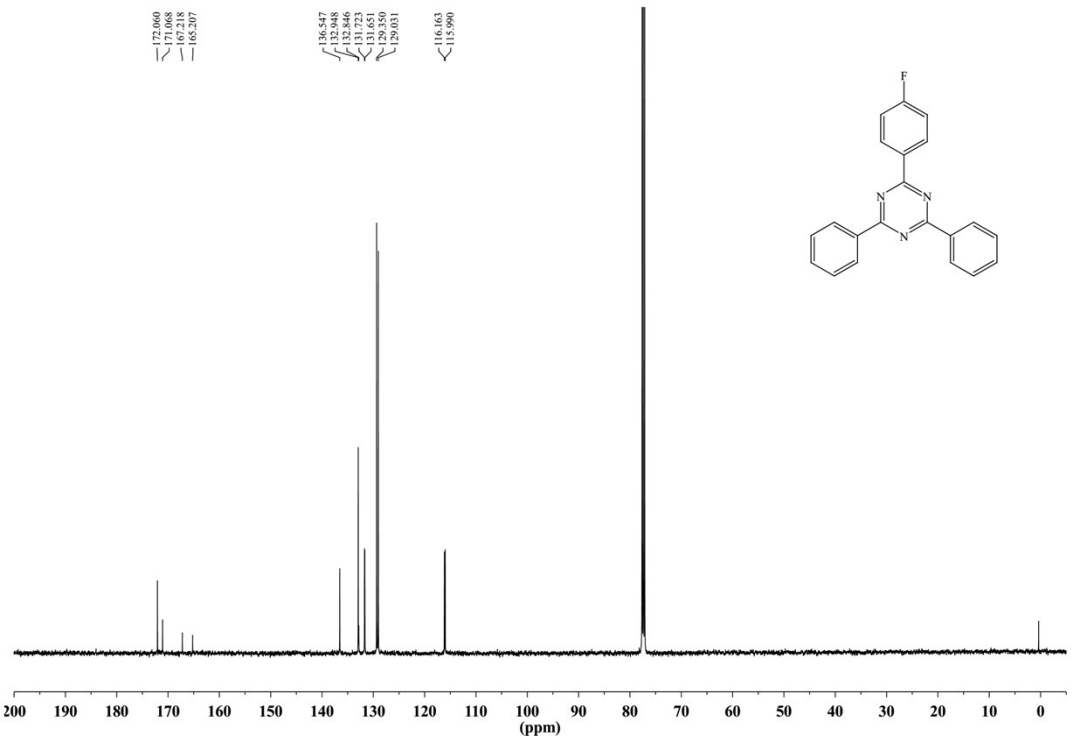

8.946
8.917
8.778
8.755
8.750
8.421
8.391
7.679
7.674
7.667
7.654
7.645
7.632
7.621
7.595
7.579
7.574
7.568
7.679
7.674
7.667
7.654
7.645
7.632
7.621
7.595
7.579
7.574
7.568
6.14
7.70
7.65
7.60
7.55
7.50
(ppm)
2.00
3.87
2.00
6.14
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)
172.421
170.257
135.972
133.383
130.212
129.423
129.164
124.123
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

3ka

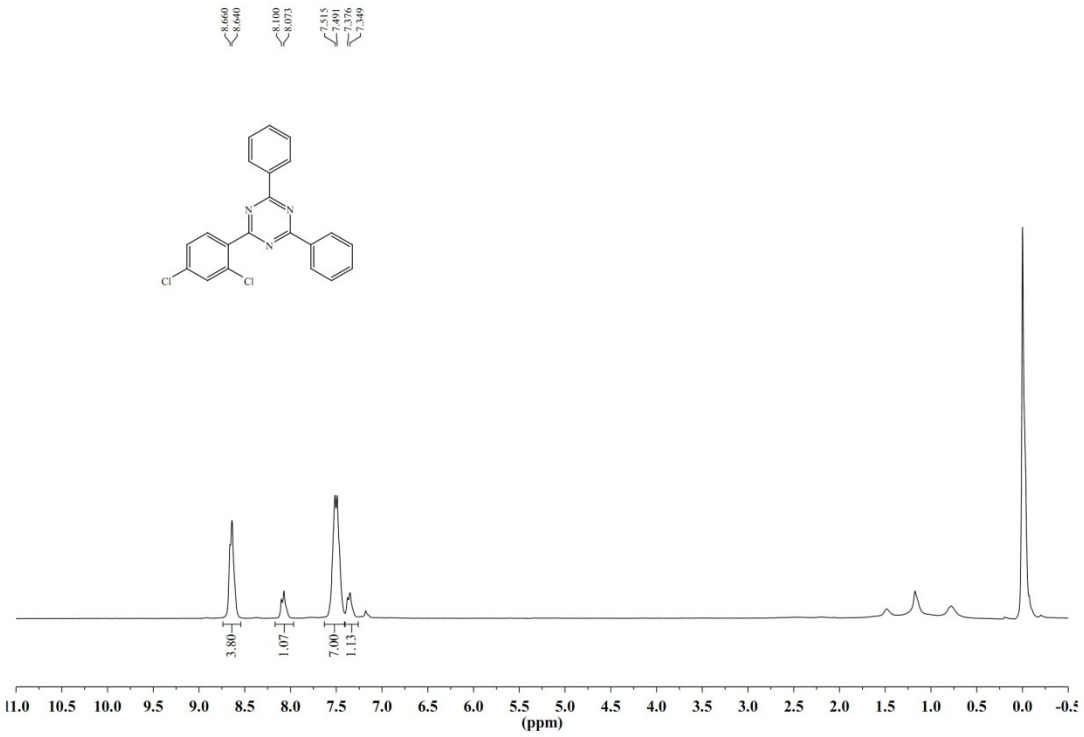


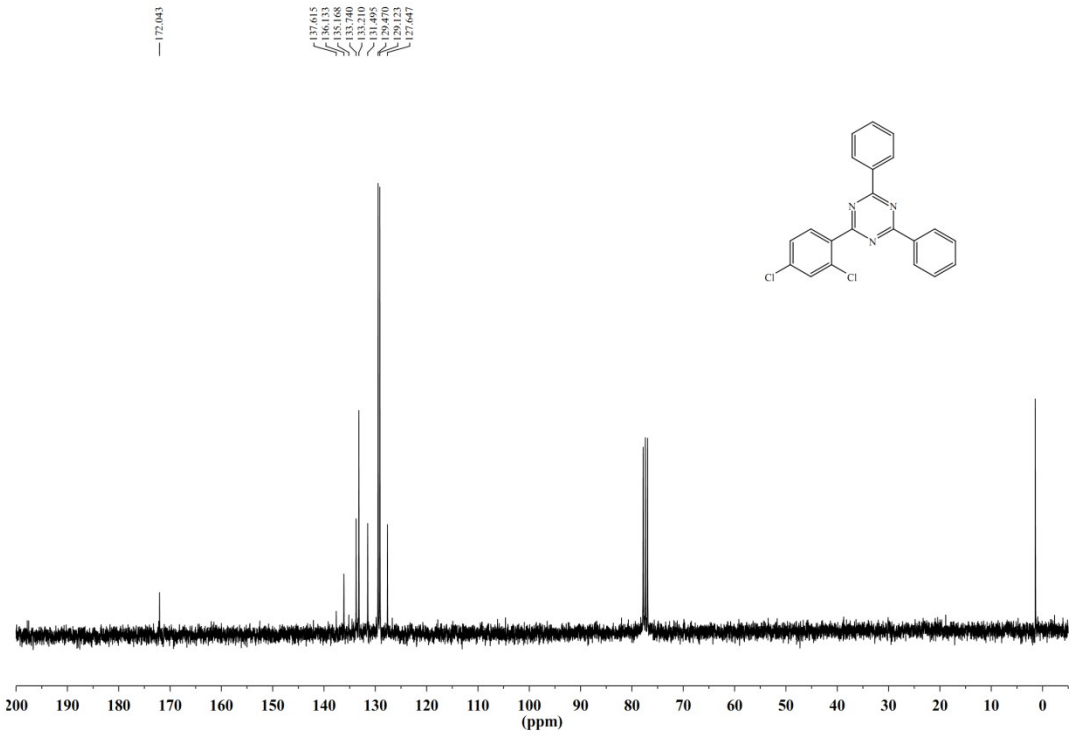
3la


8.817
8.798
8.788
8.772
8.751
7.642
7.627
7.602
7.577
7.556
7.275
7.247
7.218
F
N
N
N
6.00
6.24
2.73
.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
(ppm)

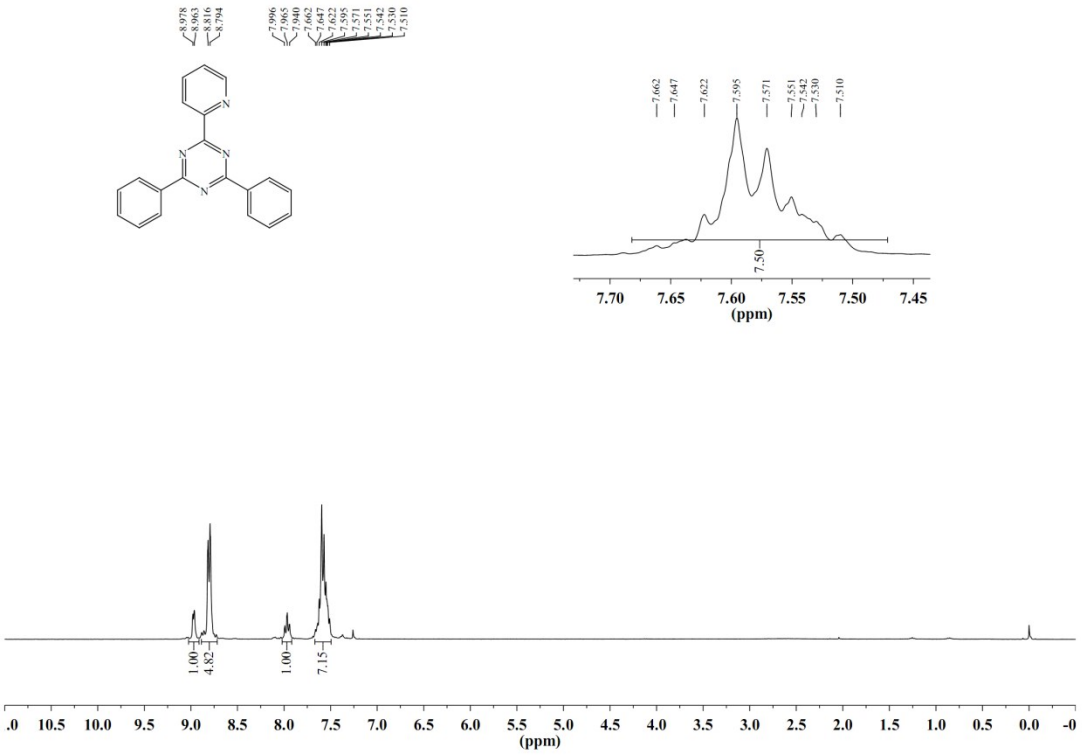

172.060
171.068
167.218
165.207
136.547
132.848
132.846
131.723
131.651
129.350
129.031
116.163
115.990
F
N
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

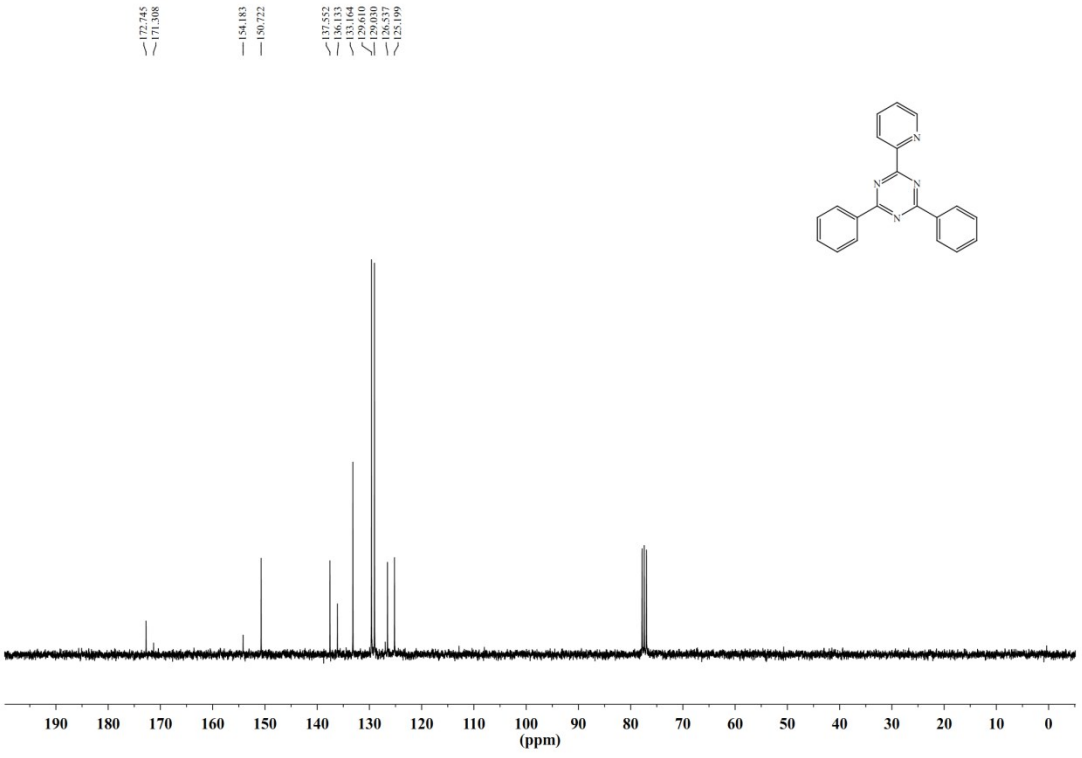
3ma


8.660
8.640
8.100
8.073
7.515
7.501
7.376
7.349
3.80
1.07
7.00
1.13
(ppm)

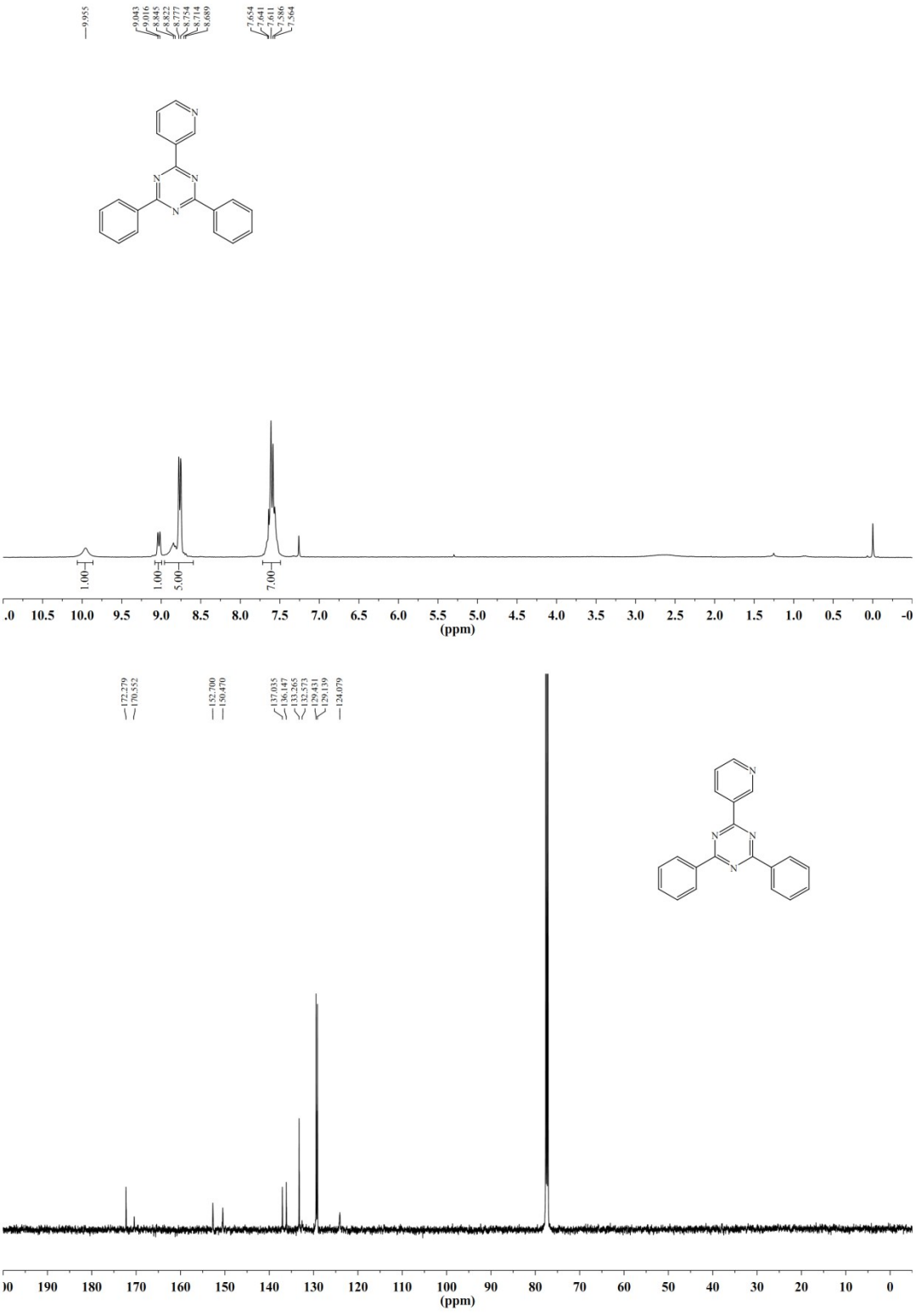

172.043
137.615
136.133
135.168
133.960
133.210
131.495
129.470
129.123
127.647
(ppm)

3na


8.978
8.963
8.816
8.794
7.996
7.965
7.940
7.662
7.647
7.622
7.595
7.571
7.551
7.542
7.530
7.510
7.50
7.70
7.65
7.60
7.55
7.50
7.45
(ppm)
1.00
4.82
1.00
7.15
(ppm)

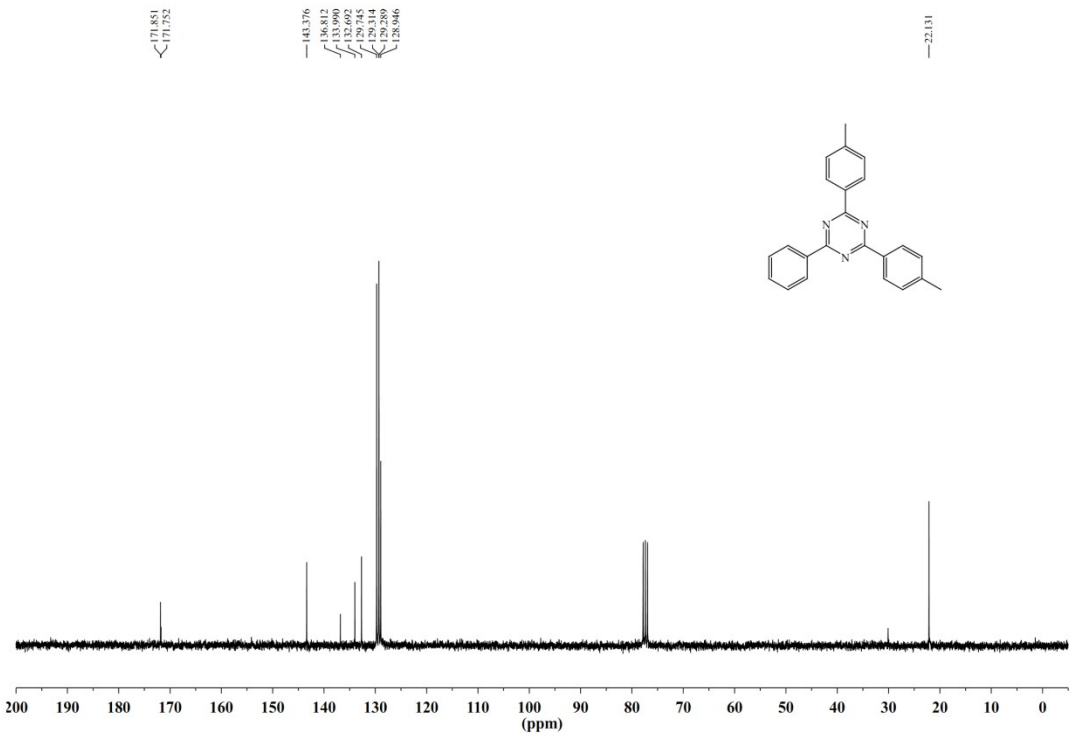

172.745
171.308
154.183
150.722
137.552
136.133
133.164
129.310
129.030
126.537
125.199
(ppm)

3oa

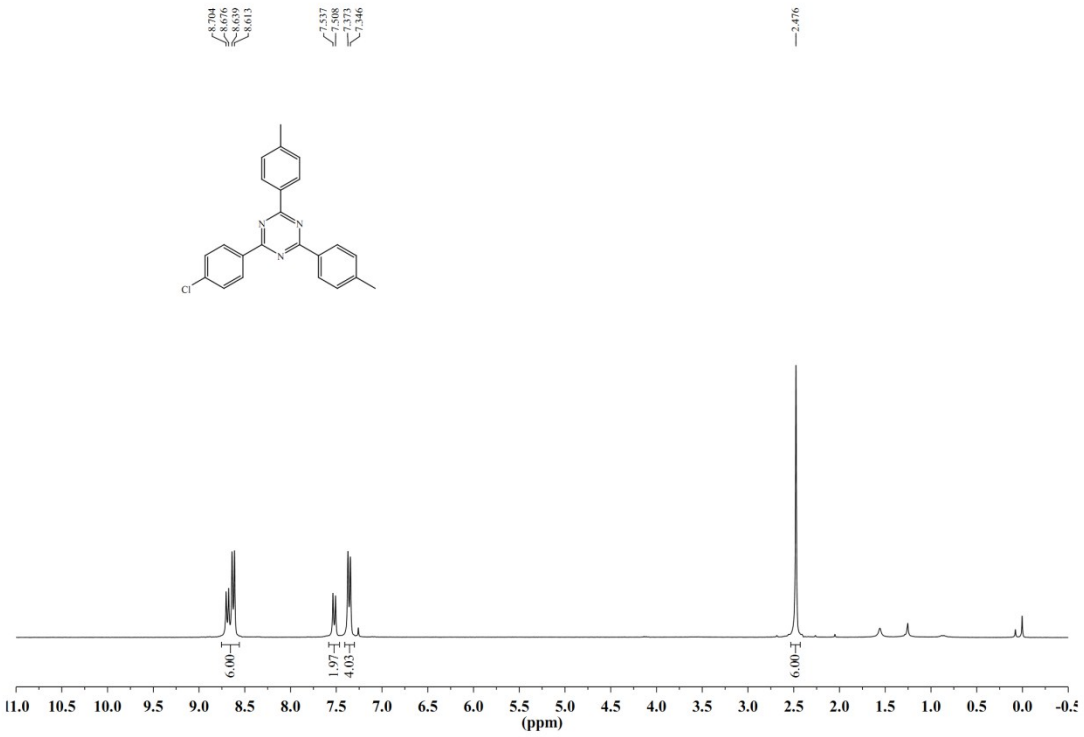

9.955
9.043
9.016
8.845
8.822
8.777
8.754
8.714
8.689
7.654
7.641
7.611
7.586
7.564
1.00
1.00
5.00
7.00
(ppm)
172.279
170.552
152.700
150.470
137.035
136.147
133.565
132.573
129.431
129.139
124.079
(ppm)

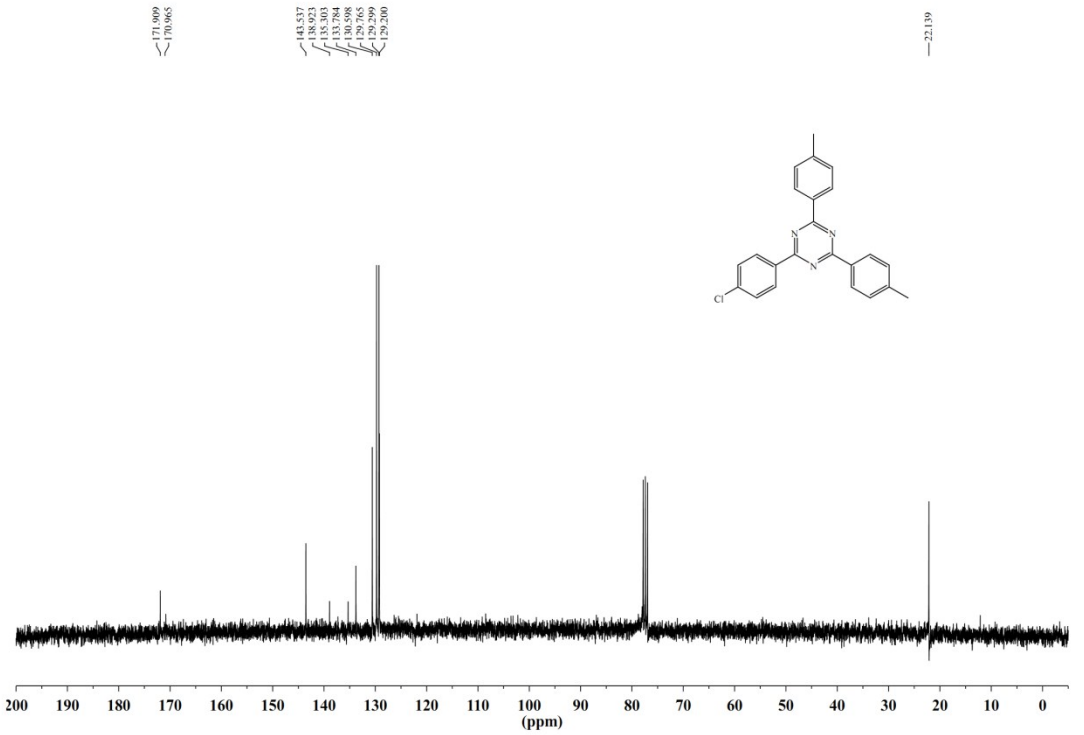
3pa


8.782
8.762
8.678
8.651
7.633
7.612
7.595
7.573
7.555
7.383
7.357
2.489
2.00
4.01
3.03
3.97
6.00
(ppm)

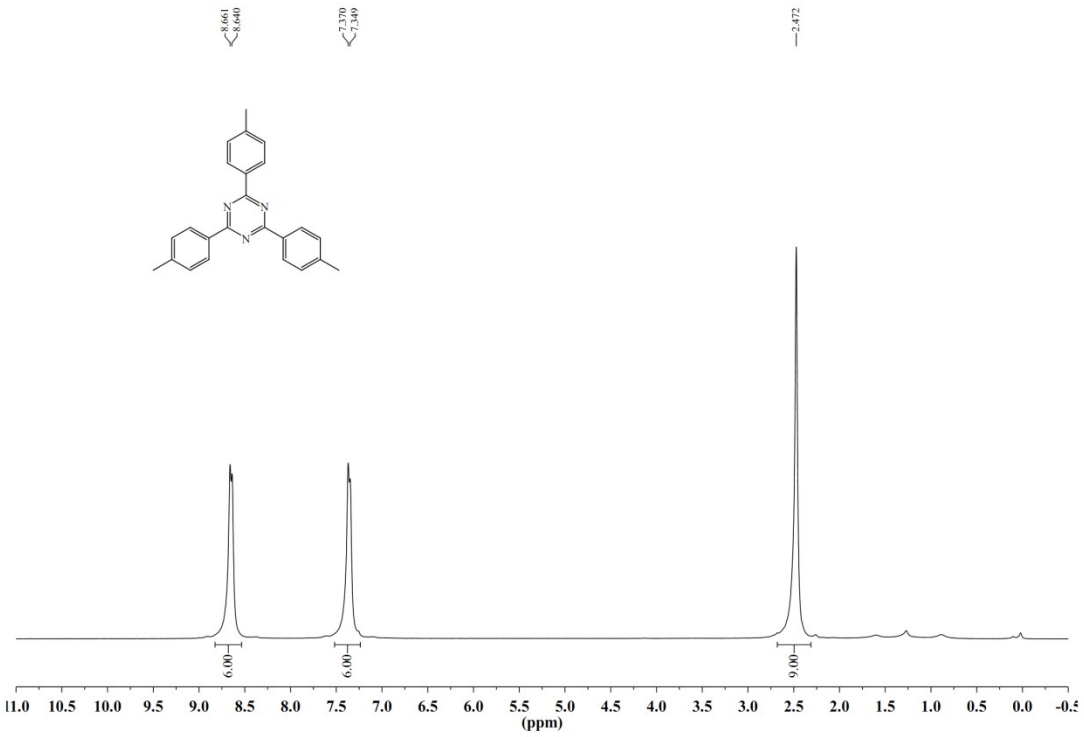

171.851
171.752
143.376
136.812
133.969
132.692
129.745
129.314
129.289
128.946
22.131
(ppm)

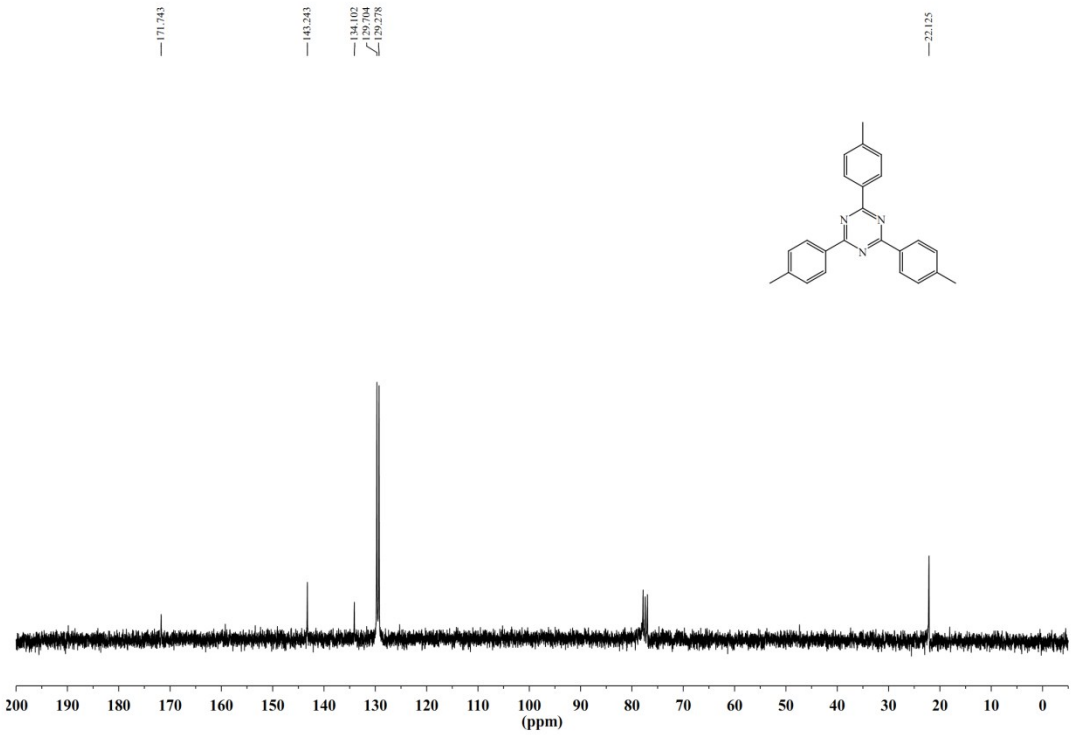
3ab


8.704
8.676
8.639
8.613
7.537
7.508
7.373
7.346
2.476
6.00
1.97
4.03
6.00
(ppm)

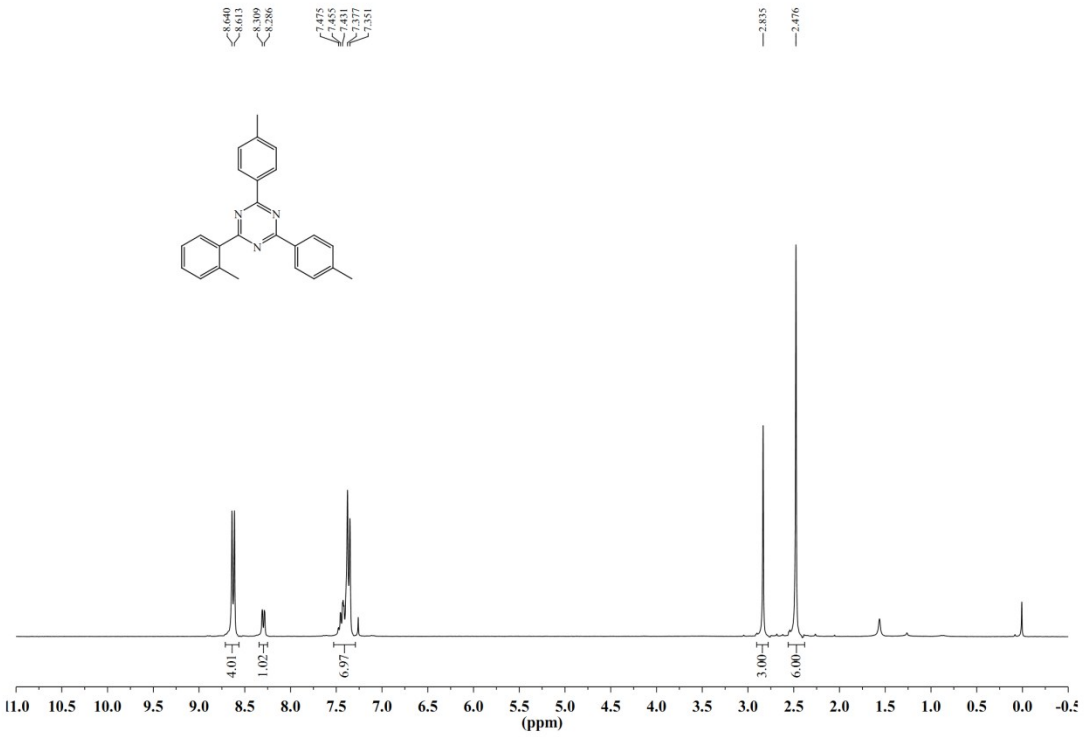

171.909
170.965
143.537
138.923
135.303
133.784
130.598
129.765
129.299
129.200
22.139
(ppm)

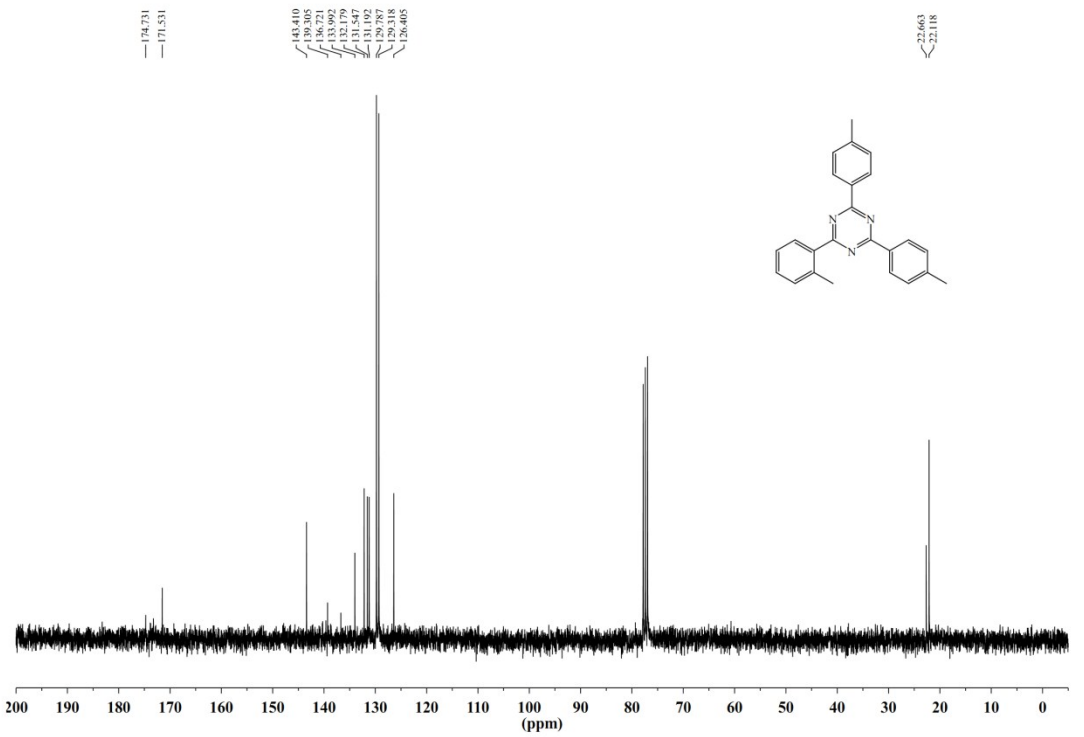
3bb


8.661
8.640
7.370
7.349
2.472
6.00
6.00
9.00
(ppm)

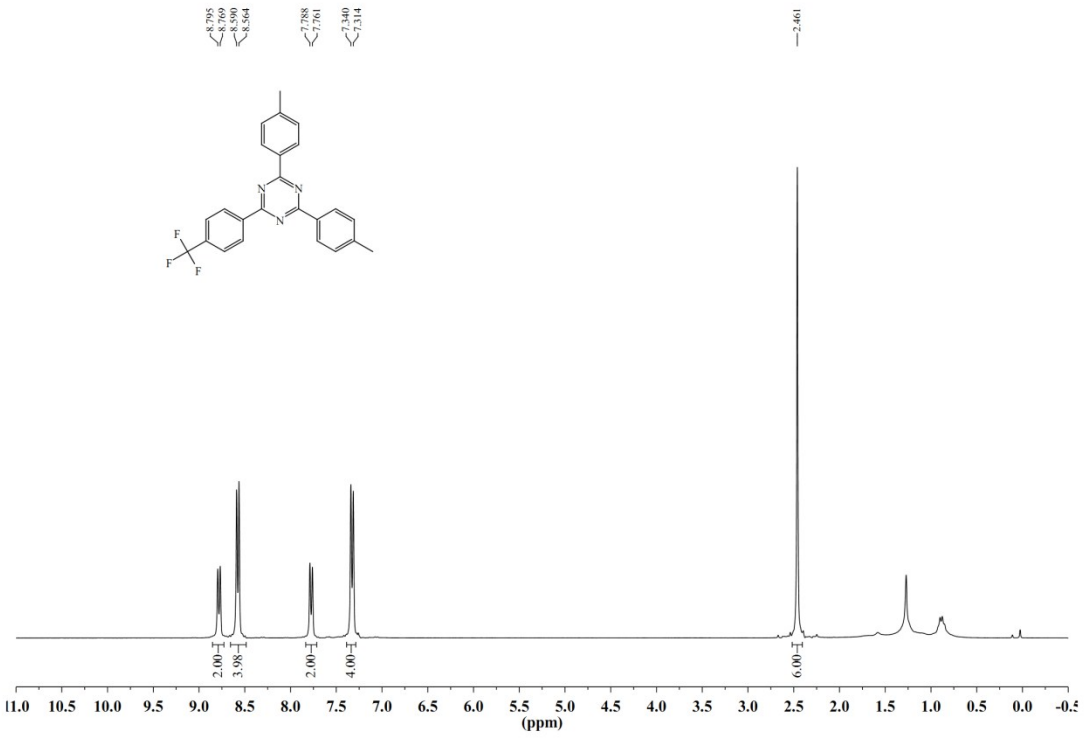

171.743
143.243
134.102
129.704
129.278
22.125
(ppm)

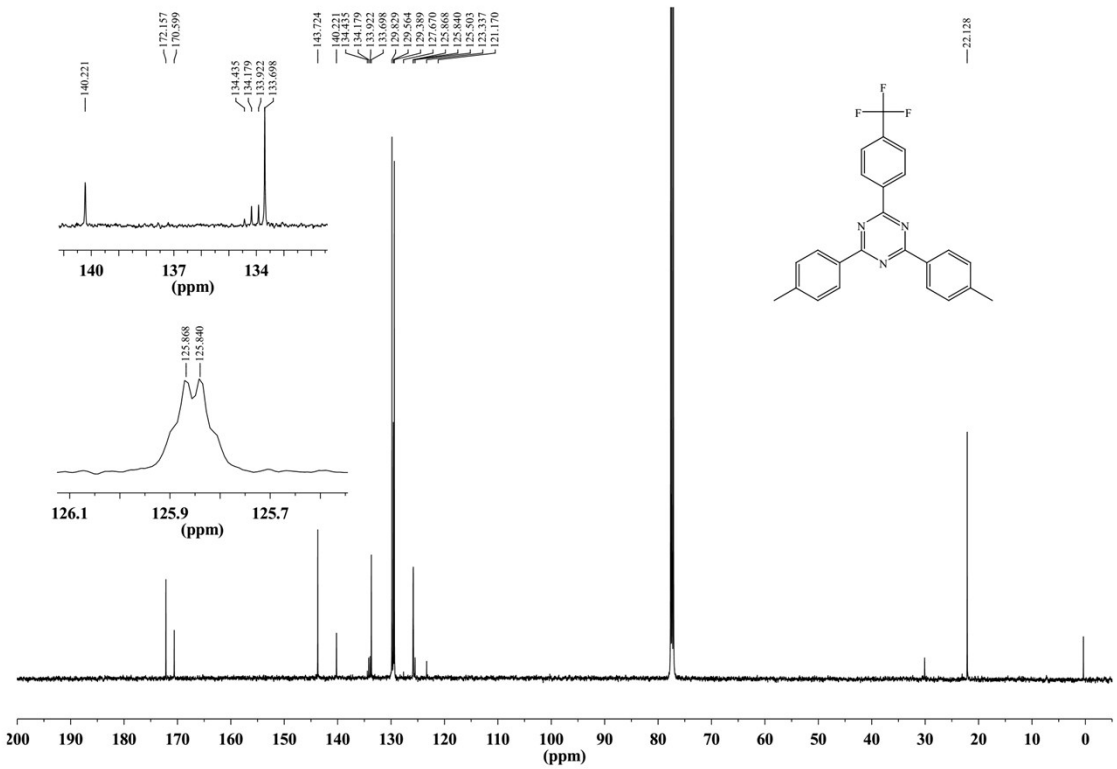
3eb


8.640
8.613
8.309
8.286
7.475
7.455
7.431
7.377
7.351
2.835
2.476
4.01
1.02
6.97
3.00
6.00
(ppm)

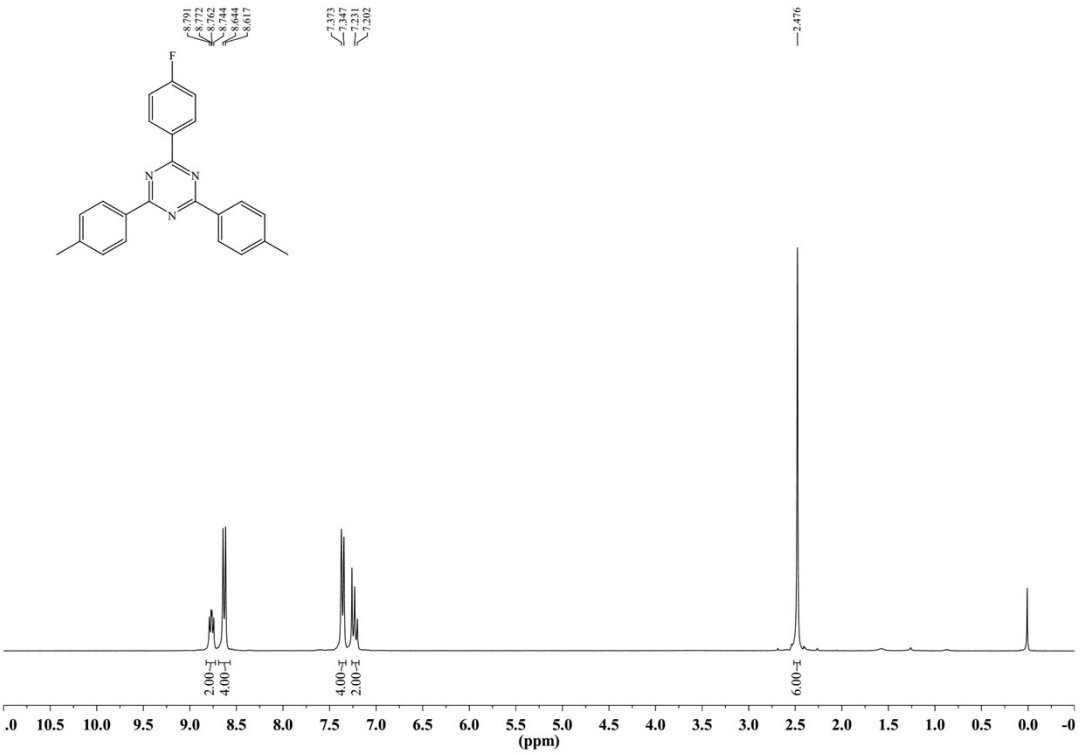

174.731
171.531
143.410
139.365
136.721
133.992
132.179
131.547
131.192
129.787
129.318
126.405
22.663
22.118
(ppm)

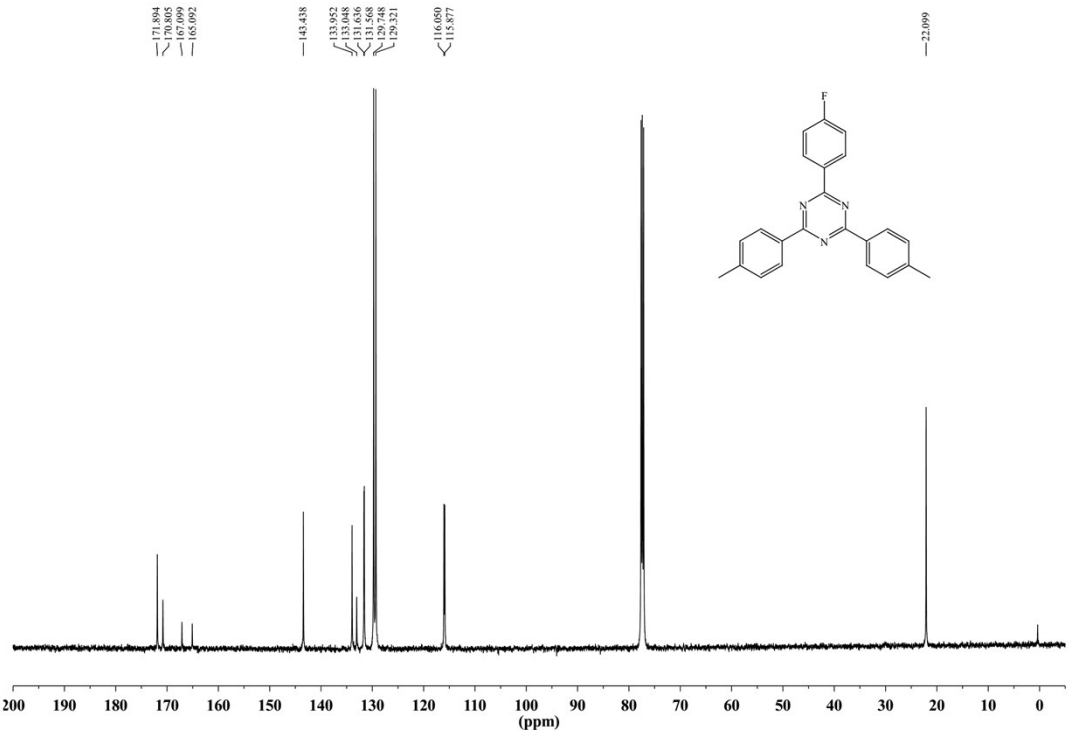
3fb


8.795
8.769
8.590
8.564
7.788
7.761
7.340
7.314
2.461
2.00
3.98
2.00
4.00
6.00
(ppm)

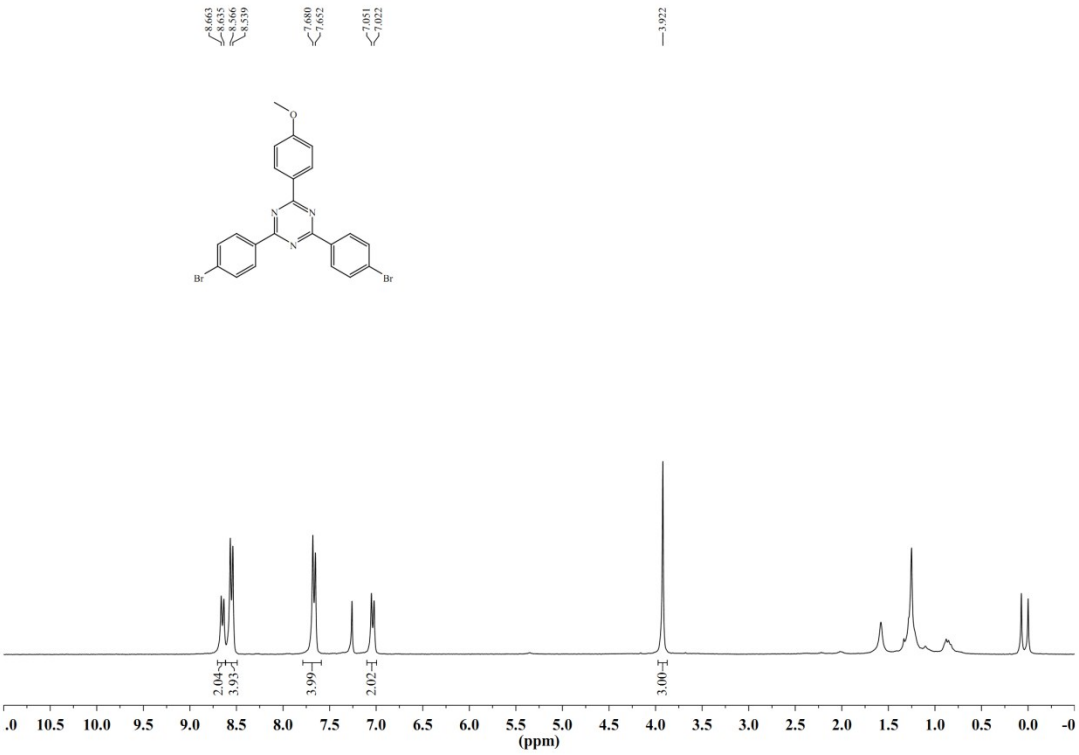

172.157
170.599
143.724
140.221
134.435
134.179
133.922
133.698
129.829
129.564
129.369
127.670
125.868
125.840
125.503
123.337
121.170
22.128
140.221
134.435
134.179
133.922
133.698
140
137
134
(ppm)
125.868
125.840
126.1
125.9
125.7
(ppm)
(ppm)

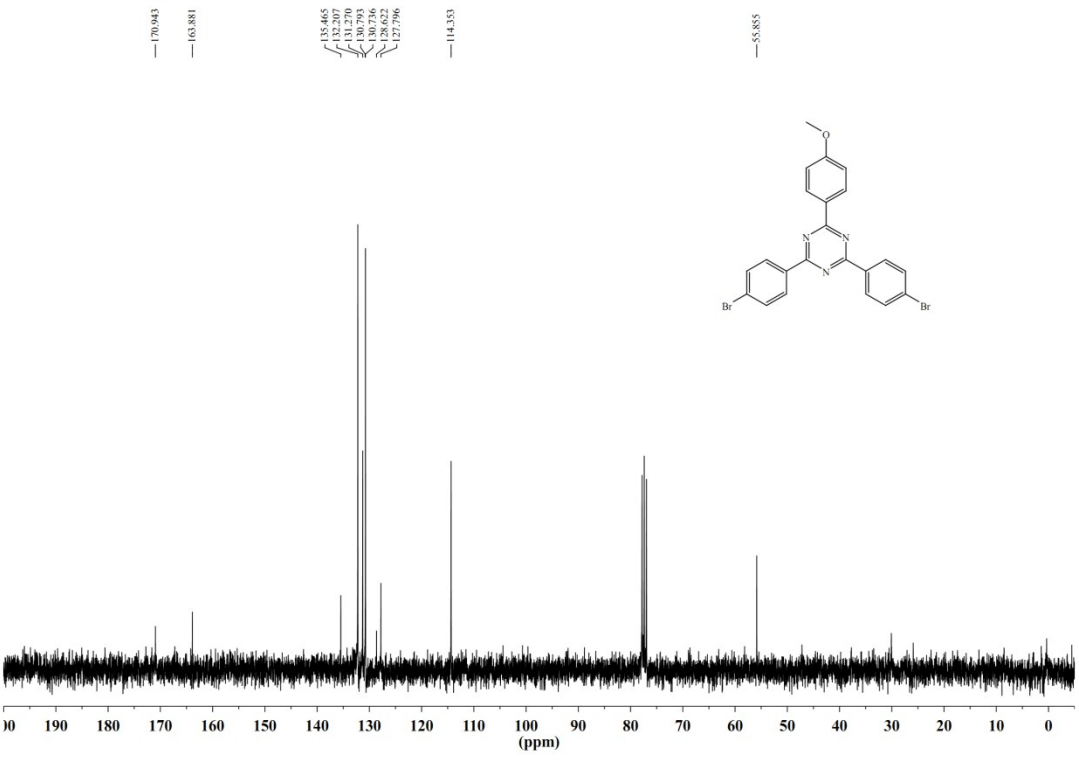
3hb


8.791
8.772
8.762
8.744
8.644
8.617
7.373
7.347
7.231
7.202
2.476
F
N
N
N
2.00
4.00
4.00
2.00
6.00
(ppm)

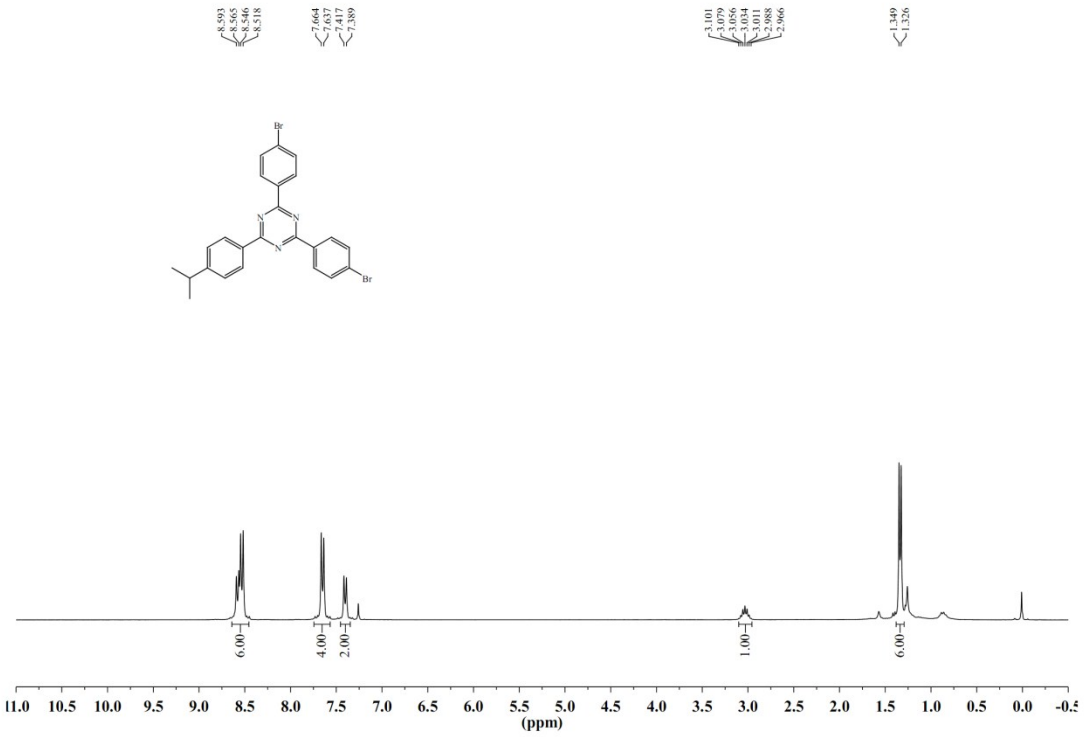

171.894
170.805
167.099
165.092
143.438
133.952
133.048
131.636
131.568
129.748
129.321
116.050
115.877
22.099
F
N
N
N
(ppm)

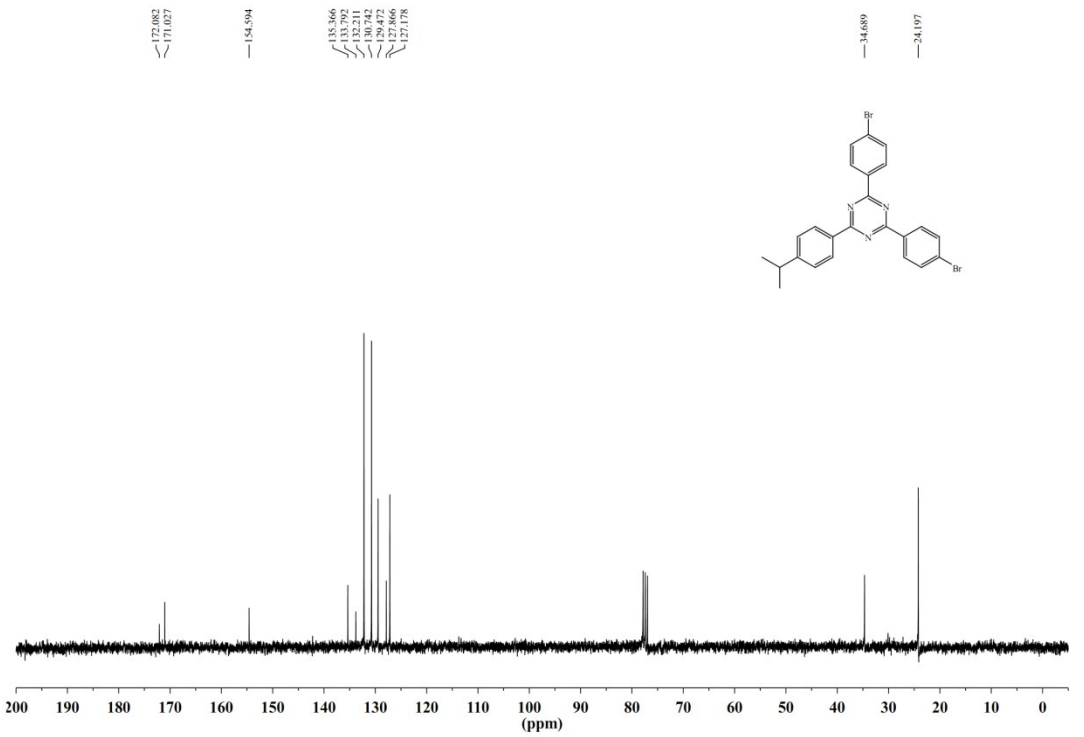
3mb


8.663
8.645
8.566
8.539
7.680
7.652
7.051
7.022
3.922
Br
Br
2.04
3.93
3.99
2.02
3.00
(ppm)

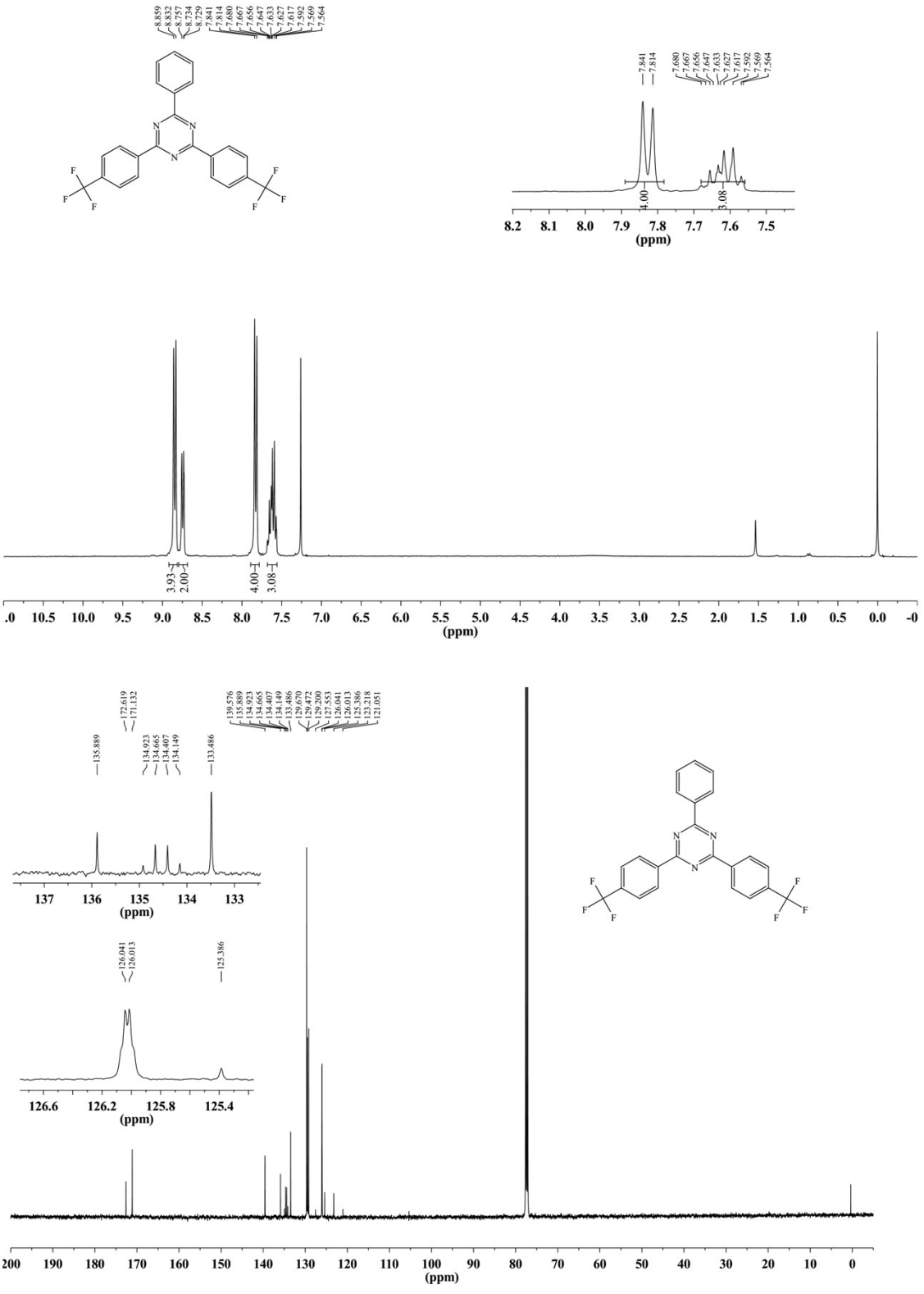

170.943
163.881
135.465
132.207
131.270
130.793
130.736
128.622
127.796
114.353
55.855
Br
Br
(ppm)

3ic

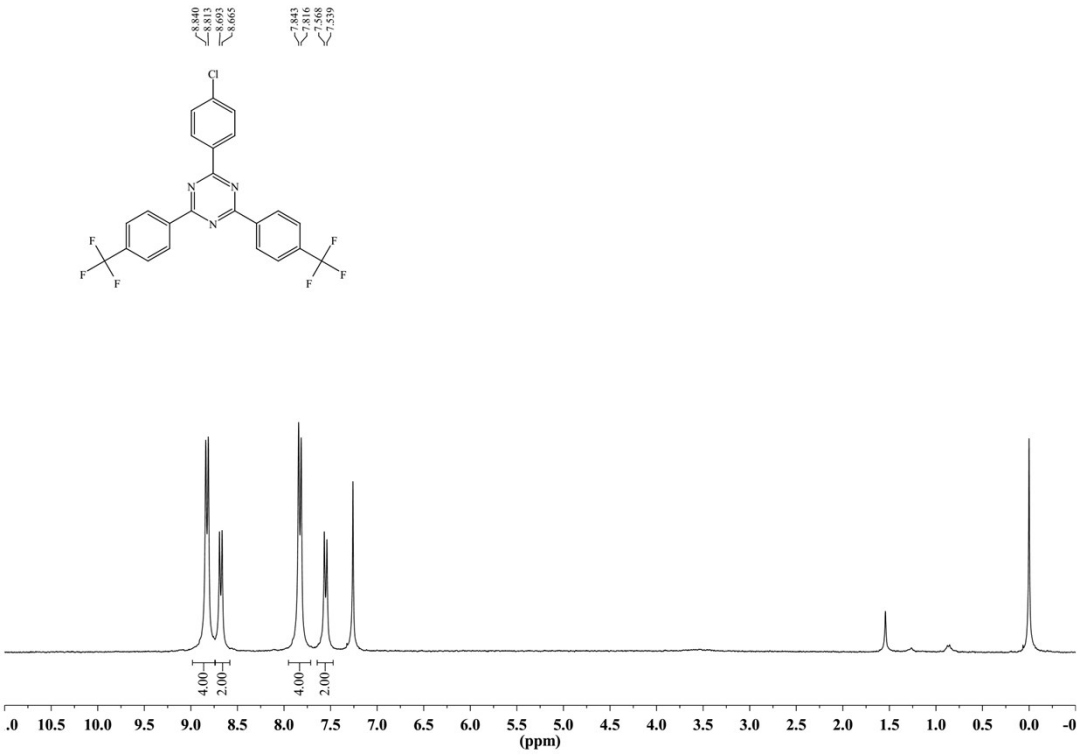

8.593
8.565
8.546
8.518
7.664
7.637
7.417
7.389
3.101
3.079
3.056
3.034
3.011
2.988
2.966
1.349
1.326
Br
Br
6.00
4.00
2.00
1.00
6.00
(ppm)

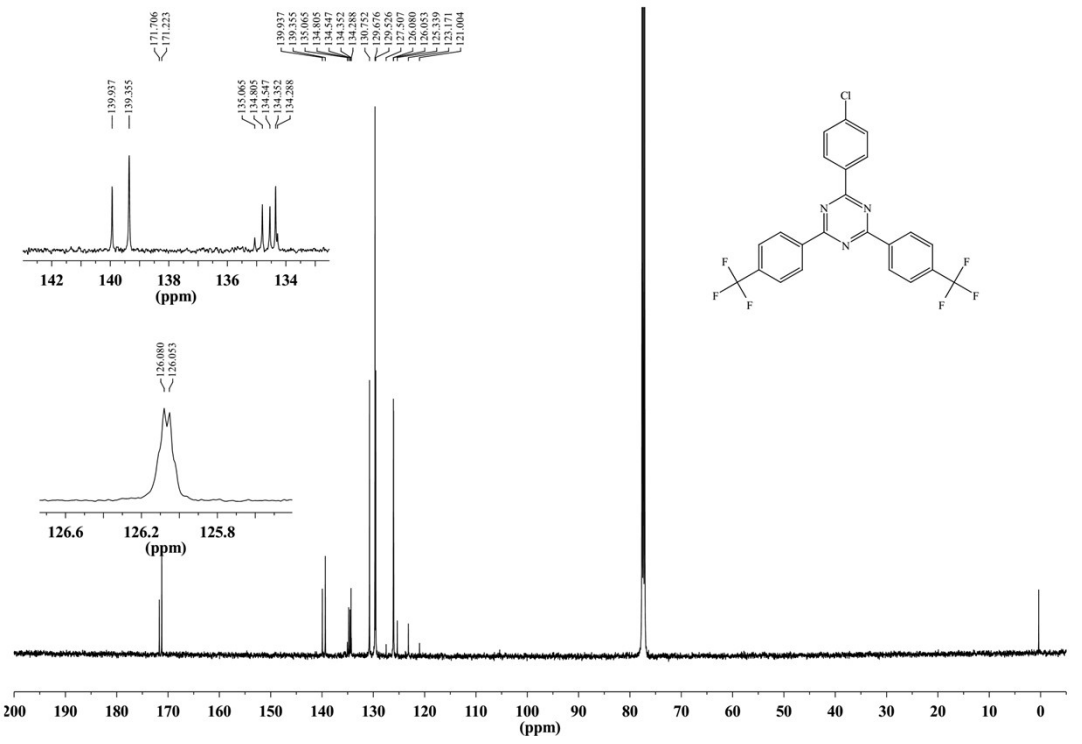

172.082
171.027
154.594
135.366
133.792
132.211
130.742
129.472
127.966
127.198
34.689
24.197
Br
Br
(ppm)

3lc

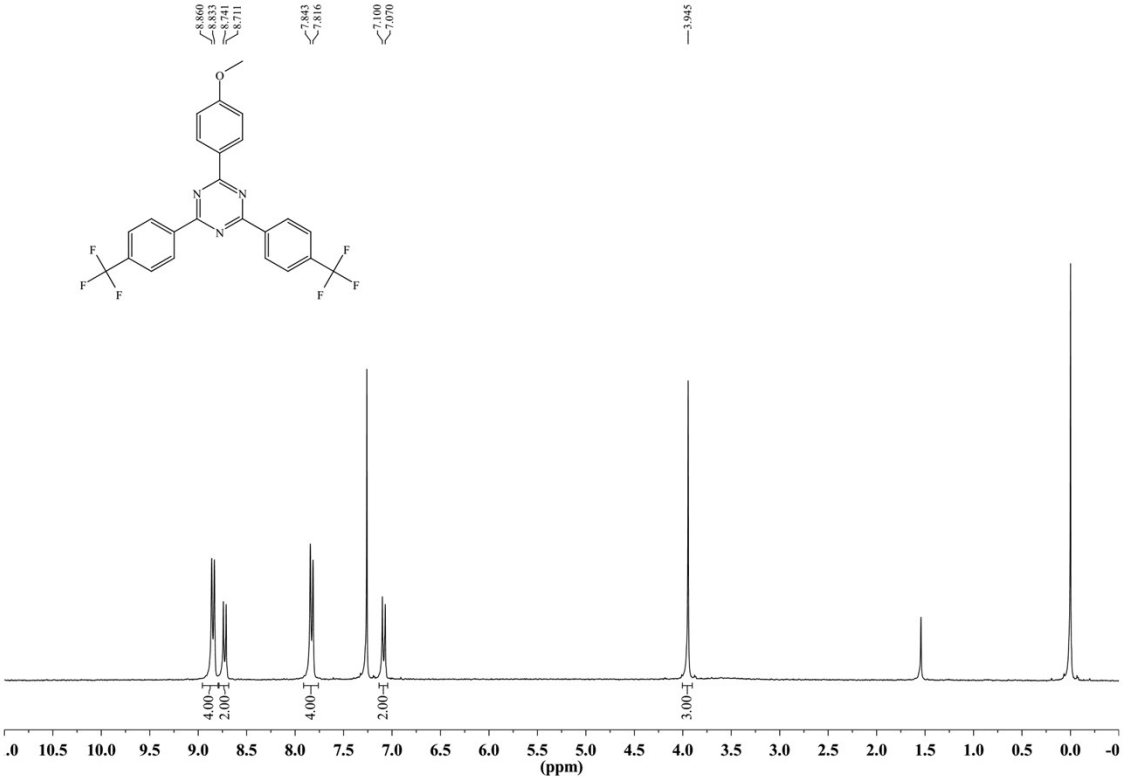


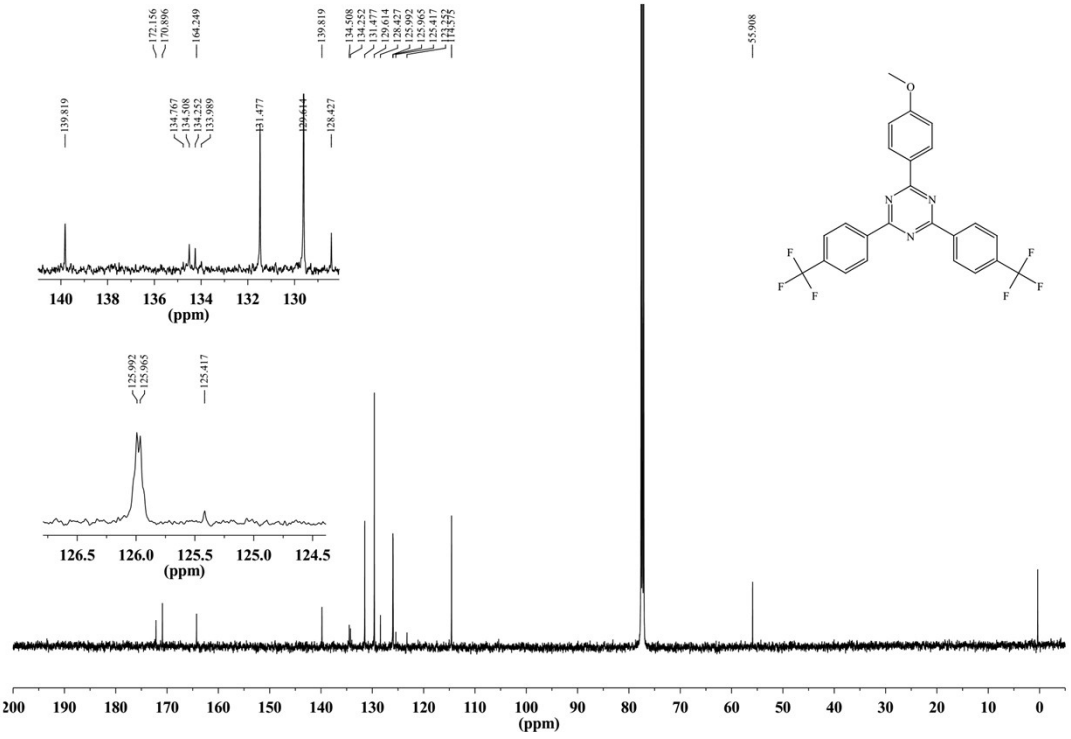
3ad



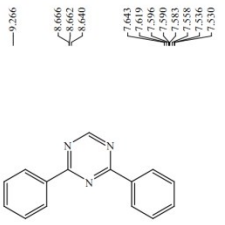


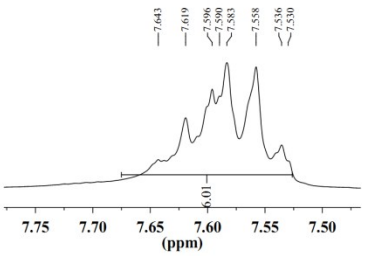
3bd

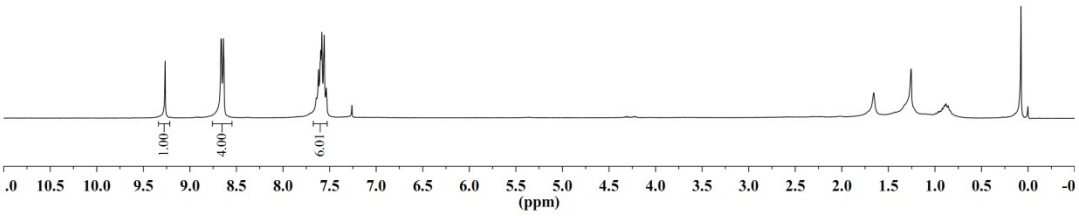

8.860
8.853
8.741
8.711
7.843
7.816
7.100
7.070
3.945
4.00
2.00
4.00
2.00
3.00
(ppm)

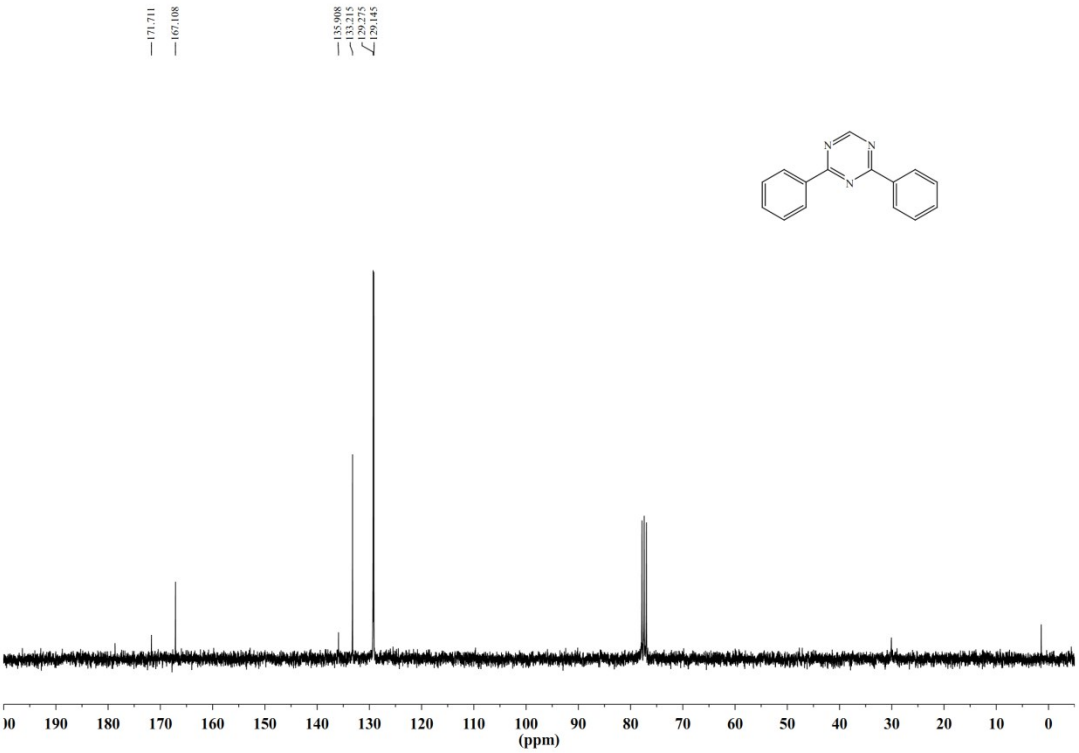

172.156
170.896
164.249
139.819
134.508
134.252
131.477
129.614
128.427
125.992
125.965
125.417
55.908
(ppm)

3id

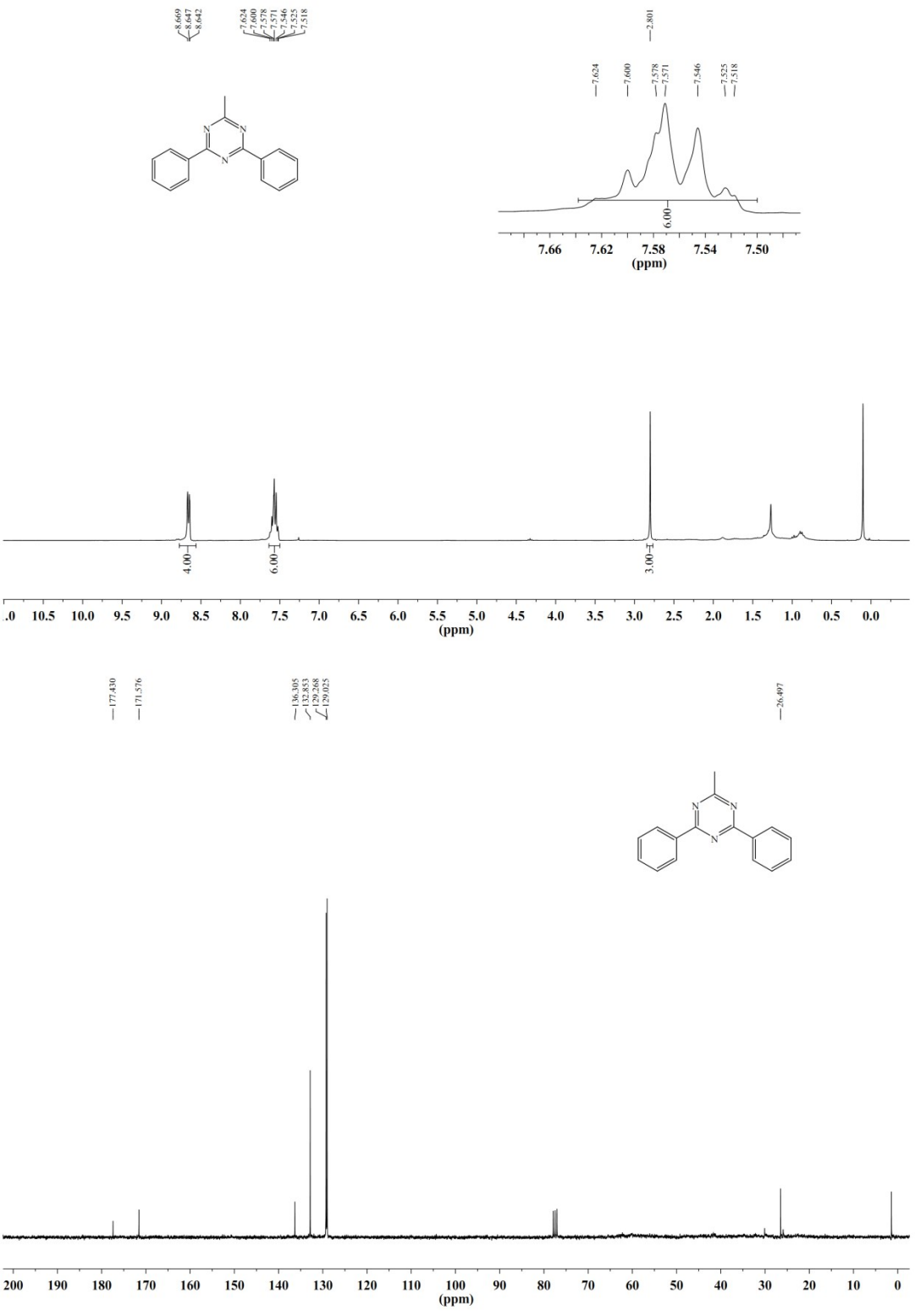

9.266
8.666
8.662
8.640
7.643
7.619
7.596
7.590
7.583
7.558
7.536
7.530


7.643
7.619
7.596
7.590
7.583
7.558
7.536
7.530
6.01
7.75
7.70
7.65
7.60
7.55
7.50
(ppm)

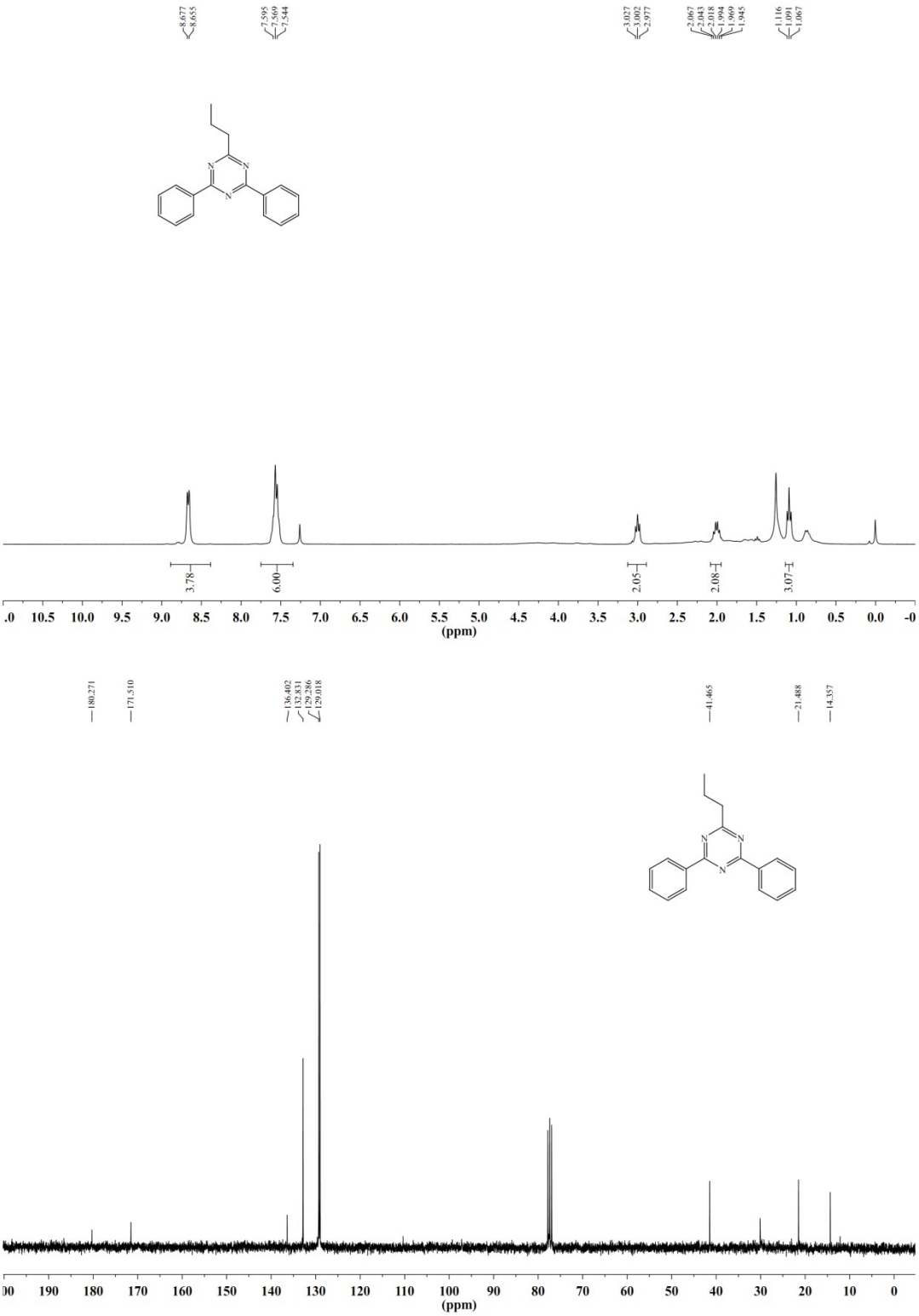

1.00
4.00
6.01
(ppm)


171.711
167.108
135.908
133.215
129.275
129.145
(ppm)

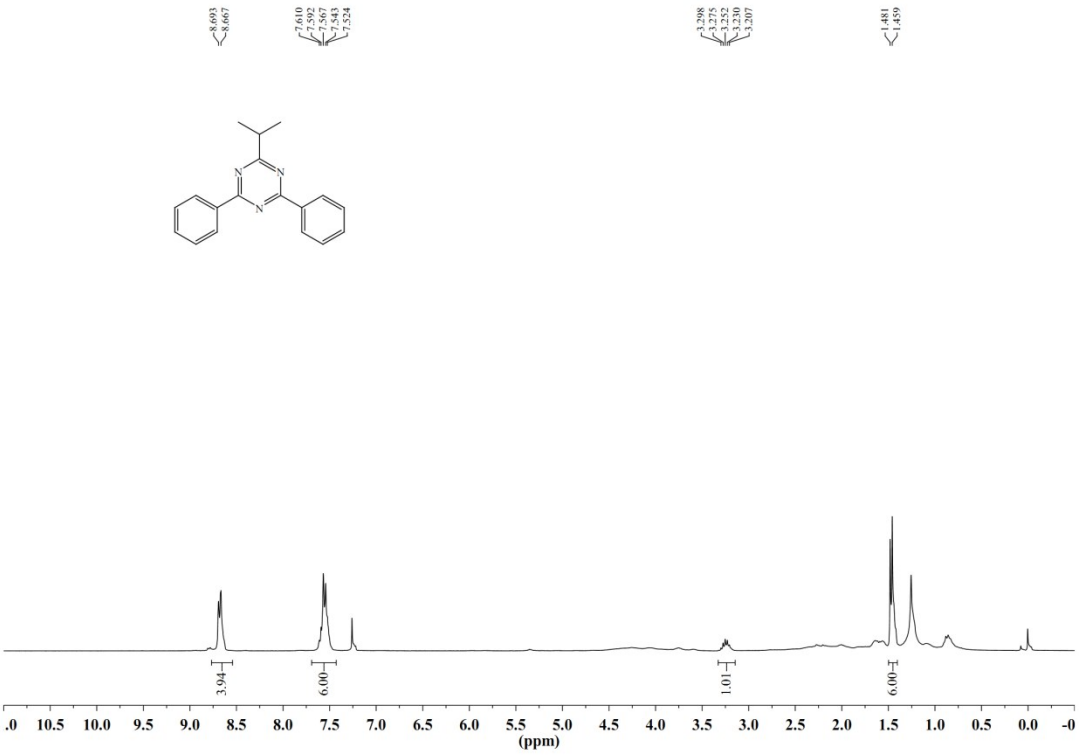
3qa

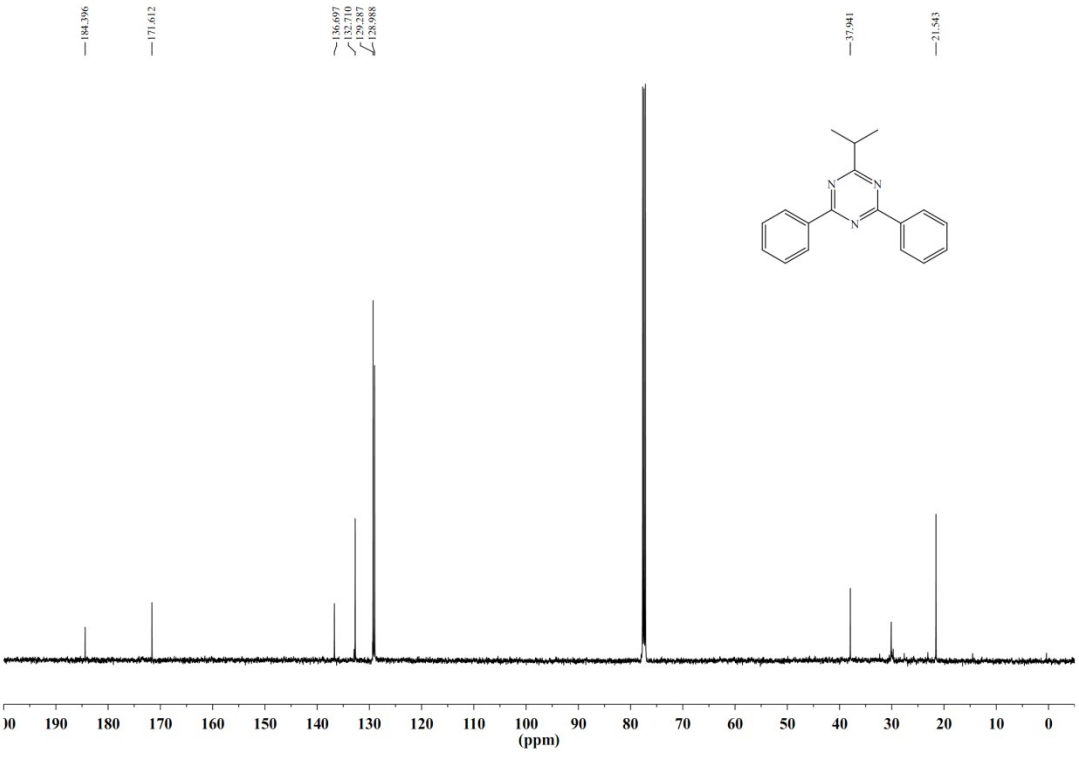

8.669
8.647
8.642
7.624
7.600
7.578
7.571
7.546
7.525
7.518
2.801
6.00
7.66
7.62
7.58
7.54
7.50
(ppm)
4.00
6.00
3.00
(ppm)
177.430
171.576
136.305
130.453
129.268
129.025
26.497
(ppm)

3ra

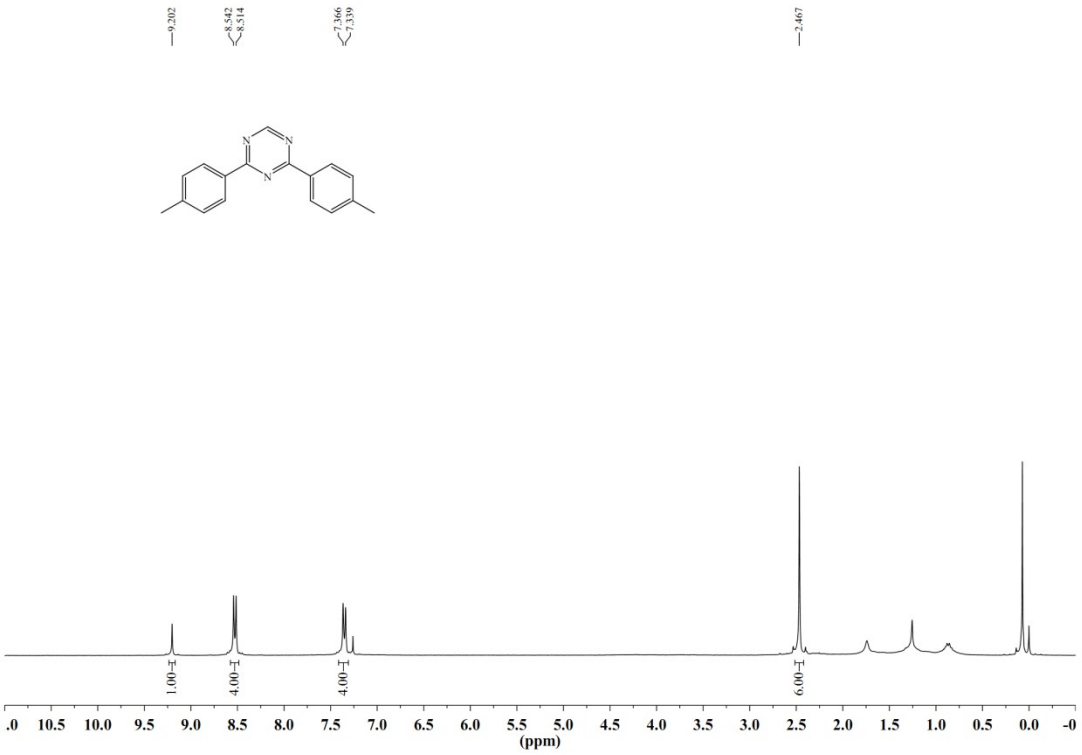

8.677
8.655
7.595
7.569
7.544
3.027
3.002
2.977
2.067
2.043
2.018
1.994
1.969
1.945
1.116
1.091
1.067
3.78
6.00
2.05
2.08
3.07
(ppm)
180.271
171.510
136.402
132.851
129.286
129.018
41.465
21.488
14.357
(ppm)

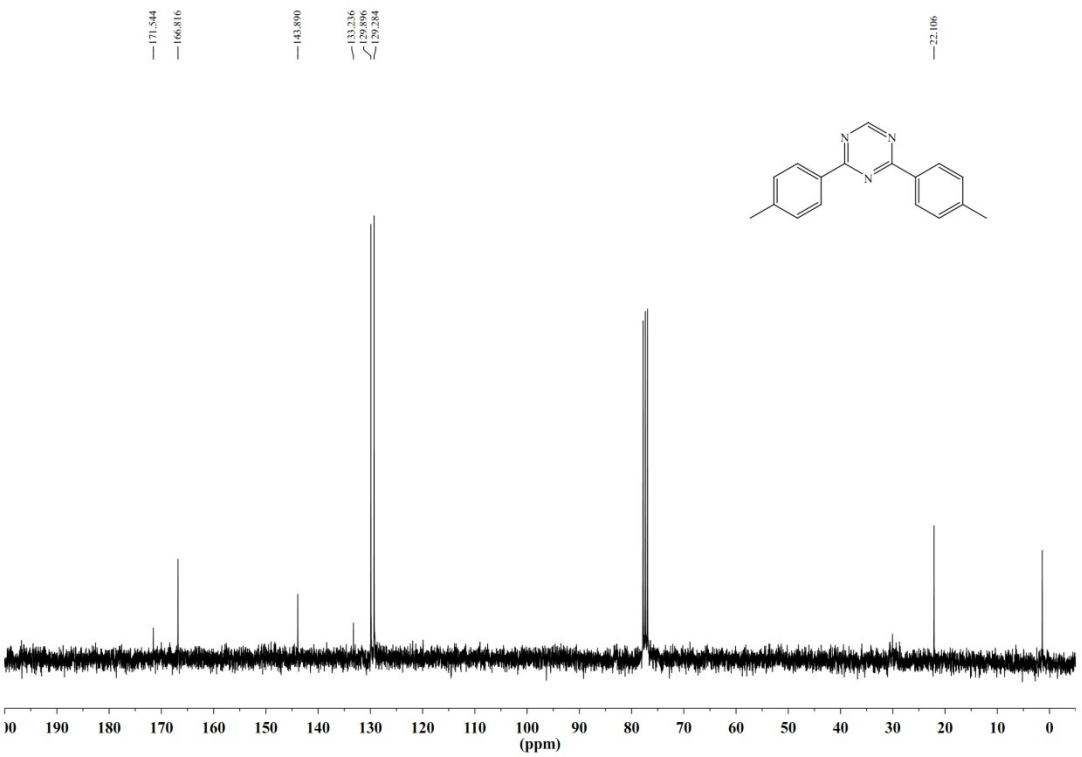
3sa


8.693
8.667
7.610
7.592
7.567
7.543
7.524
3.298
3.275
3.252
3.230
3.207
1.481
1.459
3.94
6.00
1.01
6.00
(ppm)

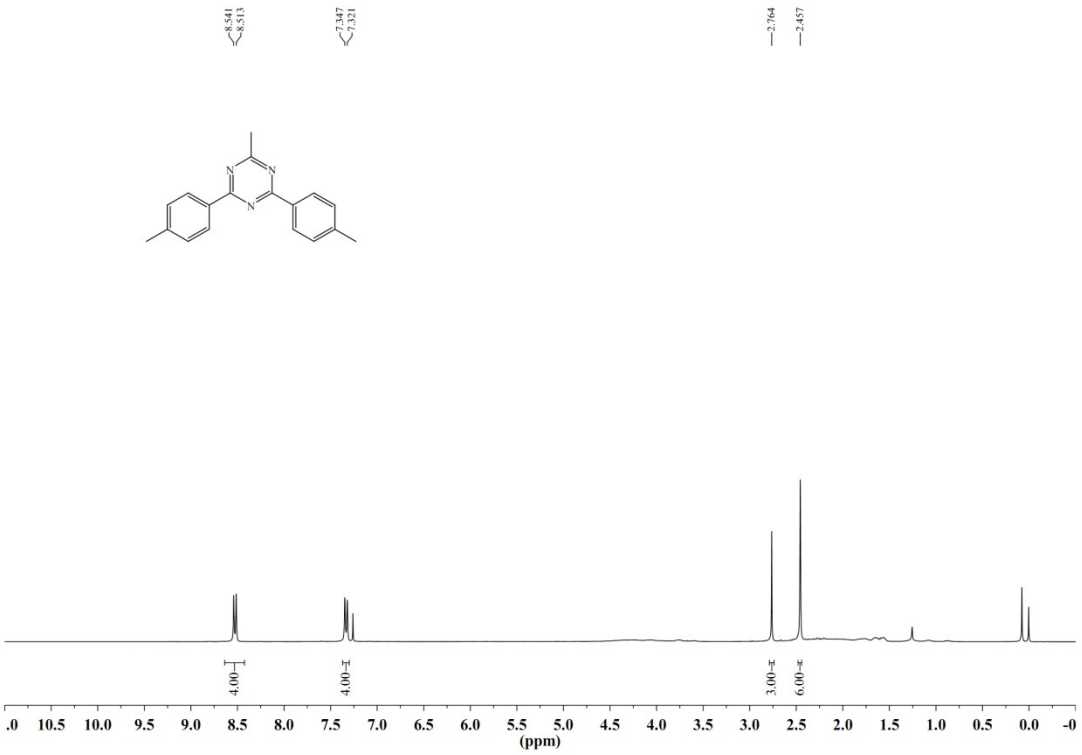

184.396
171.612
136.697
132.710
129.337
128.988
37.941
21.543
(ppm)

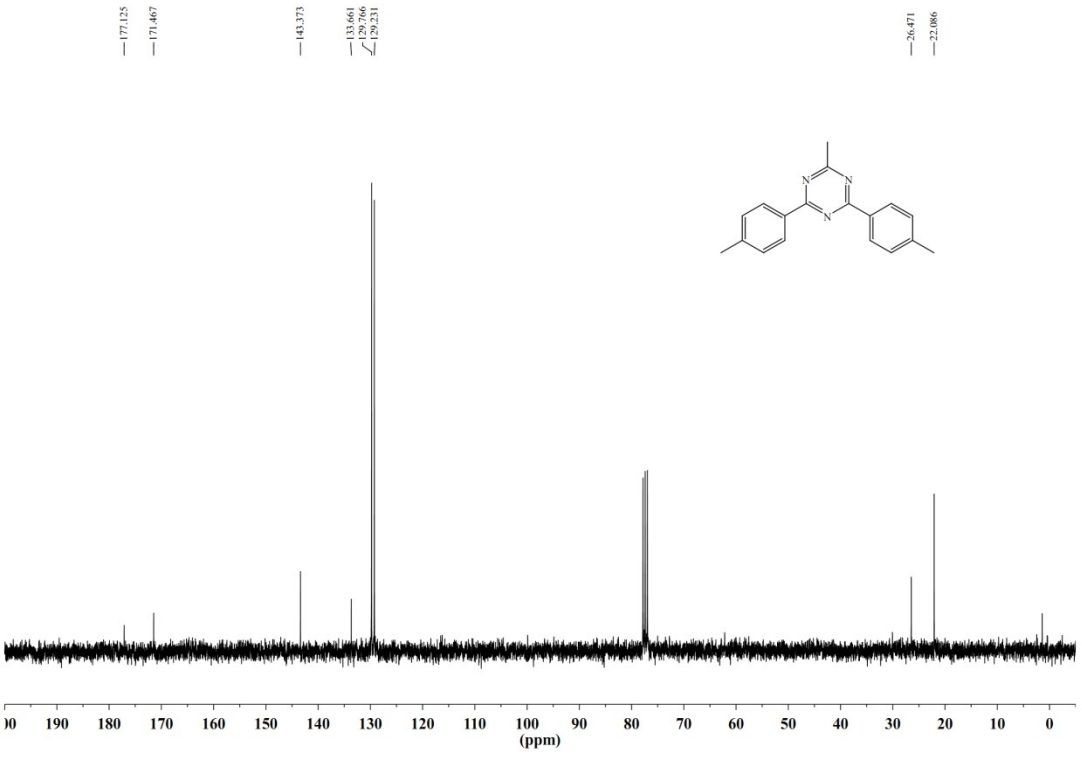
3ta


9.202
8.542
8.514
7.366
7.339
2.467
1.00
4.00
4.00
6.00
(ppm)


171.544
166.816
143.890
133.236
129.896
129.284
22.106
(ppm)

3qb


8.541
8.513
7.347
7.321
2.764
2.457
4.00
4.00
3.00
6.00
(ppm)


177.125
171.467
143.373
133.661
129.366
129.231
26.471
22.086
(ppm)

3rb

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