SUPPORTING INFORMATION

Bulky Magnesium(II) and Sodium(I) Bisphenoxide Catalysts for the Chemoselective Transesterification of Methyl (Meth)acrylates

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Abstract: Given the industrial importance of (meth)acrylate esters, various groups have devoted considerable effort to investigating their chemoselective transesterification. In 2021, we developed magnesium(II) and sodium(I) complexes derived from 2,6-di-*tert*-butyl-*p*-cresol (BHT-H) as chemoselective catalysts for the transesterification of methyl acrylate (MA) and methyl methacrylate (MMA), respectively. Based on our results, we report the discovery of magnesium(II) and sodium(I) salts derived from 6,6'-(propane-2,2'-diyl)bis(2,4-di-*tert*-butylphenol (PBTP-H_2), i.e., Mg(PBTP), and Na_2(PBTP), which are 41 and 81 times more effective catalysts than $Mg(BHT)_2$ and Na(BHT) for the transesterification of MA and MMA, respectively. These new catalysts are highly effective across an extensive range of alcohols, including primary and secondary alcohols, diols, and triols. Overall, this efficient transesterification technology can be expected to find practical applications in industrial process chemistry.

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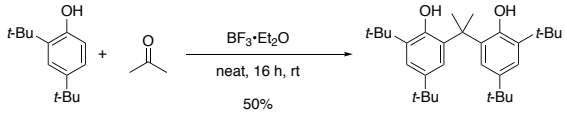
1. General methods

^{1}H NMR spectra were measured on a JEOL ECS400 (400 MHz) spectrometer at ambient temperature. Data were recorded as follows: chemical shift in ppm from internal tetramethylsilane on the δ scale, multiplicity (s = singlet; d = doublet; t = triplet; q = quartet, m = multiplet, br = broad), coupling constant (Hz), integration, and assignment. ^{13}C NMR spectra were measured on a JEOL ECS400 (100 MHz) spectrometer. Chemical shifts were recorded in ppm from the solvent resonance employed as the internal standard (deuterochloroform at 77.00 ppm). ^{19}F NMR spectra were measured on a JEOL ECS-400 (376 MHz) spectrometer. Chemical shifts were recorded in ppm from the solvent resonance employed as the external standard ($CFCl_3$ at 0 ppm). The products were purified by column chromatography on silica gel (E. Merck Art. 9385; Kanto Chemical Co., Inc. 37560). High resolution mass spectral analyses were performed at Chemical Instrument Center, Nagoya University (JEOL JMS-700 (FAB), JEOL JMS-T100GCV (EI), JEOL JMS-T100TD (DART-MS), Bruker Daltonics micrOTOF-QII (ESI)). Infrared (IR) spectra were recorded on a JASCO FT/IR 460 plus spectrometer. Melting points were measured on MPA100, Standard Research Systems. For thin-layer chromatography (TLC) analysis throughout this work, Merck precoated TLC plates (silica gel 60GF254 0.25 mm) were used. Visualization was accomplished by UV light (254 nm), anisaldehyde, $KMnO_4$, and phosphomolybdic acid. Anhydrous compounds, such as methyl acrylate (MA), methyl methacrylate (MMA), and methanol, were used as received commercially.

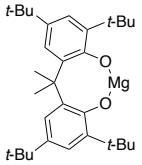
2. Synthesis of 6,6'-(Propane-2,2-diyl)bis(2,4-di-*tert*-butylphenol)[1]



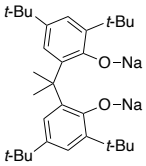
Boron trifluoride diethyl etherate (0.6 mL, 5.0 mmol, 1 equiv) was slowly added to a solution of 2,4-di-*tert*- butylphenol (2.1 g, 10.0 mmol, 2 equiv) in anhydrous acetone (368 μL, 5.0 mmol, 1 equiv) at room temperature under nitrogen. The reaction mixture was stirred at room temperature for 16 h. Methanol at 0 °C was added and stirred for 1 h. The resulting suspension was filtered, and the crude product was washed with methanol at 0 °C. The crude product was dissolved by chloroform, then purified by silica gel column chromatography (eluent: *n*-hexane:EtOAc = 8:1) to give the desired product.

6,6'-(Propane-2,2-diyl)bis(2,4-di-*tert*-butylphenol): White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.28 (s, 18H, 2C(CH_3)$_3$) 1.36 (s, 18H, 2C(CH_3)$_3$), 1.73 (s, 6H, 2CH_3), 4.99 (s, 2H, 2OH), 7.30 (d, *J* = 2.28 Hz, 2H, 2ArH), 7.40 (d, *J* = 2.28 Hz, 2H, 2ArH); ^{13}C NMR (100 MHz, $CDCl_3$): δ 29.0 (2C) 29.7 (6C), 31.9 (6C), 34.8 (2C), 35.3 (2C), 40.6 (1C),119.9 (2C), 124.2 (2C), 130.8 (2C), 137.6 (2C), 143.1 (2C), 151.9 (2C).

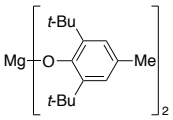
3. Preparation of metal aryloxides



Ma(PBTP): Under nitrogen atmosphere conditions, commercially available dibutylmagnesium (1.0 *M* in heptane)(100 μL, 0.10 mmol, 1.0 equiv) was slowly added to a solution of 6,6´-(propane-2,2-diyl)bis(2,4-di-*tert*-butylphenol) (PBTP-H_2, 45.2 mg, 0.10 mmol, 1.0 equiv) in dehydrated THF (200 μL) at room temperature. The reaction mixture was stirred at room temperature for 30 minutes. Volatiles were removed, and the residue was desiccated at room temperature under reduced pressure (<5 Torr) for 3 h. The resultant compound (>99% yield) as a white solid with a little pale yellow used for reaction directly. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.28 (s, 18H) 1.36 (s, 18H), 1.73 (s, 6H), 7.30 (d, *J* = 2.28 Hz, 2H, ArH), 7.40 (d, *J* = 2.28 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.0 (2C) 29.7 (6C), 31.9 (6C), 34.8 (2C), 35.3 (2C), 40.5, 119.9 (2C), 124.2 (2C), 130.7 (2C), 137.5 (2C), 143.1 (2C), 151.8 (2C).



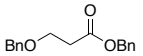
Na_2(PBTP): Under nitrogen atmosphere conditions, commercially available sodium methoxide (5.0 *M* in methanol) (10 μL, 0.05 mmol, 2 equiv) was slowly added to a solution of 6,6'-(propane-2,2-diyl)bis(2,4-di-*tert*-butylphenol) (PBTP-H_2, 11.3 mg, 0.025 mmol, 1 eq) in dehydrated THF (140 μL) at room temperature. The reaction mixture was stirred at room temperature for 30 min. Volatiles were removed, and the residue was desiccated at room temperature under reduced pressure (<5 Torr) for 3 h. The resultant compound (>99% yield) as a pale yellow solid used for reaction directly. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.28 (s, 18H), 1.36 (s, 18H), 1.73 (s, 6H), 7.30 (d, *J* = 2.28 Hz, 2H), 7.41 (d, *J* = 2.28 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.0 (2C), 29.7 (6C), 31.9 (6C), 34.8 (2C), 35.3 (2C), 40.5, 119.8 (2C), 124.2 (2C), 130.6 (2C), 137.5 (2C), 143.1 (2C), 151.8 (2C).



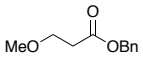
$Mg(BHT)_2$:[2] A mixture of commercially available magnesium ethoxide (229 mg, 2.0 mmol) and 2,6-di-*tert*-butyl-4-methylphenol (BHT-H, 881 mg, 4.0 mmol) in methanol (5 mL) was stirred at room temperature for 30 min. Volatiles were removed, and the residue was desiccated at room temperature under reduced pressure (<5 Torr) for 3 h. The resultant compound (>99% yield) as a white solid was stored in vial tube at room temperature. M.p. 101-104 °C (decomposition).^{1}H NMR (400 MHz, benzene-d_6) δ 1.38 (s, 36H), 2.25 (s, 6H), 7.06 (s, 4H); ^{13}C NMR (100 MHz, benzene-d_6) δ 21.5 (2C), 30.5 (12C), 34.4 (4C), 125.9 (4C), 128.5 (2C), 136.0 (4C), 152.1 (2C). IR (KBr) 3626, 2956, 2871, 1433, 1396, 1362, 1230, 1214, 1150, 1120 cm^{-1}.

4. Products in Tables 1 and 3

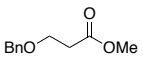
Benzyl acrylate (2a):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.19 (s, 2H), 5.84 (dd, *J* = 10.4, 1.6 Hz, 1H), 6.16 (dd, *J* = 17.4, 10.5 Hz, 1H), 6.44 (dd, *J* = 17.2, 1.4 Hz, 1H), 7.31-7.41 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 66.4, 128.3 (2C), 128.4 (2C), 128.7 (2C), 131.2, 135.9, 166.1. IR (neat) 3034, 2954, 1953, 1725, 1634, 1455, 1406, 1295, 1269, 1186, 1049 cm^{-1}. HRMS (FAB+) calcd for $C_{10}H_{10}O_2$ $[M]^+$ 162.0681, found 162.0680.



Benzyl 3-(benzyloxy)propanoate (3a):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.66 (t, *J* = 6.4 Hz, 2H), 3.76 (t, *J* = 6.4 Hz, 2H), 4.51 (s, 2H), 5.14 (s, 2H), 7.25-7.40 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 35.3, 65.6, 66.4 73.2, 127.7 (2C), 128.2 (4C), 128.4 (2C), 128.6 (2C), 135.9, 138.1, 171.5. IR (neat) 3032, 2868, 1737, 1496, 1455, 1363, 1258, 1173, 1105, 1071, 1027 cm^{-1}. HRMS (FAB+) calcd for $C_{17}H_{18}O_3$ $[M]^+$ 270.1256, found 270.1254.

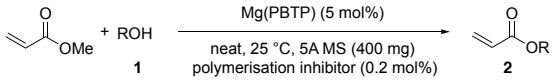


Benzyl 3-methoxypropanoate (4a):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (t, *J* = 6.4 Hz, 2H), 3.34 (s, 3H), 3.67 (t, *J* = 6.4 Hz, 2H), 5.13 (s, 2H), 7.30-7.40 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 35.1, 58.9, 66.4, 68.0, 128.3 (2C), 128.4, 128.6 (2C), 135.9, 171.5. IR (neat) 2893, 1738, 1455, 1391, 1350, 1169, 1118, 1070, 1015 cm^{-1}. HRMS (FAB+) calcd for $C_{11}H_{14}O_3$ $[M]^+$ 194.0943, found 194.0948.



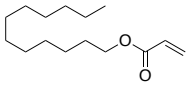
Methyl 3-(benzyloxy)propanoate (5a):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (t, *J* = 6.4 Hz, 2H), 3.69 (s, 3H), 3.75 (t, *J* = 6.4 Hz, 2H), 4.53 (s, 2H), 7.26-7.40 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 35.1, 51.8, 65.6, 73.2, 127.8 (3C), 128.5 (2C), 138.1, 172.2. IR (neat) 2868, 1741, 1437, 1366, 1195, 1176, 1105, 1073 cm^{-1}. HRMS (FAB+) calcd for $C_{11}H_{14}O_3$ $[M]^+$ 194.0943, found 194.09452.

5. Representative procedure for the transesterification of methyl acrylate (MA) catalyzed by Mg(PBTP) complex (Tables 2 and 3)

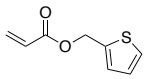


1 **2**

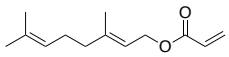
To a mixture of *in situ*-generated Mg(PBTP) (47.5 mg, 0.10 mmol), activated 5A molecular sieves (powder, 400 mg), copper(II) dimethyldithiocarbamate (1.2 mg, 0.0040 mmol) as a polymerization inhibitor, and dimethyl sulfone (18.8 mg, 0.20 mmol) as an internal standard for the crude ^{1}H NMR analysis, methyl acrylate (MA, 1.26 mL, 14 mmol) was added at 25 °C. After 1 min, alcohol (2.0 mmol) was added to the mixture at 25 °C. The mixture was stirred at room temperature for 20 min–38 h, and the reaction was monitored by TLC. After the reaction was completed, by using a drop of the mixture, the rough yield was determined by ^{1}H NMR ($CDCl_3$) analysis based on dimethyl sulfone as an internal standard.



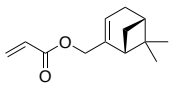
Dodecyl acrylate (2c):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.4 Hz, 3H), 1.26-1.38 (m, 18H), 1.63-1.70 (m, 2H), 4.15 (t, *J* = 6.4 Hz, 2H), 5.81 (dd, *J* = 10.5, 1.4 Hz, 1H), 6.12 (dd, *J* = 17.4, 10.0 Hz, 1H), 6.40 (dd, *J* = 17.4, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 22.8, 26.1, 28.8, 29.4, 29.5, 29.6, 29.7, 29.8 (2C), 32.1, 64.9, 128.8, 130.6, 166.5; IR (neat) 2925, 2854, 1729, 1636, 1467, 1407, 1295, 1272, 1192, 1059 cm^{-1}. HRMS (DART+) calcd for $C_{15}H_{29}O_2$ $[M+H]^+$ 241.2168, found 241.2165.



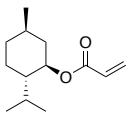
Thiophen-2-ylmethyl acrylate (2d):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.35 (s, 2H), 5.85 (dd, *J* = 10.6, 1.4 Hz, 1H), 6.14 (dd, *J* = 17.4, 10.5 Hz, 1H), 6.45 (dd, *J* = 17.4, 1.4 Hz, 1H), 6.99 (dd, *J* = 5.0, 3.2 Hz, 1H), 7.12 (d, *J* = 3.7 Hz, 1H), 7.33 (dd, *J* = 5.0, 1.4, Hz 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 60.7, 126.9, 127.0, 128.2, 128.4, 131.5, 137.9, 165.9; IR (neat) 3108, 2954, 1725, 1634, 1441, 1407, 1295, 1261, 1183 cm^{-1}. HRMS (DART+) calcd for $C_8H_8O_2S$ $[M]^+$ 168.0245, found 168.0246.



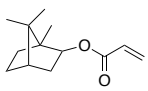
Geranyl acrylate (2e):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.60 (s, 3H), 1.68 (s, 3H), 1.72 (s, 3H), 2.03-2.14 (m, 4H), 4.68 (d, *J* = 7.4 Hz, 2H), 5.08 (m, 1H), 5.38 (m, 1H), 5.82 (dd, *J* = 10.5, 1.4 Hz, 1H), 6.13 (dd, *J* = 17.0, 10.0 Hz, 1H), 6.41 (dd, *J* = 17.4, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.6, 17.8, 25.8, 26.4, 39.7, 61.6, 118.3, 123.8, 128.7, 130.7, 132.0, 142.5, 166.4; IR (neat) 2968, 2925, 2857, 1725, 1636, 1445, 1407, 1378, 1294, 1270, 1184, 1045 cm^{-1}. HRMS (DART+) calcd for $C_{13}H_{21}O_2$ $[M+H]^+$ 209.1542, found 209.1540.



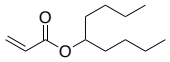
(1*R*)-(–)-Myrtenyl acrylate (2f):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.83 (s, 3H), 1.19 (d, *J* = 8.7 Hz, 1H), 1.29 (s, 3H), 2.08-2.16 (m, 2H), 2.25 (dm, *J* = 17.8 Hz, 1H), 2.32 (dm, *J* = 17.8 Hz, 1H), 2.41 (dt, *J* = 8.7, 5.8 Hz, 1H), 4.19-4.59 (m, 2H), 5.59 (m, 1H), 5.82 (dd, *J* = 10.1, 1.4 Hz, 1H), 6.12 (dd, *J* = 17.4, 10.5 Hz, 1H), 6.40 (dd, *J* = 17.0, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.2, 26.2, 31.4, 31.6, 38.2, 40.8, 43.7, 67.2, 121.7, 128.7, 130.7, 143.0, 166.2; IR (neat) 2987, 2918, 2833, 1728, 1636, 1619, 1406, 1366, 1294, 1268, 1184, 1045 cm^{-1}. HRMS (DART+) calcd for $C_{13}H_{19}O_2$ [M+H]+ 207.1385, found 207.1381.



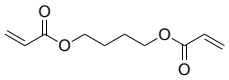
L-Menthyl acrylate (2g):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.77 (d, *J* = 6.9 Hz, 3H), 0.85-0.92 (m, 1H), 0.89 (d, *J* = 6.9 Hz, 3H), 0.91 (d, *J* = 6.9 Hz, 3H), 0.96-1.14 (m, 2H), 1.38-1.56 (m, 2H), 1.66-1.72 (m, 2H), 1.87 (m, 1H), 2.03 (m, 1H), 4.76 (td, *J* = 10.6, 4.1 Hz, 1H), 5.80 (dd, *J* = 10.1, 1.4 Hz, 1H), 6.11 (dd, *J* = 17.4, 10.1 Hz, 1H), 6.39 (dd, *J* = 17.4, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.5, 20.9, 22.2, 23.6, 26.4, 31.5, 34.4, 41.0, 47.2, 74.5, 129.2, 130.4, 166.0; IR (neat) 2956, 2871, 1723, 1633, 1456, 1405, 1296, 1270, 1199, 1046 cm^{-1}. HRMS (DART+) calcd for $C_{13}H_{23}O_2$ $[M+H]^+$ 211.1698, found 211.1700.



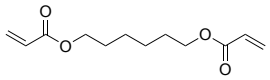
Isobornyl acrylate (2b):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.85 (d, *J* = 3.2 Hz, 6H), 1.01 (s, 3H), 1.07-1.21 (m, 2H), 1.57 (m, 1H), 1.67-1.87 (m, 4H), 4.75 (dd, *J* = 7.3, 3.7 Hz, 1H), 5.79 (dd, *J* = 10.5, 1.4 Hz, 1H), 6.09 (dd, *J* = 17.4, 10.5 Hz, 1H), 6.34 (dd, *J* = 17.4, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 11.5, 19.9, 20.2, 27.1, 33.8, 38.8, 45.1, 47.0, 48.9, 81.2, 129.3, 130.0, 165.8; IR (neat) 2956, 2879, 1720, 1636, 1619, 1455, 1406, 1390, 1296, 1276, 1199, 1109 cm^{-1}. HRMS (ESI+) calcd for $C_{13}H_{20}NaO_2$ $[M+Na]^+$ 231.1356, found 231.1353.



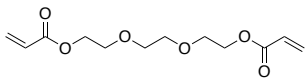
Nonan-5-yl acrylate (2h):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (m, 6H), 1.28 (m, 8H), 1.56 (m, 4H), 4.95 (m, 1H), 5.80 (dd, *J* = 10.4, 1.3 Hz, 1H), 6.11 (dd, *J* = 17.2, 10.5 Hz, 1H), 6.38 (dd, *J* = 17.2, 1.84 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.1 (2C), 22.7 (2C), 27.6 (2C), 33.9 (2C), 74.7, 129.1, 130.3, 166.2; IR (neat) 2957, 2861, 1724, 1404, 1196 cm^{-1}. HRMS (FAB^+) calcd for $C_{12}H_{23}O_2$ $[M+H]^+$199.16980, found 199.17063.



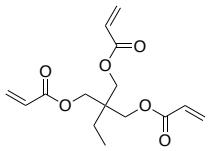
Butane-1,4-diyl diacrylate (2i):[2] Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ) 1.75–1.82 (m, 4H), 4.19–4.22 (m, 4H), 5.83 (dd, *J* = 1.4, 10.6 Hz, 2H), 6.12 (ddd, *J* = 1.8, 10.6, 17.4 Hz, 2H), 6.41 (dd, *J* = 1.4, 17.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.4(2C), 25.5(2C), 64.3(2C), 125.5(2C), 136.5(2C), 167.5(2C); IR (neat) 2970, 1730, 1636, 1620, 1468, 1410, 1297, 1272, 1186, 1061 cm^{-1}. HRMS (DART+) calcd for $C_{10}H_{15}O_4$ $[M+H]^+$ 199.0970, found 199.0966.



hexane-1,6-diyl diacrylate (2j):[2] Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.41-1.44 (m, 4H), 1.66-1.73 (m, 4H), 4.16 (t, *J* = 6.4 Hz, 4H), 5.82 (dd, *J* = 1.4, 10.1 Hz, 2H), 6.12 (dd, *J* = 10.5, 17.4 Hz, 2H), 6.40 (dd, *J* = 1.4, 17.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.7(2C), 28.6(2C), 64.6(2C), 128.6(2C), 130.7(2C), 166.4(2C); IR (neat) 2941, 2862, 1718, 1636, 1620, 1467, 1409, 1274, 1197 cm^{-1}. HRMS (DART+) calcd for $C_{12}H_{19}O_4$ $[M+H]^+$ 227.1283, found 227.1284.

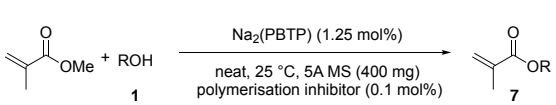


(Ethane-1,2-diylbis(oxy))bis(ethane-2,1-diyl) diacrylate (2k):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.68 (s, 4H), 3.74-3.76 (m, 4H), 4.31-4.33 (m, 4H), 5.84 (dd, *J* = 10.6, 1.4 Hz, 2H), 6.16 (dd, *J* = 17.4, 10.6 Hz, 2H), 6.43 (dd, *J* = 17.4, 1.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 63.8 (2C), 69.3 (2C), 70.7 (2C), 128.4 (2C), 131.2 (2C), 166.3 (2C). IR (neat) 2952, 2875, 1725, 1636, 1619, 1454, 1409, 1352, 1298, 1197, 1131, 1067 cm^{-1}. HRMS (DART+) calcd for $C_{12}H_{19}O_6$ $[M+H]^+$ 259.1182, found 259.1189.

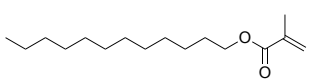


2-((Acryloyloxy)methyl)-2-ethylpropane-1,3-diyl diacrylate (2l):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.93 (t, *J* = 7.8 Hz, 3H), 1.56 (q, *J* = 6.8 Hz, 2H), 4.18 (s, 6H), 5.86 (d, *J* = 10.6 Hz, 3H), 6.11 (dd, *J* = 17.0, 10.0 Hz, 3H), 6.41 (d, *J* = 17.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 7.6, 23.3, 41.0, 64.3 (3C), 128.1 (3C), 131.5 (3C), 166.0 (3C); IR (neat) 2970, 1725, 1635, 1619, 1467, 1408, 1270, 1182, 1061 cm^{-1}. HRMS (DART+) calcd for $C_{15}H_{21}O_6$ $[M+H]^+$ 297.1338, found 297.1340.

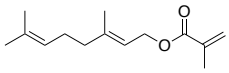
6. Representative procedure for the transesterification of methyl methacrylate (MMA) using Na_2(PBTP) complex (Table 4)



To a mixture of *in situ*-generated Na_2(PBTP) (12.4 mg, 0.025 mmol), activated 5A molecular sieves (powder, 400 mg), 4-acetamido-2,2,6,6-tetramethylpiperidine 1-oxyl (0.42 mg, 0.0020 mmol) as a polymerization inhibitor, and dimethyl sulfone (18.8 mg, 0.20 mmol) as an internal standard for the crude ^{1}H NMR analysis, methyl methacrylate (MMA, 1.49 mL, 14 mmol) was added at 25 °C. After 1 min, **1** (2.0 mmol) was added to the mixture at 25 °C. The mixture was stirred at room temperature for 10 min–38 h, and the reaction was monitored by TLC. After the reaction was completed, by using a drop of the mixture, the rough yield was determined by ^{1}H NMR ($CDCl_3$) analysis based on dimethyl sulfone as an internal standard.

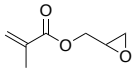


Dodecyl methacrylate (7c):[2] Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.88 (t, *J* = 6.9 Hz, 3H), 1.26-1.39 (m, 18H), 1.63-1.70 (m, 2H), 1.95 (s, 3H), 4.14 (t, *J* = 6.9 Hz, 2H), 5.55 (m, 1H), 6.10 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.3, 18.5, 22.8, 26.1, 28.7, 29.4, 29.5, 29.7 (2C), 29.8 (2C), 32.1, 65.0, 125.3, 136.7, 167.6; IR (neat) 2921, 2854, 1719, 1638, 1467, 1321, 1296, 1165 cm^{-1}. HRMS (FAB+) calcd for $C_{16}H_{31}O_2$ $[M+H]^+$ 255.2324, found 255.2324.

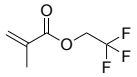


Geranyl methacrylate (7e):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.60 (s, 3H), 1.68 (s, 3H), 1.72 (s, 3H), 1.94-1.96 (m, 3H), 2.03-2.14 (m, 4H), 4.67 (d, *J* = 7.3 Hz, 2H), 5.08 (tm, *J* = 6.9 Hz, 1H), 5.38 (tm, *J* = 6.9 Hz, 1H), 5.55 (m, 1H), 6.10 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.6, 17.8, 18.5, 25.8, 26.4, 39.6, 61.8, 118.6, 123.9, 125.4, 131.9, 136.7, 142.1, 167.7; IR (neat) 2926, 1719, 1638, 1451, 1377, 1313, 1293, 1162, 1010 cm^{-1}. HRMS (DART+) calcd for $C_{14}H_{23}O_2$ $[M+H]^+$ 223.1698, found 223.1696.

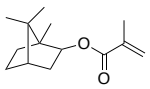
Benzyl methacrylate (7a):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.97 (s, 3H), 5.20 (s, 2H), 5.59 (s, 1H), 6.16 (s, 1H), 7.30-7.40 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.5, 66.5, 125.9, 128.1 (2C), 128.2, 128.6 (2C), 136.2, 136.3, 167.3; IR (neat) 3034, 2957, 1719, 1637, 1454, 1319, 1294, 1159 cm^{-1}. HRMS (DART+) calcd for $C_{11}H_{13}O_2$ $[M+H]^+$ 177.0916, found 177.0912.



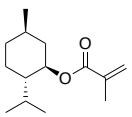
Oxiran-2-ylmethyl methacrylate (7m):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.97 (s, 3H), 2.68 (dd, *J* = 4.6, 2.5 Hz, 1H), 2.87 (dd, *J* = 4.6, 4.1 Hz, 1H), 3.26 (m, 1H), 4.01 (dd, *J* = 6.0, 12.4 Hz, 1H), 4.49 (dd, *J* = 3.2, 12.4 Hz, 1H), 5.62 (m, 1H), 6.17 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.4, 44.7, 49.5, 65.2, 126.3, 135.9, 167.1; IR (neat) 3002, 2958, 2930, 1722, 1637, 1454, 1349, 1317, 1296, 1170 cm^{-1}. HRMS (DART+) calcd for C7H11O3 [M+H]+ 143.0708, found 143.0707.



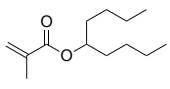
2,2,2-Trifluoromethyl methacrylate (7n):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.99 (s, 3H), 4.54 (q, *J* = 7.8 Hz, 2H), 5.71 (s, 1H), 6.23 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.2, 60.7 (q, *J* = 36.2 Hz), 123.2 (q, *J* = 275 Hz), 127.8, 134.9, 165.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ –73.8; IR (neat) 2974, 1758, 1284, 1183, 1150 cm^{-1}. HRMS (DART+) calcd for $C_6H_8F_3O_2$ $[M+H]^+$ 169.0476, found 169.0469.



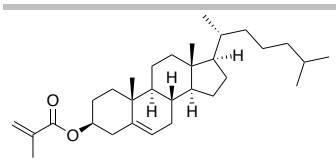
Isobornyl methacrylate (7b):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.85 (s, 3H), 0.86 (s, 3H), 1.02 (s, 3H), 1.07-1.21 (m, 2H), 1.57 (m, 1H), 1.67-1.88 (m, 4H), 1.93 (s, 3H), 4.71 (m, 1H), 5.52 (d, J = 1.4 Hz, 1H), 6.07 (s, 1H); ^{13}C NMR (100 MHz, CDCl3) d 11.5, 18.4, 19.9, 20.1, 27.1, 33.7, 38.9, 45.1, 47.0, 48.9, 81.2, 125.0, 136.9, 166.9. IR (neat) 2955, 2879, 1717, 1638, 1455, 1327, 1298, 1163, 1054 cm^{-1}. HRMS (FAB+) calcd for $C_{14}H_{22}NaO_2$ $[M+Na]^+$ 245.1517, found 245.1509.



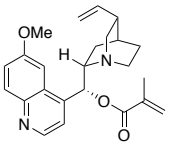
L-Menthyl methacrylate (7g):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.77 (d, *J* = 6.9 Hz, 3H), 0.82-0.93 (m, 1H), 0.89 (d, *J* = 6.4 Hz, 3H), 0.91 (d, *J* = 6.4 Hz, 3H), 0.95-1.14 (m, 2H), 1.40-1.58 (m, 2H), 1.66-1.73 (m, 2H), 1.88 (m, 1H), 1.94 (m, 3H), 2.03 (m, 1H), 4.73 (td, *J* = 11.0, 4.1 Hz, 1H), 5.53 (m, 1H), 6.08 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 16.6, 18.6, 20.9, 22.2, 23.7, 26.5, 31.5, 34.4, 41.0, 47.3, 74.6, 125.1, 137.0, 167.1; IR (neat) 2956, 2871, 1715, 1638, 1456, 1316, 1297, 1171 cm^{-1}. HRMS (DART+) calcd for $C_{14}H_{25}O_2$ $[M+H]^+$ 225.1855, found 225.1856.



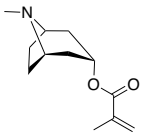
Nonan-5-yl methacrylate 7h):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) d 0.89 (t, *J* = 6.9 Hz, 6H), 1.23–1.37 (m, 8H), 1.53–1.62 (m, 4H), 1.95 (s, 3H), 4.93 (m, 1H), 5.53 (m, 1H), 6.09 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) d 14.2 (2C), 18.6, 22.8 (2C), 27.6 (2C), 33.9 (2C), 74.8 124.9, 137.0, 167.4; IR (neat) 2958, 2932, 2862, 1717, 1638, 1456, 1319, 1296, 1170 cm^{-1}. HRMS (DART+) calcd for $C_{13}H_{25}O_2$ $[M+H]^+$ 213.1855, found 213.1853.



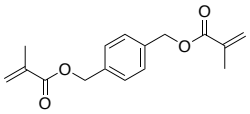
Cholesteryl methacrylate (7o):[2] White solid. M.p. 112-114 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.68 (s, 3H), 0.86 (d, *J* = 6.6 Hz, 3H), 0.87 (d, *J* = 6.6 Hz, 3H), 0.92 (d, *J* = 6.4 Hz, 3H), 0.95-1.69 (m, 24H), 1.77-2.04 (m, 8H), 2.36 (d, *J* = 8.2 Hz, 2H), 4.67 (m, 1H), 5.38 (d, *J* = 4.6 Hz, 1H), 5.53 (m, 1H), 6.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 12.0, 18.5, 18.9, 19.5, 21.2, 22.7, 23.0, 24.0, 24.4, 27.9, 28.2, 28.4, 32.0, 32.1, 36.0, 36.3, 36.8, 37.2, 38.3, 39.7, 39.9, 42.5, 50.2, 56.3, 56.8, 74.4, 122.8, 125.1, 137.0, 139.9, 167.0; IR (KBr) 2947, 1718, 1638, 1467, 1375, 1324, 1295, 1171, 1012 cm^{-1}. HRMS (EI) calcd for $C_{31}H_{50}O_2$ $[M]^+$ 454.3811, found 454.3818.



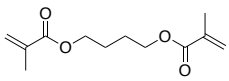
Quinine methacrylate (7p):[2] White solid. M.p. 124-129 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.50-1.65 (m, 2H), 1.72 (m, 1H), 1.83-1.91 (m, 2H), 1.98 (s, 3H), 2.28 (m, 1H), 2.58-2.73 (m, 2H), 3.06 (dd, *J* = 13.7, 10.1 Hz, 1H), 3.15 (m, 1H), 3.41 (q, *J* = 7.8 Hz, 1H), 3.96 (s, 3H), 4.98-5.03 (m, 2H), 5.66 (m, 1H), 5.83 (m, 1H), 6.23 (s, 1H), 6.34 (d, *J* = 6.9 Hz, 1H), 7.34 (d, *J* = 4.6 Hz, 1H), 7.34 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.44 (d, *J* = 2.3 Hz, 1H), 8.02 (d, *J* = 9.2 Hz, 1H), 8.73 (d, *J* = 4.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.5, 24.3, 27.7, 28.0, 39.8, 42.6, 55.7, 56.8, 59.4, 74.5, 101.5, 114.6, 118.8, 121.9, 126.5, 127.0, 131.9, 136.2, 141.9, 143.8, 144.9, 147.6, 158.0, 166.4; IR (KBr) 2925, 1715, 1622, 1594, 1508, 1469, 1446, 1375, 1324, 1303, 1230, 1156 cm^{-1}. HRMS (DART+) calcd for $C_{24}H_{29}N_2O_3$ $[M+H]^+$ 393.2178, found 393.2187.



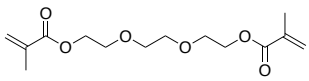
Tropinyl methacrylate (7q):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.74 (d, *J* = 14.7 Hz, 2H), 1.92-2.06 (m, 4H), 1.97 (s, 3H), 2.15 (dt, *J* = 14.7, 4.4 Hz, 2H), 2.29 (s, 3H), 3.20-3.05 (m, 2H), 5.06 (t, *J* = 5.5 Hz, 1H), 5.57 (t, *J* = 1.6 Hz, 1H), 6.09 (s, 1H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 18.2, 25.5(2C), 36.5(2C), 40.3(2C), 59.6, 67.5, 125.0, 136.7, 166.5.; IR (neat) 2943, 1715, 1448, 1316, 1296, 1170, 1063, 1036 cm^{-1}. HRMS (FAB+) calcd for $C_{12}H_{20}NO_2$ $[M+H]^+$ 210.1494, found 210.1485.



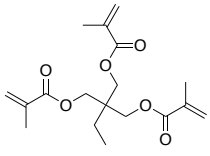
1,4-Phenylenebis(methylene) bis(2-methylacrylate) (7r):[2] White solid. M.p. 68-70 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.97 (s, 6H), 5.20 (s, 4H), 5.59-5.60 (m, 2H), 6.16 (s, 2H), 7.38 (s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.5 (2C), 66.2 (2C), 126.1 (2C), 128.4 (4C), 136.2 (2C), 136.3 (2C), 167.3 (2C); IR (neat) 3040, 2966, 2931, 1701, 1635, 1456, 1373, 1319, 1295, 1156 cm^{-1}. HRMS (FAB+) calcd for $C_{16}H_{18}O_4Na$ $[M+Na]^+$ 297.1103, found 297.1099.



Butane-1,4-diyl dimethacrylate (7i):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.76–1.83 (m, 4H), 1.95 (t, *J* = 1.4 Hz, 6H), 4.17–4.22 (m, 4H), 5.55–5.57 (m, 2H), 6.10 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.4(2C), 25.5(2C), 64.3(2C), 125.5(2C), 136.5(2C), 167.5(2C); IR (neat) 2959, 2928, 2855, 1713, 1637, 1453, 1404, 1377, 1323, 1297, 1165 cm^{-1}. HRMS (DART+) calcd for $C_{12}H_{19}O_4$ $[M+H]^+$ 227.1283, found 227.1287.



(Ethane-1,2-diylbis(oxy))bis(ethane-2,1-diyl) dimethacrylate (7k):[2] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.95 (s, 6H), 3.68 (s, 4H), 3.74-3.77 (m, 4H), 4.29-4.32 (m, 4H), 5.57-5.59 (m, 2H), 6.13-6.14 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.4 (2C), 63.9 (2C), 69.3 (2C), 70.7 (2C), 125.9 (2C), 136.2 (2C), 167.5 (2C); IR (neat) 2955, 2874, 1719, 1637, 1454, 1319, 1297, 1171, 1043 cm^{-1}. HRMS (DART+) calcd for $C_{14}H_{23}O_6$ $[M+H]^+$ 287.1495, found 287.1495.



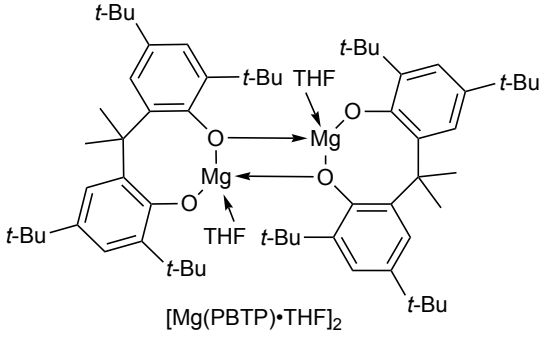
1,1,1-Trimethylolpropane trimethacrylate (7i):[2] Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.95 (t, *J* = 7.6 Hz, 3H), 1.59 (q, *J* = 7.9 Hz, 2H), 1.94 (s, 9H), 4.16 (s, 6H), 5.58-5.60 (m, 3H), 6.10 (s, 3H); ^{13}C NMR (100 MHz,$CDCl_3$) δ 7.3, 18.1(3C), 23.3, 41.0, 64.1(3C), 125.9(3C), 135.8(3C), 166.8(3C); IR (neat) 2967, 1724, 1638, 1455, 1322, 1294, 1154 cm^{-1}. HRMS (FAB+) calcd for $C_{18}H_{26}NaO_6$ $[M+Na]^+$ 361.1627, found 361.1623.

7. X-ray diffraction analysis of Mg(PBTP) and Na_2(PBTP)

Single Crystal Structure of [Mg(PBTP)·THF]$_2$

In a solution of PBTP-H_2 (136 mg, 0.3 mmol) in THF (3 mL), dibutylmagnesium (300 μL, 1.0 *M* in hepatne) was added under argon atmosphere. After 0.5 h, the resultant solution was concentrated *in vacuo* to give white solid. The solid was dissolved in toluene and hexane and recrystallized overnight. All manipulations were carried out in glove box.

Crystal data of [Mga(PBTP)·THF]$_2$ (Figure S1): Formula $C_{70}H_{108}Mg_2O_6$, colorless, monoclinic, space group *P* 21/c, *a* = 16.2490(5) Å, *b* = 10.6440(3) Å, *c* =19.0878(5) Å, α = 90°, β = 96.071(3)°, γ = 90 °, *V* = 3282.80(16) Å^3, Z = 2, ρcalc = 1.107 g/cm^3, λ(MoKα) = 0.71073 Å, *T* = 93 K. 8210 reflections collected, and 6084 parameters were used for the solution of the structure. R_1 = 0.0659 and wR_2 = 0.1828. GOF = 1.044. Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-2151275. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [Fax: int. code + 44(1223)336-033; E-mail: deposit@ccdc.cam.ac.uk; Web page: http://www.ccdc.cam.ac.uk/pages/Home.aspx].



[Mg(PBTP)•THF]$_2$

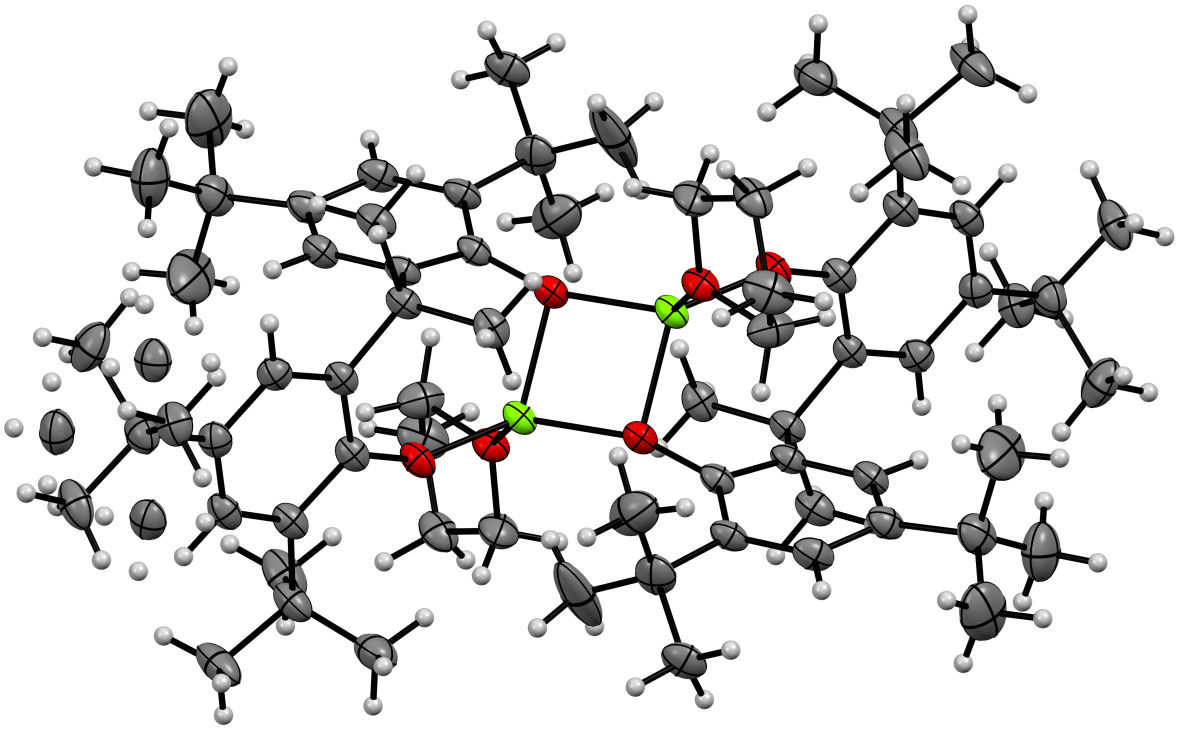


Figure S1. X-ray crystal structure of [Mg(PBTP)·THF]$_2$ with thermal ellipsoids at 50% probability.

Single Crystal Structure of Na_2(PBTP)·4THF

In a solution of PBTP-H_2 (136 mg, 0.3 mmol) in THF (3 mL), sodium hydride (9 mmol) was added under argon atmosphere. After 14 h, the resultant mixture was filtrated through celite pad, and concentrated *in vacuo* to give white solid. The solid was dissolved in THF and recrystallized by adsorption of THF using alumina overnight. All manipulations were carried out in glove box.

Crystal data of Na_2(PBTP)·4THF (Figure S2): Formula $C_{47}H_{78}Na_2O_6$, colorless, monoclinic, space group *C* 2/c, *a* = 13.2993(4) Å, *b* = 14.9598(4) Å, *c* =23.1561(7) Å, α = 90°, β = 92.864(3)°, γ = 90 °, *V* = 4601.3(2) Å^3, Z = 4, ρcalc = 1.133 g/cm^3, λ(MoKα) = 0.71073 Å, *T* = 93 K. 5819 reflections collected, and 4503 parameters were used for the solution of the structure. R_1 = 0.0572 and wR_2 = 0.1463. GOF = 1.016. Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-2152692. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [Fax: int. code + 44(1223)336-033; E-mail: deposit@ccdc.cam.ac.uk; Web page: http://www.ccdc.cam.ac.uk/pages/Home.aspx].

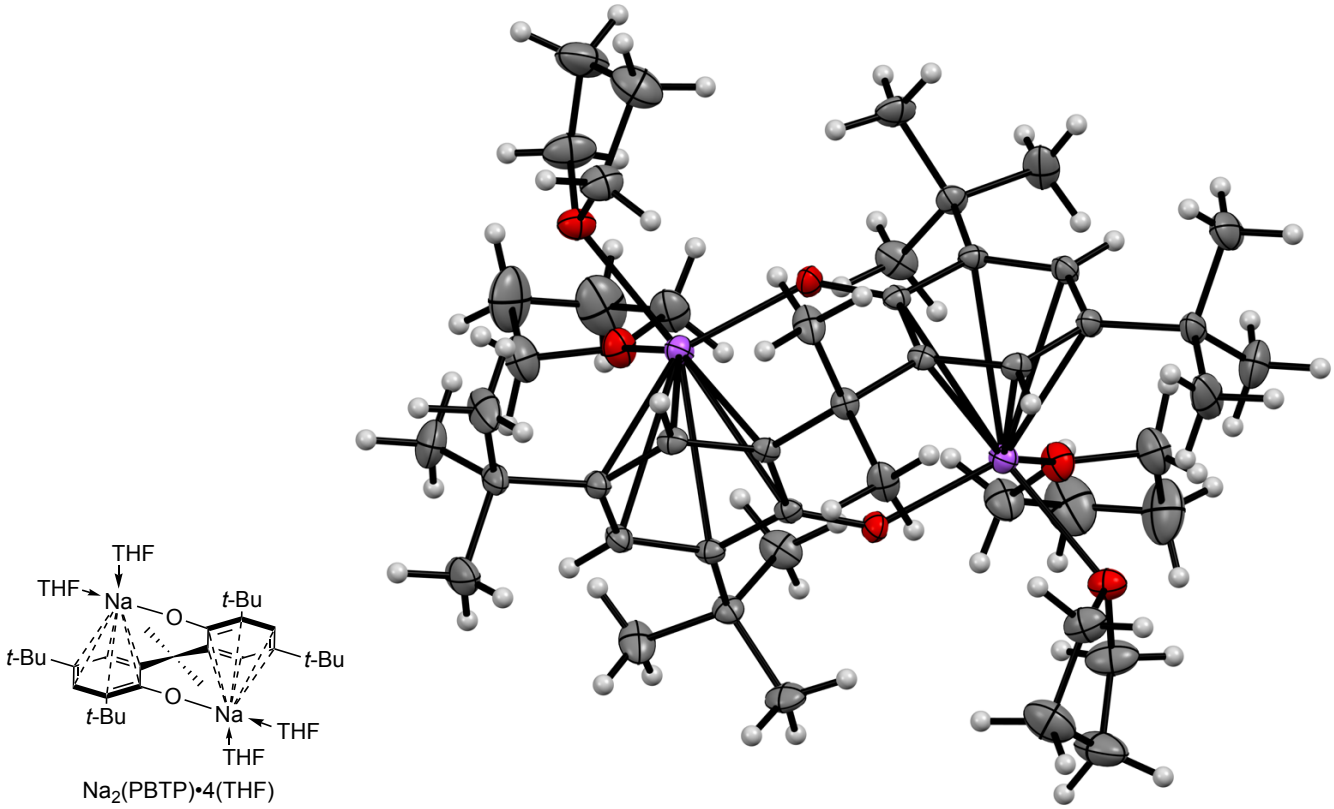


Figure S2. X-crystal structure of Na_2(PBTP)·4THF with thermal ellipsoids at 50% probability.

8. DFT calculations for potential energy profile including Mg(II) and Na(I) species.

8-1. Computational details.

DFT calculations were performed at the wb97XD[3]/6-31G(d,p)[4] level. Solvent effect was taken into account by a self-consistent reaction field method with polarizable continuum model.[5] Solvent parameters for methylpropanoate was adopted because of the structural similarity to methyl acrylate (MA). For computational software, Gaussian 16 package[6] was used. For the structural optimization, frequency analysis was performed to check number of imaginary frequency of energy minimum and transition state.

8-2. Comparison between X-ray structure and DFT optimized structure for [Mg(PBTP)•THF]$_2$ and Na$_2$(PBTP)•4(THF).

The computed geometrical parameter (bond lengths are given in Å) of the X-ray structures of [Mg(PBTP)•THF]$_2$ and Na$_2$(PBTP)•4(THF) are represented in **Figure S3** and **Figure S4**, respectively. Calculated bond lengths around the Mg and Na moieties were in good agreement with the X-ray structures, indicating that the reliability of the present DFT calculation set-up.

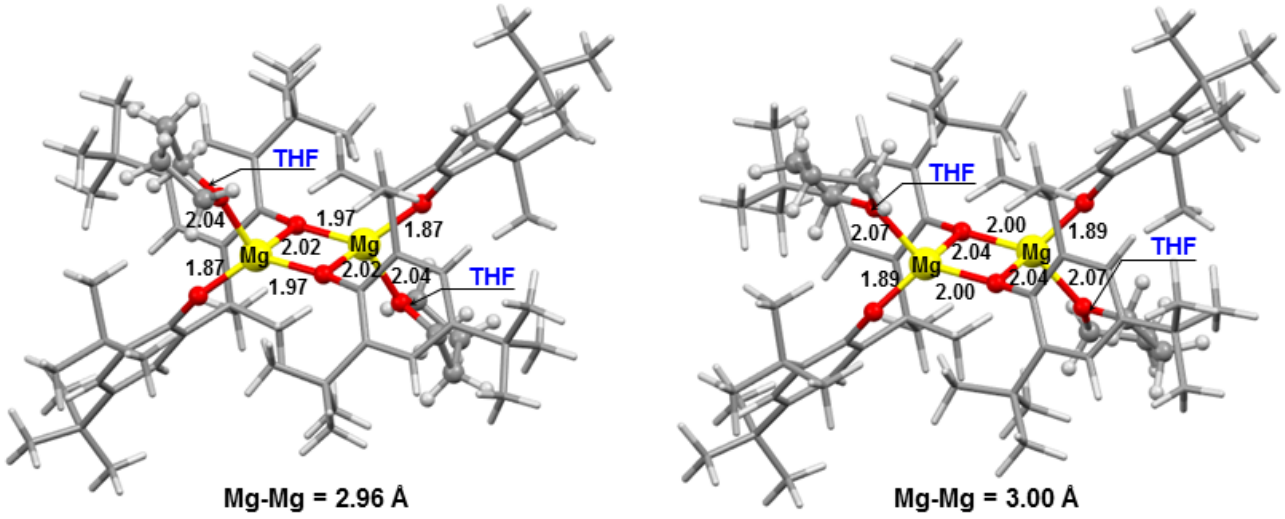


Figure S3. X-ray structure of [Mg(PBTP)•THF]$_2$ (left) and optimized structure from the DFT calculation (right). Bond lengths are given in Å.

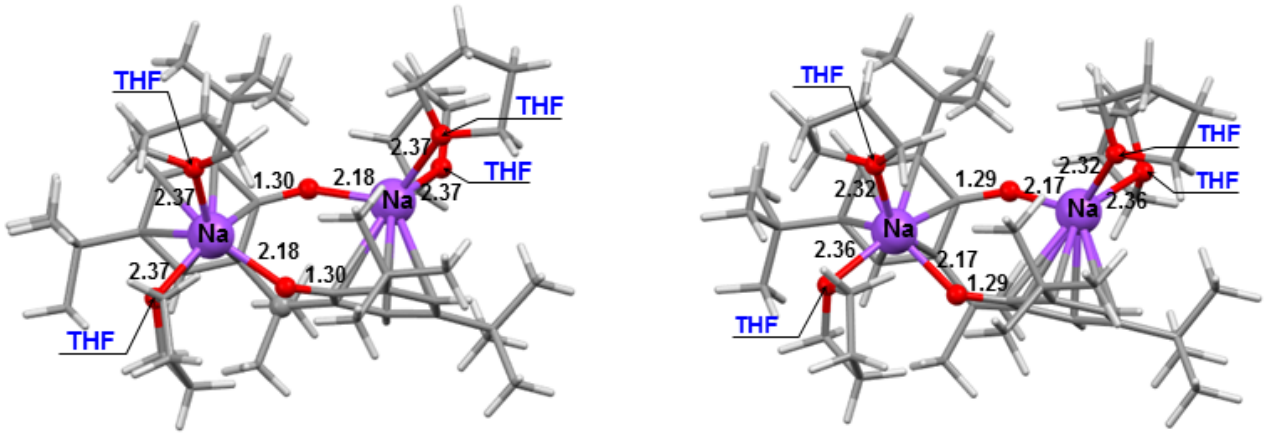


Figure S4. X-ray structure of Na$_2$(PBTP)•4(THF) (left) and optimized structure from the DFT calculation (right). Bond lengths are given in Å.

8-3. Optimized structures for intermediate and transition states shown in Figure 2 for the transesterification of MA with 1a using [Mg(PBTP)]$_2$ catalyst.

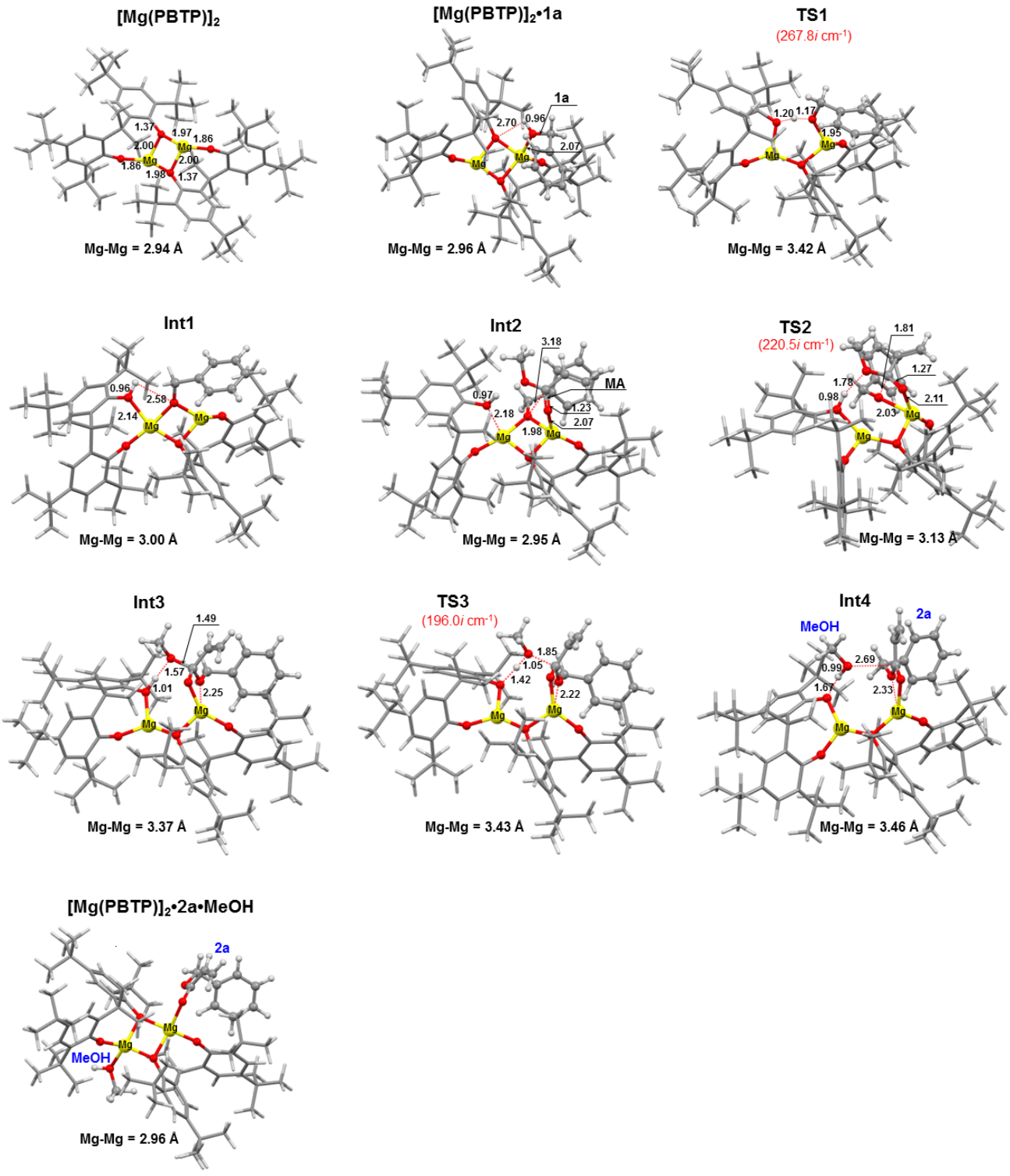


Figure S5. Optimized structures of intermediates and transition states for the transesterification of MA with **1a** using [Mg(PBTP)]$_2$ catalyst. Bond lengths are given in Å.

8-4. Optimized structures for intermediate and transition states at the rate determining step (RDS) in Table 5 for the transesterification of MMA with 1a using Na_2(PBTP)

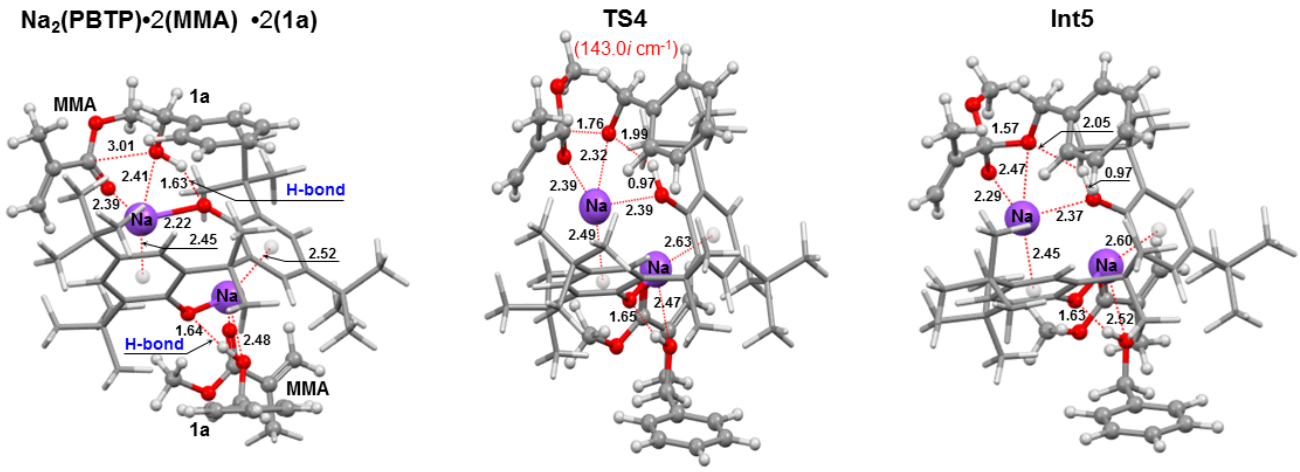


Figure S6. Optimized structures of intermediates and transition at the RDS for the transesterification of MMA with 1a using Na_2(PBTP) catalyst. Bond lengths are given in Å.

8-5. Optimized structures for intermediate and transition states at the rate determining step (RDS) in Table 5 for the transesterification of MA with 1a using Mg(PBTP) catalyst.

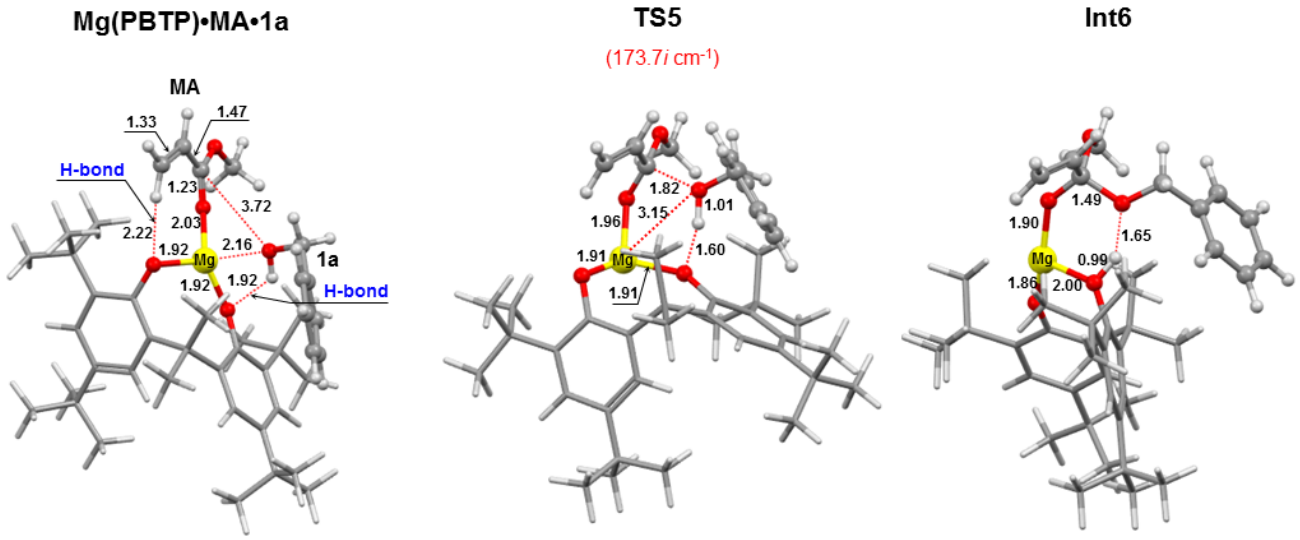


Figure S7. Optimized structures of intermediates and transition states for the transesterification of MA with **1a** using Mg(PBTP) catalyst. Bond lengths are given in Å

8-6. Optimized structures for intermediate and transition states at the rate determining step (RDS) in Table 5 for the transesterification of MMA with 1a using Na(BHT) catalyst.

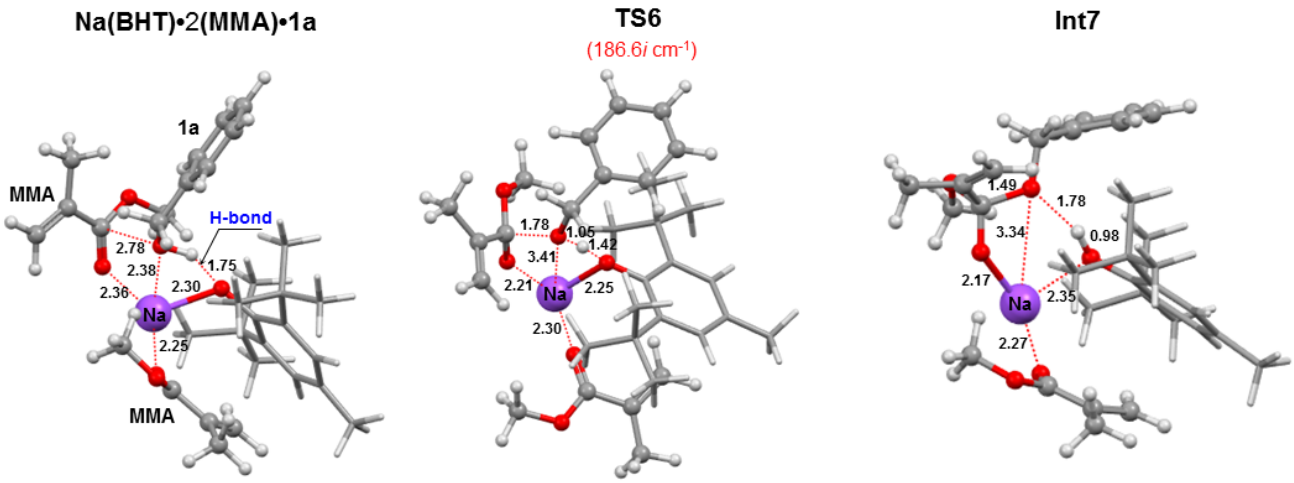


Figure S8. Optimized structures of intermediates and transition at the RDS for the transesterification of MMA with 1a using Na(BHT) catalyst. Bond lengths are given in Å.

8-7. Atomic coordinates of the optimized structures

[Mg(PBTP)•THF]2-optXray-byDFT

Mg	-1.065000	-0.163000	-1.044000	H	-0.866000	4.252000	-2.066000	H	-0.510000	0.226000	-4.198000
O	-0.610000	1.100000	0.487000	H	-0.033000	2.755000	-1.634000	H	-0.221000	1.973000	-3.975000
O	-2.784000	-0.955000	-0.974000	C	-0.619000	5.597000	0.232000	C	-2.173000	1.523000	-4.836000
O	-1.522000	1.088000	-2.628000	H	-0.933000	5.852000	1.249000	H	-1.870000	2.010000	-5.764000
C	-1.703000	1.884000	0.719000	H	-1.345000	6.015000	-0.471000	H	-2.731000	0.617000	-5.083000
C	-2.922000	1.276000	1.109000	H	0.333000	6.100000	0.038000	C	-2.993000	2.437000	-3.920000
C	-4.099000	2.014000	0.997000	C	-3.950000	-1.227000	-0.420000	H	-4.055000	2.446000	-4.173000
H	-5.031000	1.498000	1.205000	C	-4.204000	-0.878000	0.939000	H	-2.619000	3.464000	-3.980000
C	-4.136000	3.349000	0.624000	C	-5.442000	-1.164000	1.502000	C	-2.755000	1.864000	-2.526000
C	-2.908000	3.965000	0.417000	H	-5.618000	-0.894000	2.537000	H	-2.611000	2.631000	-1.767000
H	-2.896000	5.017000	0.176000	C	-6.481000	-1.759000	0.788000	H	-3.532000	1.175000	-2.195000
C	-1.687000	3.282000	0.445000	C	-6.218000	-2.087000	-0.538000	Mg	1.066000	0.161000	1.044000
C	-3.135000	-0.125000	1.747000	H	-7.007000	-2.547000	-1.116000	O	0.610000	-1.102000	-0.487000
C	-1.910000	-1.031000	1.926000	C	-4.991000	-1.852000	-1.166000	O	2.786000	0.951000	0.976000
H	-2.210000	-1.906000	2.513000	C	-7.836000	-1.999000	1.465000	O	1.521000	-1.090000	2.629000
H	-1.129000	-0.517000	2.490000	C	-7.658000	-2.973000	2.646000	C	1.704000	-1.886000	-0.718000
H	-1.500000	-1.416000	0.998000	H	-6.955000	-2.579000	3.387000	C	2.922000	-1.276000	-1.108000
C	-3.584000	0.173000	3.200000	H	-8.615000	-3.148000	3.150000	C	4.100000	-2.015000	-0.996000
H	-4.479000	0.796000	3.254000	H	-7.272000	-3.936000	2.296000	H	5.032000	-1.498000	-1.204000
H	-2.780000	0.712000	3.713000	C	-8.869000	-2.599000	0.502000	C	4.138000	-3.349000	-0.622000
H	-3.773000	-0.753000	3.752000	H	-9.056000	-1.938000	-0.351000	C	2.909000	-3.965000	-0.415000
C	-5.484000	4.052000	0.439000	H	-8.548000	-3.572000	0.117000	H	2.898000	-5.018000	-0.175000
C	-6.253000	3.344000	-0.694000	H	-9.820000	-2.746000	1.024000	C	1.688000	-3.283000	-0.444000
H	-6.424000	2.288000	-0.465000	C	-8.394000	-0.662000	1.989000	C	3.134000	0.124000	-1.747000
H	-5.692000	3.397000	-1.633000	H	-8.520000	0.053000	1.169000	C	1.909000	1.030000	-1.926000
H	-7.228000	3.819000	-0.851000	H	-9.369000	-0.812000	2.468000	H	2.210000	1.904000	-2.512000
C	-5.321000	5.531000	0.064000	H	-7.727000	-0.208000	2.729000	H	1.129000	0.516000	-2.490000
H	-6.306000	5.992000	-0.058000	C	-4.796000	-2.271000	-2.637000	H	1.499000	1.414000	-0.998000
H	-4.780000	5.651000	-0.881000	C	-3.687000	-3.332000	-2.735000	C	3.583000	-0.175000	-3.200000
H	-4.786000	6.089000	0.839000	H	-3.941000	-4.219000	-2.145000	H	4.479000	-0.797000	-3.254000
C	-6.306000	3.971000	1.739000	H	-2.748000	-2.927000	-2.361000	H	2.780000	-0.715000	-3.712000
H	-7.272000	4.471000	1.610000	H	-3.546000	-3.645000	-3.777000	H	3.771000	0.752000	-3.753000
H	-5.776000	4.457000	2.565000	C	-6.069000	-2.874000	-3.253000	C	5.486000	-4.052000	-0.438000
H	-6.505000	2.935000	2.028000	H	-5.867000	-3.146000	-4.294000	C	6.255000	-3.343000	0.695000
C	-0.421000	4.077000	0.061000	H	-6.902000	-2.163000	-3.253000	H	6.425000	-2.287000	0.466000
C	0.780000	3.709000	0.942000	H	-6.390000	-3.782000	-2.733000	H	5.694000	-3.396000	1.635000
H	0.515000	3.761000	2.004000	C	-4.400000	-1.063000	-3.504000	H	7.230000	-3.817000	0.852000
H	1.599000	4.415000	0.771000	H	-3.435000	-0.674000	-3.181000	C	5.323000	-5.530000	-0.062000
H	1.174000	2.720000	0.729000	H	-5.146000	-0.263000	-3.429000	H	6.309000	-5.991000	0.060000
C	-0.091000	3.821000	-1.421000	H	-4.326000	-1.359000	-4.558000	H	4.783000	-5.650000	0.883000
H	0.867000	4.281000	-1.687000	C	-0.980000	1.182000	-3.960000	H	4.788000	-6.088000	-0.837000

C	6.307000	-3.971000	-1.738000
H	7.274000	-4.470000	-1.609000
H	5.778000	-4.457000	-2.563000
H	6.506000	-2.934000	-2.027000
C	0.423000	-4.079000	-0.060000
C	-0.778000	-3.712000	-0.942000
H	-0.512000	-3.763000	-2.004000
H	-1.596000	-4.418000	-0.772000
H	-1.173000	-2.723000	-0.729000
C	0.092000	-3.823000	1.422000
H	-0.867000	-4.283000	1.687000
H	0.866000	-4.253000	2.067000
H	0.033000	-2.756000	1.634000
C	0.621000	-5.599000	-0.231000
H	0.936000	-5.854000	-1.248000
H	1.348000	-6.016000	0.472000
H	-0.331000	-6.102000	-0.037000
C	3.951000	1.225000	0.420000
C	4.204000	0.878000	-0.940000
C	5.440000	1.166000	-1.504000
H	5.616000	0.897000	-2.540000
C	6.479000	1.763000	-0.790000
C	6.216000	2.090000	0.536000
H	7.005000	2.551000	1.113000
C	4.991000	1.852000	1.165000
C	7.833000	2.005000	-1.469000
C	7.652000	2.979000	-2.649000
H	6.949000	2.585000	-3.389000
H	8.609000	3.156000	-3.154000
H	7.266000	3.941000	-2.298000
C	8.866000	2.606000	-0.506000
H	9.055000	1.945000	0.346000
H	8.544000	3.579000	-0.121000
H	9.817000	2.755000	-1.029000
C	8.392000	0.669000	-1.994000
H	8.520000	-0.046000	-1.175000
H	9.367000	0.820000	-2.473000
H	7.726000	0.214000	-2.733000
C	4.797000	2.270000	2.637000
C	3.686000	3.329000	2.737000
H	3.939000	4.217000	2.148000
H	2.748000	2.923000	2.363000
H	3.546000	3.640000	3.779000
C	6.070000	2.874000	3.252000
H	5.869000	3.145000	4.293000
H	6.904000	2.164000	3.251000
H	6.389000	3.783000	2.732000
C	4.404000	1.060000	3.503000
H	3.439000	0.670000	3.181000
H	5.151000	0.262000	3.426000
H	4.332000	1.355000	4.557000
C	0.979000	-1.181000	3.961000
H	0.511000	-0.223000	4.198000
H	0.219000	-1.970000	3.978000
C	2.171000	-1.523000	4.838000
H	1.868000	-2.009000	5.767000
H	2.732000	-0.618000	5.083000
C	2.989000	-2.440000	3.922000
H	4.051000	-2.451000	4.176000
H	2.612000	-3.465000	3.982000
C	2.753000	-1.867000	2.528000
H	2.610000	-2.633000	1.768000
H	3.531000	-1.178000	2.198000

Na2(PBTP)•4(THF)-optXray-byDFT

Na	-2.283000	-0.392000	0.119000
O	-0.762000	-1.736000	-0.648000
C	0.499000	-1.647000	-0.915000
C	0.983000	-0.833000	-1.997000
C	2.333000	-0.883000	-2.346000
H	2.662000	-0.300000	-3.196000
C	3.287000	-1.621000	-1.640000
C	2.827000	-2.313000	-0.514000
H	3.553000	-2.855000	0.082000
C	1.489000	-2.337000	-0.121000
C	0.000000	0.002000	-2.840000
C	-0.725000	-1.011000	-3.752000
H	0.024000	-1.600000	-4.289000
H	-1.356000	-0.523000	-4.502000
H	-1.334000	-1.692000	-3.151000
C	4.768000	-1.688000	-2.034000
C	5.170000	-3.155000	-2.279000
H	4.571000	-3.590000	-3.085000
H	5.021000	-3.767000	-1.384000
H	6.227000	-3.224000	-2.560000
C	5.066000	-0.899000	-3.317000
H	6.126000	-0.998000	-3.573000
H	4.855000	0.169000	-3.197000
H	4.481000	-1.270000	-4.165000
C	5.639000	-1.107000	-0.904000
H	6.701000	-1.150000	-1.172000
H	5.507000	-1.667000	0.027000
H	5.372000	-0.063000	-0.709000
C	1.058000	-3.096000	1.145000
C	0.107000	-4.246000	0.767000
H	0.623000	-4.982000	0.141000
H	-0.743000	-3.848000	0.212000
H	-0.255000	-4.759000	1.667000
C	2.245000	-3.698000	1.910000
H	1.876000	-4.206000	2.808000
H	2.951000	-2.924000	2.234000
H	2.791000	-4.437000	1.315000
C	0.350000	-2.127000	2.110000
H	0.020000	-2.654000	3.014000
H	-0.520000	-1.681000	1.629000
H	1.037000	-1.328000	2.410000
O	-3.996000	-1.991000	-0.130000
C	-3.609000	-3.059000	0.750000
H	-4.329000	-3.107000	1.572000
H	-2.616000	-2.836000	1.160000
C	-3.569000	-4.319000	-0.109000
H	-4.557000	-4.790000	-0.151000
H	-2.852000	-5.050000	0.270000
C	-3.183000	-3.750000	-1.478000
H	-2.112000	-3.528000	-1.508000
H	-3.450000	-4.404000	-2.311000
C	-3.952000	-2.437000	-1.495000
H	-3.457000	-1.662000	-2.087000
H	-4.980000	-2.563000	-1.859000
O	-2.971000	-0.274000	2.333000
C	-4.363000	0.071000	2.439000
H	-4.897000	-0.399000	1.610000
H	-4.453000	1.160000	2.345000
C	-4.816000	-0.420000	3.813000
H	-5.603000	0.206000	4.237000
H	-5.192000	-1.446000	3.747000
C	-3.511000	-0.387000	4.613000
H	-3.522000	-1.038000	5.488000
H	-3.287000	0.634000	4.940000
C	-2.506000	-0.836000	3.563000
H	-1.488000	-0.477000	3.737000
H	-2.479000	-1.931000	3.476000
O	0.762000	1.737000	-0.645000
C	-0.498000	1.648000	-0.913000
C	-0.983000	0.836000	-1.995000
C	-2.332000	0.886000	-2.345000
H	-2.661000	0.303000	-3.195000
C	-3.287000	1.623000	-1.638000
C	-2.827000	2.314000	-0.511000
H	-3.553000	2.855000	0.086000
C	-1.489000	2.337000	-0.117000
C	0.726000	1.017000	-3.749000
H	-0.023000	1.607000	-4.286000
H	1.357000	0.531000	-4.501000
H	1.335000	1.697000	-3.148000
C	-4.768000	1.690000	-2.032000
C	-5.169000	3.158000	-2.275000
H	-4.570000	3.594000	-3.081000
H	-5.021000	3.768000	-1.379000
H	-6.226000	3.228000	-2.557000
C	-5.065000	0.903000	-3.316000
H	-6.125000	1.003000	-3.573000
H	-4.855000	-0.164000	-3.197000
H	-4.480000	1.276000	-4.163000
C	-5.639000	1.108000	-0.903000
H	-6.701000	1.152000	-1.171000
H	-5.507000	1.667000	0.029000
H	-5.372000	0.064000	-0.709000
C	-1.058000	3.094000	1.150000
C	-0.107000	4.245000	0.773000
H	-0.624000	4.982000	0.148000
H	0.742000	3.848000	0.218000
H	0.255000	4.757000	1.674000
C	-2.246000	3.695000	1.916000
H	-1.876000	4.202000	2.813000
H	-2.951000	2.921000	2.238000
H	-2.791000	4.435000	1.321000
C	-0.350000	2.124000	2.113000
H	-0.020000	2.650000	3.018000
H	0.520000	1.679000	1.631000
H	-1.037000	1.325000	2.412000
Na	2.284000	0.392000	0.119000
O	3.996000	1.991000	-0.127000
C	3.608000	3.058000	0.755000
H	4.329000	3.104000	1.577000
H	2.616000	2.834000	1.164000
C	3.568000	4.319000	-0.102000
H	4.555000	4.791000	-0.142000
H	2.850000	5.049000	0.279000
C	3.182000	3.753000	-1.472000
H	2.112000	3.530000	-1.503000
H	3.450000	4.408000	-2.303000
C	3.953000	2.440000	-1.491000
H	3.459000	1.666000	-2.085000
H	4.981000	2.568000	-1.854000
O	2.971000	0.270000	2.333000
C	4.363000	-0.075000	2.439000
H	4.897000	0.398000	1.611000
H	4.453000	-1.164000	2.343000
C	4.815000	0.413000	3.814000
H	5.602000	-0.214000	4.238000
H	5.192000	1.439000	3.750000
C	3.510000	0.379000	4.613000
H	3.521000	1.029000	5.490000
H	3.285000	-0.642000	4.938000
C	2.505000	0.830000	3.564000
H	1.487000	0.472000	3.737000
H	2.479000	1.925000	3.479000

[Mg(PBTP)]2

Mg	0.966000	-0.413000	0.994000
O	0.655000	1.189000	-0.164000
O	2.773000	-0.824000	1.095000
C	1.723000	2.048000	-0.198000
C	2.979000	1.591000	-0.661000
C	4.098000	2.387000	-0.416000
H	5.067000	1.984000	-0.693000
C	4.035000	3.647000	0.159000
C	2.767000	4.120000	0.478000
H	2.681000	5.115000	0.887000
C	1.602000	3.362000	0.325000
C	3.305000	0.318000	-1.490000
C	2.132000	-0.563000	-1.944000
H	2.519000	-1.331000	-2.620000
H	1.400000	0.023000	-2.509000
H	1.629000	-1.103000	-1.148000
C	3.886000	0.843000	-2.830000
H	4.791000	1.440000	-2.706000
H	3.138000	1.480000	-3.311000
H	4.112000	0.017000	-3.512000
C	5.321000	4.449000	0.387000
C	6.260000	3.649000	1.310000
H	6.521000	2.678000	0.879000
H	5.787000	3.468000	2.281000
H	7.191000	4.202000	1.479000
C	5.050000	5.812000	1.038000
H	5.996000	6.341000	1.191000
H	4.567000	5.704000	2.014000
H	4.416000	6.443000	0.407000

C	6.021000	4.690000	-0.965000
H	6.943000	5.264000	-0.821000
H	5.370000	5.251000	-1.643000
H	6.287000	3.748000	-1.454000
C	0.265000	3.977000	0.797000
C	-0.878000	3.745000	-0.212000
H	-0.536000	3.898000	-1.240000
H	-1.696000	4.448000	-0.028000
H	-1.324000	2.755000	-0.135000
C	-0.100000	3.398000	2.177000
H	-1.076000	3.772000	2.508000
H	0.649000	3.690000	2.919000
H	-0.151000	2.310000	2.156000
C	0.366000	5.507000	0.965000
H	0.675000	5.997000	0.036000
H	1.059000	5.801000	1.758000
H	-0.617000	5.899000	1.242000
C	3.956000	-1.082000	0.561000
C	4.304000	-0.559000	-0.715000
C	5.557000	-0.844000	-1.247000
H	5.815000	-0.442000	-2.220000
C	6.506000	-1.617000	-0.578000
C	6.149000	-2.106000	0.675000
H	6.868000	-2.702000	1.220000
C	4.909000	-1.860000	1.269000
C	7.872000	-1.876000	-1.228000
C	7.676000	-2.607000	-2.570000
H	7.067000	-2.020000	-3.264000
H	8.643000	-2.795000	-3.050000
H	7.177000	-3.569000	-2.417000
C	8.782000	-2.739000	-0.344000
H	8.988000	-2.257000	0.617000
H	8.341000	-3.722000	-0.147000
H	9.741000	-2.900000	-0.848000
C	8.583000	-0.533000	-1.480000
H	8.735000	0.006000	-0.539000
H	9.563000	-0.697000	-1.944000
H	8.002000	0.112000	-2.146000
C	4.595000	-2.407000	2.674000
C	3.375000	-3.347000	2.622000
H	3.571000	-4.195000	1.957000
H	2.496000	-2.822000	2.251000
H	3.157000	-3.743000	3.621000
C	5.762000	-3.215000	3.265000
H	5.482000	-3.570000	4.262000
H	6.668000	-2.610000	3.374000
H	6.003000	-4.093000	2.657000
C	4.320000	-1.235000	3.637000
H	3.494000	-0.622000	3.274000
H	5.207000	-0.599000	3.726000
H	4.072000	-1.612000	4.636000
Mg	-0.967000	0.470000	-1.030000
O	-0.647000	-1.145000	0.109000
O	-2.786000	0.829000	-1.107000
C	-1.706000	-2.014000	0.167000
C	-2.952000	-1.577000	0.678000
C	-4.066000	-2.394000	0.483000
H	-5.030000	-2.005000	0.793000
C	-4.005000	-3.658000	-0.084000
C	-2.746000	-4.105000	-0.467000
H	-2.661000	-5.097000	-0.882000
C	-1.591000	-3.321000	-0.376000
C	-3.272000	-0.297000	1.497000
C	-2.098000	0.595000	1.920000
H	-2.478000	1.375000	2.586000
H	-1.360000	0.020000	2.488000
H	-1.606000	1.121000	1.109000
C	-3.826000	-0.803000	2.856000
H	-4.729000	-1.408000	2.763000
H	-3.065000	-1.426000	3.335000
H	-4.045000	0.034000	3.527000
C	-5.285000	-4.485000	-0.247000
C	-6.278000	-3.713000	-1.136000
H	-6.540000	-2.743000	-0.704000
H	-5.851000	-3.534000	-2.128000
H	-7.204000	-4.286000	-1.259000
C	-5.017000	-5.850000	-0.894000
H	-5.958000	-6.400000	-0.996000
H	-4.583000	-5.745000	-1.894000
H	-4.340000	-6.460000	-0.287000
C	-5.920000	-4.723000	1.137000
H	-6.837000	-5.316000	1.040000
H	-5.231000	-5.265000	1.792000
H	-6.182000	-3.781000	1.628000
C	-0.278000	-3.893000	-0.956000
C	0.912000	-3.726000	0.007000
H	0.655000	-4.093000	1.007000
H	1.770000	-4.305000	-0.349000
H	1.259000	-2.701000	0.097000
C	-0.000000	-3.215000	-2.311000
H	0.974000	-3.521000	-2.708000
H	-0.770000	-3.497000	-3.036000
H	-0.003000	-2.129000	-2.226000
C	-0.372000	-5.408000	-1.229000
H	-0.612000	-5.971000	-0.321000
H	-1.112000	-5.654000	-1.996000
H	0.597000	-5.761000	-1.595000
C	-3.966000	1.074000	-0.561000
C	-4.291000	0.560000	0.726000
C	-5.542000	0.833000	1.268000
H	-5.783000	0.439000	2.249000
C	-6.511000	1.584000	0.602000
C	-6.177000	2.063000	-0.661000
H	-6.911000	2.641000	-1.205000
C	-4.940000	1.829000	-1.267000
C	-7.873000	1.828000	1.265000
C	-7.674000	2.576000	2.597000
H	-7.048000	2.006000	3.290000
H	-8.638000	2.754000	3.086000
H	-7.192000	3.544000	2.428000
C	-8.807000	2.667000	0.382000
H	-9.017000	2.170000	-0.571000
H	-8.384000	3.654000	0.169000
H	-9.762000	2.818000	0.896000
C	-8.560000	0.476000	1.540000
H	-8.713000	-0.076000	0.606000
H	-9.537000	0.629000	2.012000
H	-7.961000	-0.152000	2.206000
C	-4.651000	2.362000	-2.682000
C	-3.447000	3.322000	-2.657000
H	-3.651000	4.179000	-2.007000
H	-2.556000	2.819000	-2.282000
H	-3.242000	3.703000	-3.665000
C	-5.838000	3.143000	-3.270000
H	-5.575000	3.491000	-4.274000
H	-6.735000	2.522000	-3.360000
H	-6.087000	4.025000	-2.670000
C	-4.368000	1.182000	-3.633000
H	-3.529000	0.587000	-3.271000
H	-5.246000	0.531000	-3.703000
H	-4.138000	1.550000	-4.640000

[Mg(PBTP)]2-1a

Mg	-0.981000	-0.306000	-1.422000
O	-0.723000	1.198000	-0.153000
O	-2.780000	-0.722000	-1.650000
C	-1.793000	2.031000	0.011000
C	-3.042000	1.507000	0.426000
C	-4.165000	2.331000	0.333000
H	-5.129000	1.884000	0.554000
C	-4.114000	3.667000	-0.030000
C	-2.854000	4.184000	-0.311000
H	-2.777000	5.230000	-0.564000
C	-1.690000	3.411000	-0.321000
C	-3.364000	0.115000	1.040000
C	-2.203000	-0.844000	1.337000
H	-2.581000	-1.659000	1.961000
H	-1.406000	-0.360000	1.901000
H	-1.787000	-1.330000	0.461000
C	-3.937000	0.415000	2.451000
H	-4.814000	1.063000	2.442000
H	-3.168000	0.929000	3.037000
H	-4.198000	-0.510000	2.975000
C	-5.404000	4.492000	-0.096000
C	-6.344000	3.874000	-1.149000
H	-6.591000	2.835000	-0.911000
H	-5.877000	3.889000	-2.139000
H	-7.282000	4.439000	-1.204000
C	-5.140000	5.954000	-0.479000
H	-6.088000	6.501000	-0.514000
H	-4.672000	6.037000	-1.465000
H	-4.495000	6.454000	0.251000
C	-6.099000	4.472000	1.279000
H	-7.022000	5.062000	1.250000
H	-5.446000	4.894000	2.050000
H	-6.365000	3.454000	1.582000
C	-0.381000	4.080000	-0.794000
C	0.820000	3.746000	0.110000
H	0.563000	3.860000	1.168000
H	1.650000	4.429000	-0.100000
H	1.215000	2.746000	-0.045000
C	-0.108000	3.649000	-2.247000
H	0.862000	4.027000	-2.590000
H	-0.885000	4.042000	-2.910000
H	-0.100000	2.564000	-2.345000
C	-0.483000	5.619000	-0.795000
H	-0.727000	6.012000	0.198000
H	-1.224000	5.993000	-1.507000
H	0.483000	6.038000	-1.093000
C	-3.985000	-1.008000	-1.182000
C	-4.367000	-0.615000	0.132000
C	-5.656000	-0.887000	0.575000
H	-5.940000	-0.568000	1.572000
C	-6.606000	-1.539000	-0.210000
C	-6.204000	-1.935000	-1.483000
H	-6.918000	-2.450000	-2.111000
C	-4.926000	-1.694000	-1.994000
C	-8.023000	-1.759000	0.337000
C	-7.959000	-2.544000	1.661000
H	-7.382000	-2.010000	2.422000
H	-8.966000	-2.706000	2.060000
H	-7.490000	-3.522000	1.508000
C	-8.908000	-2.548000	-0.638000
H	-9.036000	-2.021000	-1.589000
H	-8.490000	-3.538000	-0.847000
H	-9.902000	-2.690000	-0.201000
C	-8.685000	-0.390000	0.589000
H	-8.760000	0.178000	-0.344000
H	-9.694000	-0.517000	0.997000
H	-8.108000	0.209000	1.300000
C	-4.555000	-2.149000	-3.417000
C	-3.366000	-3.129000	-3.366000
H	-3.628000	-4.021000	-2.786000
H	-2.497000	-2.665000	-2.902000
H	-3.096000	-3.452000	-4.379000
C	-5.710000	-2.879000	-4.123000
H	-5.385000	-3.180000	-5.124000
H	-6.590000	-2.238000	-4.241000
H	-6.012000	-3.784000	-3.587000
C	-4.195000	-0.926000	-4.283000
H	-3.358000	-0.379000	-3.849000
H	-5.050000	-0.245000	-4.355000
H	-3.927000	-1.243000	-5.298000
Mg	0.905000	0.428000	0.738000
O	0.617000	-1.078000	-0.597000
O	2.730000	0.842000	0.628000
O	0.258000	1.240000	2.527000
C	1.695000	-1.903000	-0.768000
C	2.890000	-1.396000	-1.324000
C	4.044000	-2.175000	-1.226000
H	4.975000	-1.732000	-1.566000
C	4.065000	-3.456000	-0.697000
C	2.844000	-3.977000	-0.281000
H	2.818000	-4.987000	0.100000
C	1.656000	-3.241000	-0.291000
C	3.114000	-0.055000	-2.072000
C	1.895000	0.834000	-2.354000
H	2.220000	1.678000	-2.969000
H	1.139000	0.297000	-2.939000
H	1.439000	1.263000	-1.469000

C	3.605000	-0.444000	-3.491000
H	4.528000	-1.027000	-3.489000
H	2.835000	-1.054000	-3.975000
H	3.766000	0.445000	-4.108000
C	5.393000	-4.213000	-0.583000
C	6.354000	-3.398000	0.306000
H	6.551000	-2.408000	-0.117000
H	5.929000	-3.257000	1.305000
H	7.313000	-3.917000	0.410000
C	5.218000	-5.603000	0.045000
H	6.191000	-6.097000	0.124000
H	4.793000	-5.540000	1.052000
H	4.569000	-6.242000	-0.563000
C	6.016000	-4.387000	-1.980000
H	6.976000	-4.910000	-1.908000
H	5.356000	-4.972000	-2.629000
H	6.197000	-3.422000	-2.464000
C	0.385000	-3.885000	0.297000
C	-0.803000	-3.797000	-0.680000
H	-0.570000	-4.318000	-1.614000
H	-1.690000	-4.266000	-0.243000
H	-1.079000	-2.776000	-0.931000
C	0.068000	-3.215000	1.644000
H	-0.861000	-3.609000	2.071000
H	0.873000	-3.403000	2.359000
H	-0.045000	-2.138000	1.542000
C	0.565000	-5.388000	0.587000
H	0.840000	-5.949000	-0.312000
H	1.319000	-5.575000	1.358000
H	-0.382000	-5.792000	0.957000
C	3.874000	1.164000	0.051000
C	4.147000	0.774000	-1.291000
C	5.364000	1.117000	-1.868000
H	5.563000	0.803000	-2.887000
C	6.352000	1.830000	-1.190000
C	6.071000	2.194000	0.123000
H	6.822000	2.739000	0.678000
C	4.872000	1.880000	0.768000
C	7.691000	2.122000	-1.880000
C	7.451000	2.870000	-3.205000
H	6.829000	2.288000	-3.892000
H	8.403000	3.071000	-3.709000
H	6.949000	3.826000	-3.026000
C	8.618000	2.983000	-1.011000
H	8.877000	2.480000	-0.073000
H	8.159000	3.947000	-0.768000
H	9.551000	3.181000	-1.548000
C	8.405000	0.788000	-2.173000
H	8.594000	0.243000	-1.242000
H	9.367000	0.963000	-2.670000
H	7.802000	0.146000	-2.822000
C	4.662000	2.257000	2.245000
C	3.426000	3.162000	2.404000
H	3.560000	4.096000	1.849000
H	2.531000	2.669000	2.027000
H	3.275000	3.417000	3.460000
C	5.857000	3.017000	2.841000
H	5.648000	3.244000	3.892000
H	6.779000	2.428000	2.810000
H	6.037000	3.968000	2.327000
C	4.485000	0.968000	3.070000
H	3.655000	0.379000	2.678000
H	5.392000	0.356000	3.023000
H	4.293000	1.208000	4.124000
C	0.721000	1.079000	3.889000
H	1.768000	1.386000	3.902000
H	0.150000	1.763000	4.520000
H	-0.536000	1.783000	2.480000
C	0.571000	-0.346000	4.347000
C	-0.699000	-0.888000	4.572000
C	1.696000	-1.142000	4.561000
C	-0.839000	-2.205000	4.993000
H	-1.584000	-0.276000	4.419000
C	1.558000	-2.458000	4.997000
H	2.686000	-0.726000	4.398000
C	0.292000	-2.991000	5.210000
H	-1.829000	-2.617000	5.158000
H	2.442000	-3.065000	5.165000
H	0.182000	-4.018000	5.543000

[Mg(PBTP)]2-1a-TS1

Mg	1.019000	0.071000	-0.707000
O	1.218000	-1.665000	0.188000
O	2.656000	0.856000	-1.122000
C	2.423000	-2.290000	-0.030000
C	3.621000	-1.627000	0.298000
C	4.812000	-2.167000	-0.193000
H	5.726000	-1.608000	-0.018000
C	4.876000	-3.362000	-0.896000
C	3.679000	-4.050000	-1.085000
H	3.707000	-5.003000	-1.592000
C	2.442000	-3.545000	-0.681000
C	3.807000	-0.382000	1.209000
C	2.563000	0.209000	1.898000
H	2.903000	0.919000	2.658000
H	1.952000	-0.548000	2.393000
H	1.927000	0.797000	1.241000
C	4.667000	-0.883000	2.397000
H	5.627000	-1.301000	2.091000
H	4.117000	-1.673000	2.918000
H	4.857000	-0.078000	3.114000
C	6.225000	-3.862000	-1.429000
C	6.774000	-2.832000	-2.436000
H	6.922000	-1.854000	-1.969000
H	6.079000	-2.702000	-3.272000
H	7.737000	-3.166000	-2.838000
C	6.103000	-5.217000	-2.140000
H	7.086000	-5.529000	-2.506000
H	5.429000	-5.164000	-3.001000
H	5.737000	-5.996000	-1.463000
C	7.222000	-4.017000	-0.266000
H	8.186000	-4.379000	-0.638000
H	6.849000	-4.735000	0.472000
H	7.398000	-3.066000	0.246000
C	1.153000	-4.329000	-1.013000
C	0.233000	-4.463000	0.217000
H	0.783000	-4.873000	1.071000
H	-0.590000	-5.148000	-0.011000
H	-0.204000	-3.511000	0.513000
C	0.405000	-3.619000	-2.154000
H	-0.527000	-4.145000	-2.390000
H	1.020000	-3.590000	-3.060000
H	0.148000	-2.597000	-1.877000
C	1.459000	-5.761000	-1.488000
H	2.028000	-6.326000	-0.742000
H	2.012000	-5.779000	-2.432000
H	0.515000	-6.287000	-1.658000
C	3.852000	1.281000	-0.747000
C	4.493000	0.733000	0.401000
C	5.750000	1.203000	0.766000
H	6.230000	0.781000	1.642000
C	6.429000	2.187000	0.048000
C	5.792000	2.694000	-1.081000
H	6.301000	3.450000	-1.663000
C	4.530000	2.270000	-1.506000
C	7.816000	2.649000	0.511000
C	7.710000	3.255000	1.924000
H	7.331000	2.525000	2.646000
H	8.691000	3.595000	2.274000
H	7.030000	4.113000	1.925000
C	8.418000	3.710000	-0.421000
H	8.543000	3.328000	-1.439000
H	7.795000	4.610000	-0.466000
H	9.405000	4.007000	-0.053000
C	8.776000	1.444000	0.546000
H	8.865000	0.992000	-0.447000
H	9.775000	1.757000	0.871000
H	8.429000	0.671000	1.237000
C	3.912000	2.842000	-2.796000
C	2.570000	3.536000	-2.498000
H	2.707000	4.345000	-1.772000
H	1.848000	2.831000	-2.088000
H	2.155000	3.970000	-3.415000
C	4.820000	3.888000	-3.465000
H	4.333000	4.257000	-4.374000
H	5.787000	3.467000	-3.757000
H	5.001000	4.751000	-2.815000
C	3.697000	1.707000	-3.818000
H	3.036000	0.941000	-3.411000
H	4.653000	1.238000	-4.074000
H	3.256000	2.105000	-4.739000
Mg	-1.663000	-0.459000	1.353000
O	-0.629000	0.732000	0.107000
O	-3.272000	-0.958000	0.600000
O	-0.244000	-1.612000	2.026000
C	-1.553000	1.728000	-0.115000
C	-2.646000	1.489000	-0.974000
C	-3.678000	2.429000	-0.991000
H	-4.551000	2.201000	-1.595000
C	-3.660000	3.604000	-0.255000
C	-2.535000	3.837000	0.532000
H	-2.489000	4.753000	1.103000
C	-1.481000	2.928000	0.642000
C	-2.875000	0.291000	-1.936000
C	-1.779000	-0.786000	-2.047000
H	-2.094000	-1.513000	-2.801000
H	-0.841000	-0.357000	-2.420000
H	-1.612000	-1.341000	-1.129000
C	-2.942000	0.899000	-3.359000
H	-3.731000	1.644000	-3.475000
H	-1.991000	1.396000	-3.576000
H	-3.093000	0.120000	-4.112000
C	-4.859000	4.558000	-0.314000
C	-6.096000	3.839000	0.258000
H	-6.328000	2.927000	-0.302000
H	-5.930000	3.558000	1.303000
H	-6.973000	4.494000	0.215000
C	-4.623000	5.839000	0.497000
H	-5.496000	6.493000	0.415000
H	-4.470000	5.625000	1.560000
H	-3.754000	6.394000	0.129000
C	-5.133000	4.958000	-1.776000
H	-5.978000	5.653000	-1.827000
H	-4.259000	5.450000	-2.215000
H	-5.379000	4.091000	-2.396000
C	-0.295000	3.252000	1.576000
C	1.000000	3.387000	0.756000
H	0.919000	4.227000	0.059000
H	1.856000	3.572000	1.414000
H	1.233000	2.502000	0.165000
C	-0.148000	2.185000	2.678000
H	0.662000	2.454000	3.364000
H	-1.067000	2.121000	3.273000
H	0.090000	1.199000	2.282000
C	-0.481000	4.594000	2.309000
H	-0.555000	5.436000	1.615000
H	-1.366000	4.593000	2.954000
H	0.391000	4.771000	2.946000
C	-4.289000	-1.003000	-0.240000
C	-4.183000	-0.407000	-1.526000
C	-5.276000	-0.452000	-2.385000
H	-5.190000	0.011000	-3.362000
C	-6.485000	-1.056000	-2.039000
C	-6.559000	-1.647000	-0.780000
H	-7.483000	-2.128000	-0.491000
C	-5.499000	-1.644000	0.130000
C	-7.657000	-1.034000	-3.029000
C	-7.252000	-1.760000	-4.326000
H	-6.381000	-1.293000	-4.795000
H	-8.073000	-1.740000	-5.052000
H	-7.003000	-2.806000	-4.121000
C	-8.908000	-1.722000	-2.467000
H	-9.264000	-1.234000	-1.554000
H	-8.723000	-2.778000	-2.243000
H	-9.715000	-1.677000	-3.206000
C	-8.022000	0.427000	-3.357000
H	-8.313000	0.965000	-2.449000
H	-8.859000	0.465000	-4.063000
H	-7.180000	0.961000	-3.809000
C	-5.641000	-2.309000	1.512000

C	-4.578000	-3.413000	1.681000
H	-4.716000	-4.196000	0.927000
H	-3.573000	-3.006000	1.573000
H	-4.670000	-3.879000	2.670000
C	-7.016000	-2.967000	1.708000
H	-7.055000	-3.431000	2.699000
H	-7.831000	-2.238000	1.653000
H	-7.204000	-3.751000	0.967000
C	-5.480000	-1.249000	2.619000
H	-4.514000	-0.750000	2.538000
H	-6.268000	-0.492000	2.542000
H	-5.553000	-1.717000	3.608000
C	-0.125000	-2.322000	3.247000
H	-0.529000	-3.335000	3.131000
H	0.937000	-2.410000	3.508000
H	0.575000	-1.761000	1.202000
C	-0.872000	-1.570000	4.320000
C	-0.273000	-0.478000	4.955000
C	-2.208000	-1.870000	4.601000
C	-0.994000	0.297000	5.857000
H	0.763000	-0.234000	4.734000
C	-2.934000	-1.092000	5.501000
H	-2.686000	-2.712000	4.105000
C	-2.327000	-0.007000	6.129000
H	-0.519000	1.143000	6.344000
H	-3.972000	-1.331000	5.708000
H	-2.891000	0.600000	6.829000

[Mg(PBTP)]2-1a-Int1

Mg	1.005000	-0.786000	0.933000
O	2.256000	-2.515000	0.963000
O	2.391000	0.291000	0.212000
C	3.302000	-2.577000	0.043000
C	4.391000	-1.746000	0.288000
C	5.346000	-1.662000	-0.726000
H	6.154000	-0.950000	-0.598000
C	5.274000	-2.393000	-1.905000
C	4.189000	-3.253000	-2.064000
H	4.115000	-3.834000	-2.972000
C	3.166000	-3.353000	-1.120000
C	4.639000	-0.839000	1.522000
C	3.677000	-0.942000	2.727000
H	4.143000	-0.421000	3.569000
H	3.487000	-1.974000	3.027000
H	2.729000	-0.431000	2.561000
C	6.010000	-1.265000	2.098000
H	6.821000	-1.211000	1.370000
H	5.942000	-2.301000	2.445000
H	6.285000	-0.644000	2.956000
C	6.336000	-2.180000	-2.991000
C	6.213000	-0.736000	-3.519000
H	6.348000	-0.001000	-2.719000
H	5.225000	-0.570000	-3.960000
H	6.970000	-0.545000	-4.288000
C	6.162000	-3.144000	-4.173000
H	6.948000	-2.964000	-4.912000
H	5.200000	-3.002000	-4.676000
H	6.235000	-4.190000	-3.856000
C	7.742000	-2.392000	-2.401000
H	8.502000	-2.258000	-3.178000
H	7.846000	-3.403000	-1.993000
H	7.960000	-1.680000	-1.600000
C	1.929000	-4.241000	-1.383000
C	1.860000	-5.400000	-0.365000
H	2.740000	-6.043000	-0.456000
H	0.968000	-6.006000	-0.547000
H	1.812000	-5.085000	0.685000
C	0.626000	-3.406000	-1.344000
H	-0.183000	-3.953000	-1.837000
H	0.758000	-2.459000	-1.877000
H	0.275000	-3.186000	-0.333000
C	1.992000	-4.891000	-2.776000
H	2.872000	-5.530000	-2.893000
H	1.997000	-4.139000	-3.571000
H	1.109000	-5.520000	-2.917000
C	3.485000	1.031000	0.239000
C	4.628000	0.593000	0.969000
C	5.751000	1.405000	1.055000
H	6.609000	1.052000	1.617000
C	5.832000	2.642000	0.415000
C	4.743000	3.011000	-0.370000
H	4.800000	3.943000	-0.916000
C	3.586000	2.238000	-0.504000
C	7.108000	3.484000	0.534000
C	7.416000	3.760000	2.018000
H	7.566000	2.832000	2.578000
H	8.329000	4.359000	2.116000
H	6.593000	4.307000	2.488000
C	6.984000	4.835000	-0.184000
H	6.824000	4.709000	-1.259000
H	6.158000	5.430000	0.218000
H	7.907000	5.408000	-0.051000
C	8.285000	2.713000	-0.095000
H	8.093000	2.514000	-1.154000
H	9.214000	3.290000	-0.017000
H	8.445000	1.751000	0.403000
C	2.483000	2.659000	-1.492000
C	1.163000	2.928000	-0.755000
H	1.297000	3.686000	0.022000
H	0.789000	2.020000	-0.287000
H	0.401000	3.296000	-1.451000
C	2.843000	3.936000	-2.268000
H	2.044000	4.158000	-2.982000
H	3.773000	3.826000	-2.835000
H	2.943000	4.804000	-1.607000
C	2.281000	1.537000	-2.531000
H	2.023000	0.597000	-2.041000
H	3.199000	1.383000	-3.110000
H	1.479000	1.804000	-3.230000
Mg	-1.948000	-1.130000	1.333000
O	-0.649000	0.307000	0.936000
O	-3.427000	-1.209000	0.224000
O	-0.309000	-2.092000	1.775000
C	-1.385000	1.439000	0.842000
C	-2.237000	1.625000	-0.268000
C	-3.128000	2.698000	-0.229000
H	-3.829000	2.800000	-1.051000
C	-3.181000	3.616000	0.811000
C	-2.281000	3.436000	1.860000
H	-2.296000	4.144000	2.675000
C	-1.386000	2.367000	1.918000
C	-2.306000	0.766000	-1.566000
C	-1.278000	-0.376000	-1.739000
H	-1.346000	-0.735000	-2.772000
H	-0.259000	-0.013000	-1.580000
H	-1.465000	-1.241000	-1.105000
C	-1.959000	1.726000	-2.731000
H	-2.574000	2.628000	-2.754000
H	-0.919000	2.041000	-2.623000
H	-2.059000	1.219000	-3.696000
C	-4.205000	4.757000	0.763000
C	-5.624000	4.166000	0.644000
H	-5.741000	3.567000	-0.264000
H	-5.848000	3.523000	1.501000
H	-6.369000	4.969000	0.613000
C	-4.157000	5.638000	2.018000
H	-4.911000	6.427000	1.942000
H	-4.368000	5.062000	2.925000
H	-3.182000	6.122000	2.138000
C	-3.919000	5.645000	-0.463000
H	-4.647000	6.462000	-0.522000
H	-2.918000	6.083000	-0.399000
H	-3.979000	5.075000	-1.395000
C	-0.459000	2.205000	3.144000
C	1.021000	2.309000	2.730000
H	1.255000	3.328000	2.406000
H	1.670000	2.072000	3.581000
H	1.284000	1.648000	1.902000
C	-0.710000	0.862000	3.865000
H	-0.197000	0.853000	4.833000
H	-1.780000	0.716000	4.056000
H	-0.341000	0.011000	3.292000
C	-0.697000	3.305000	4.196000
H	-0.526000	4.306000	3.788000
H	-1.709000	3.266000	4.612000
H	0.008000	3.164000	5.021000
C	-4.210000	-0.764000	-0.745000
C	-3.735000	0.198000	-1.681000
C	-4.607000	0.663000	-2.661000
H	-4.251000	1.410000	-3.362000
C	-5.928000	0.231000	-2.774000
C	-6.358000	-0.730000	-1.863000
H	-7.375000	-1.090000	-1.935000
C	-5.540000	-1.246000	-0.855000
C	-6.839000	0.837000	-3.849000
C	-6.231000	0.603000	-5.244000
H	-5.246000	1.071000	-5.340000
H	-6.877000	1.026000	-6.021000
H	-6.115000	-0.467000	-5.440000
C	-8.246000	0.224000	-3.833000
H	-8.750000	0.391000	-2.876000
H	-8.218000	-0.855000	-4.022000
H	-8.858000	0.683000	-4.616000
C	-6.975000	2.353000	-3.602000
H	-7.413000	2.545000	-2.617000
H	-7.621000	2.811000	-4.360000
H	-6.004000	2.855000	-3.641000
C	-6.079000	-2.308000	0.123000
C	-5.242000	-3.598000	0.013000
H	-5.308000	-4.011000	-1.000000
H	-4.194000	-3.404000	0.243000
H	-5.618000	-4.354000	0.712000
C	-7.538000	-2.691000	-0.175000
H	-7.863000	-3.449000	0.545000
H	-8.216000	-1.836000	-0.081000
H	-7.656000	-3.117000	-1.177000
C	-6.040000	-1.779000	1.570000
H	-5.020000	-1.539000	1.870000
H	-6.652000	-0.876000	1.663000
H	-6.434000	-2.533000	2.262000
C	-0.270000	-3.239000	2.586000
H	-0.057000	-4.139000	1.984000
H	0.528000	-3.148000	3.336000
H	1.811000	-3.364000	1.037000
C	-1.604000	-3.425000	3.277000
C	-1.934000	-2.637000	4.388000
C	-2.566000	-4.295000	2.756000
C	-3.199000	-2.719000	4.962000
H	-1.191000	-1.959000	4.801000
C	-3.831000	-4.382000	3.334000
H	-2.322000	-4.905000	1.890000
C	-4.149000	-3.593000	4.435000
H	-3.442000	-2.107000	5.825000
H	-4.568000	-5.061000	2.919000
H	-5.135000	-3.659000	4.883000

[Mg(PBTP)]2-1a-MA-Int2

Mg	-0.955000	-0.484000	0.288000
O	-2.300000	-1.989000	-0.550000
O	-2.469000	0.528000	0.803000
C	-3.658000	-2.159000	-0.238000
C	-4.552000	-1.123000	-0.526000
C	-5.829000	-1.214000	0.031000
H	-6.497000	-0.371000	-0.101000
C	-6.267000	-2.310000	0.762000
C	-5.370000	-3.361000	0.930000
H	-5.694000	-4.237000	1.472000
C	-4.053000	-3.312000	0.468000
C	-4.296000	0.129000	-1.395000
C	-3.012000	0.139000	-2.245000
H	-3.100000	0.933000	-2.991000
H	-2.861000	-0.799000	-2.786000
H	-2.114000	0.383000	-1.686000
C	-5.421000	0.151000	-2.461000
H	-6.429000	0.178000	-2.045000
H	-5.343000	-0.751000	-3.077000
H	-5.307000	1.016000	-3.121000
C	-7.684000	-2.316000	1.347000
C	-7.831000	-1.126000	2.316000

H	-7.666000	-0.169000	1.812000
H	-7.109000	-1.203000	3.135000
H	-8.838000	-1.111000	2.746000
C	-7.991000	-3.607000	2.118000
H	-9.008000	-3.561000	2.518000
H	-7.308000	-3.747000	2.962000
H	-7.928000	-4.489000	1.473000
C	-8.711000	-2.178000	0.207000
H	-9.729000	-2.179000	0.611000
H	-8.622000	-3.010000	-0.499000
H	-8.574000	-1.246000	-0.350000
C	-3.088000	-4.459000	0.825000
C	-2.301000	-4.953000	-0.405000
H	-2.990000	-5.269000	-1.196000
H	-1.685000	-5.816000	-0.131000
H	-1.627000	-4.199000	-0.810000
C	-2.151000	-3.961000	1.942000
H	-1.391000	-4.714000	2.179000
H	-2.730000	-3.760000	2.849000
H	-1.642000	-3.040000	1.660000
C	-3.828000	-5.696000	1.369000
H	-4.563000	-6.078000	0.654000
H	-4.335000	-5.496000	2.317000
H	-3.098000	-6.489000	1.558000
C	-3.397000	1.451000	0.610000
C	-4.329000	1.350000	-0.465000
C	-5.285000	2.343000	-0.639000
H	-5.988000	2.254000	-1.460000
C	-5.385000	3.452000	0.201000
C	-4.474000	3.528000	1.249000
H	-4.532000	4.375000	1.919000
C	-3.488000	2.567000	1.484000
C	-6.469000	4.507000	-0.053000
C	-6.284000	5.110000	-1.459000
H	-6.360000	4.346000	-2.239000
H	-7.050000	5.868000	-1.657000
H	-5.300000	5.583000	-1.548000
C	-6.417000	5.653000	0.966000
H	-6.575000	5.292000	1.988000
H	-5.458000	6.179000	0.933000
H	-7.205000	6.380000	0.745000
C	-7.859000	3.848000	0.038000
H	-8.015000	3.412000	1.030000
H	-8.649000	4.586000	-0.141000
H	-7.975000	3.049000	-0.701000
C	-2.504000	2.734000	2.657000
C	-1.075000	2.949000	2.122000
H	-1.014000	3.874000	1.539000
H	-0.754000	2.133000	1.475000
H	-0.369000	3.029000	2.957000
C	-2.841000	3.951000	3.535000
H	-2.126000	4.005000	4.362000
H	-3.845000	3.878000	3.967000
H	-2.771000	4.892000	2.980000
C	-2.544000	1.496000	3.575000
H	-2.284000	0.594000	3.023000
H	-3.547000	1.365000	3.996000
H	-1.841000	1.621000	4.408000
Mg	1.666000	-0.833000	-1.011000
O	0.507000	0.723000	-0.465000
O	3.457000	-0.366000	-0.741000
O	0.461000	-1.902000	0.136000
C	1.291000	1.838000	-0.549000
C	2.396000	2.006000	0.325000
C	3.333000	2.994000	0.023000
H	4.224000	3.040000	0.642000
C	3.218000	3.875000	-1.039000
C	2.066000	3.765000	-1.808000
H	1.923000	4.461000	-2.622000
C	1.098000	2.780000	-1.603000
C	2.762000	1.207000	1.609000
C	1.731000	0.199000	2.143000
H	2.115000	-0.215000	3.081000
H	0.785000	0.702000	2.369000
H	1.540000	-0.634000	1.475000
C	2.853000	2.264000	2.744000
H	3.684000	2.960000	2.623000
H	1.927000	2.845000	2.757000
H	2.955000	1.786000	3.723000
C	4.336000	4.884000	-1.324000
C	5.626000	4.113000	-1.664000
H	5.926000	3.449000	-0.847000
H	5.480000	3.495000	-2.556000
H	6.451000	4.808000	-1.858000
C	4.001000	5.806000	-2.504000
H	4.824000	6.509000	-2.669000
H	3.857000	5.241000	-3.431000
H	3.095000	6.391000	-2.315000
C	4.578000	5.762000	-0.082000
H	5.378000	6.486000	-0.275000
H	3.671000	6.316000	0.183000
H	4.872000	5.164000	0.785000
C	-0.128000	2.762000	-2.541000
C	-1.397000	2.904000	-1.690000
H	-1.411000	3.880000	-1.194000
H	-2.302000	2.828000	-2.302000
H	-1.448000	2.145000	-0.913000
C	-0.153000	1.477000	-3.391000
H	-1.006000	1.491000	-4.078000
H	0.761000	1.409000	-3.993000
H	-0.226000	0.577000	-2.786000
C	-0.132000	3.933000	-3.540000
H	-0.115000	4.905000	-3.037000
H	0.709000	3.889000	-4.240000
H	-1.053000	3.885000	-4.130000
C	4.404000	-0.152000	0.147000
C	4.120000	0.506000	1.378000
C	5.109000	0.547000	2.356000
H	4.875000	1.011000	3.309000
C	6.394000	0.037000	2.163000
C	6.689000	-0.456000	0.894000
H	7.699000	-0.786000	0.688000
C	5.744000	-0.535000	-0.131000
C	7.416000	0.088000	3.305000
C	6.876000	-0.702000	4.512000
H	5.930000	-0.288000	4.873000
H	7.591000	-0.677000	5.343000
H	6.702000	-1.749000	4.241000
C	8.767000	-0.521000	2.905000
H	9.230000	0.027000	2.078000
H	8.663000	-1.569000	2.604000
H	9.456000	-0.484000	3.755000
C	7.658000	1.551000	3.725000
H	8.045000	2.134000	2.883000
H	8.387000	1.603000	4.542000
H	6.736000	2.030000	4.068000
C	6.152000	-0.949000	-1.557000
C	5.442000	-2.240000	-2.002000
H	5.808000	-3.099000	-1.433000
H	4.366000	-2.168000	-1.843000
H	5.638000	-2.431000	-3.065000
C	7.663000	-1.201000	-1.685000
H	7.899000	-1.458000	-2.723000
H	8.250000	-0.314000	-1.421000
H	7.996000	-2.034000	-1.056000
C	5.803000	0.205000	-2.520000
H	4.738000	0.438000	-2.478000
H	6.360000	1.107000	-2.247000
H	6.070000	-0.063000	-3.550000
C	0.701000	-3.030000	0.936000
H	0.680000	-2.748000	2.001000
H	-0.092000	-3.772000	0.797000
H	-2.046000	-2.375000	-1.399000
C	2.026000	-3.702000	0.652000
C	2.075000	-4.895000	-0.073000
C	3.221000	-3.153000	1.126000
C	3.289000	-5.535000	-0.311000
H	1.149000	-5.335000	-0.436000
C	4.435000	-3.788000	0.892000
H	3.207000	-2.222000	1.684000
C	4.471000	-4.985000	0.178000
H	3.312000	-6.466000	-0.869000
H	5.353000	-3.335000	1.254000
H	5.418000	-5.483000	-0.002000
C	0.472000	-2.891000	-2.883000
O	0.774000	-1.722000	-2.649000
O	-0.801000	-3.231000	-2.727000
C	-1.293000	-4.507000	-3.186000
H	-0.937000	-5.309000	-2.537000
H	-2.376000	-4.435000	-3.116000
H	-1.000000	-4.679000	-4.221000
C	1.460000	-3.894000	-3.313000
C	2.660000	-3.496000	-3.740000
H	1.203000	-4.945000	-3.268000
H	3.412000	-4.216000	-4.042000
H	2.917000	-2.444000	-3.800000

[Mg(PBTP)]2-1a-MA-TS2

Mg	-0.914000	-0.498000	-0.048000
O	-1.955000	-2.255000	-0.409000
O	-2.397000	0.358000	0.747000
C	-3.294000	-2.434000	-0.010000
C	-4.254000	-1.504000	-0.420000
C	-5.511000	-1.589000	0.182000
H	-6.236000	-0.821000	-0.060000
C	-5.854000	-2.562000	1.108000
C	-4.886000	-3.513000	1.420000
H	-5.134000	-4.294000	2.122000
C	-3.593000	-3.472000	0.895000
C	-4.104000	-0.340000	-1.430000
C	-2.824000	-0.278000	-2.291000
H	-3.010000	0.404000	-3.125000
H	-2.536000	-1.240000	-2.716000
H	-1.964000	0.178000	-1.800000
C	-5.222000	-0.537000	-2.485000
H	-6.227000	-0.556000	-2.062000
H	-5.060000	-1.490000	-2.998000
H	-5.189000	0.256000	-3.237000
C	-7.246000	-2.536000	1.751000
C	-7.441000	-1.184000	2.465000
H	-7.376000	-0.342000	1.770000
H	-6.678000	-1.040000	3.237000
H	-8.426000	-1.147000	2.943000
C	-7.433000	-3.656000	2.782000
H	-8.431000	-3.585000	3.224000
H	-6.703000	-3.582000	3.595000
H	-7.341000	-4.647000	2.326000
C	-8.319000	-2.698000	0.657000
H	-9.319000	-2.667000	1.101000
H	-8.203000	-3.656000	0.140000
H	-8.258000	-1.901000	-0.090000
C	-2.558000	-4.517000	1.349000
C	-1.988000	-5.263000	0.129000
H	-2.783000	-5.815000	-0.383000
H	-1.223000	-5.982000	0.445000
H	-1.531000	-4.591000	-0.594000
C	-1.455000	-3.822000	2.170000
H	-0.669000	-4.535000	2.439000
H	-1.878000	-3.414000	3.093000
H	-0.998000	-3.001000	1.621000
C	-3.169000	-5.596000	2.262000
H	-3.978000	-6.142000	1.767000
H	-3.552000	-5.178000	3.197000
H	-2.391000	-6.319000	2.523000
C	-3.387000	1.198000	0.483000
C	-4.261000	0.954000	-0.615000
C	-5.261000	1.870000	-0.914000
H	-5.915000	1.672000	-1.757000
C	-5.464000	3.032000	-0.170000
C	-4.625000	3.232000	0.923000
H	-4.769000	4.118000	1.525000
C	-3.600000	2.352000	1.280000
C	-6.576000	4.009000	-0.569000
C	-6.328000	4.507000	-2.006000
H	-6.331000	3.682000	-2.725000
H	-7.107000	5.217000	-2.308000
H	-5.358000	5.010000	-2.078000
C	-6.633000	5.234000	0.354000
H	-6.841000	4.951000	1.391000
H	-5.695000	5.797000	0.334000

H	-7.432000	5.906000	0.026000
C	-7.939000	3.295000	-0.506000
H	-8.136000	2.928000	0.507000
H	-8.747000	3.980000	-0.787000
H	-7.976000	2.438000	-1.186000
C	-2.700000	2.652000	2.493000
C	-1.255000	2.904000	2.026000
H	-1.208000	3.735000	1.315000
H	-0.837000	2.026000	1.534000
H	-0.619000	3.158000	2.883000
C	-3.152000	3.905000	3.262000
H	-2.494000	4.050000	4.125000
H	-4.176000	3.807000	3.639000
H	-3.094000	4.810000	2.650000
C	-2.730000	1.475000	3.487000
H	-2.394000	0.555000	3.008000
H	-3.746000	1.318000	3.865000
H	-2.079000	1.688000	4.343000
Mg	1.708000	-0.383000	-1.760000
O	0.418000	0.758000	-0.740000
O	3.368000	0.050000	-1.027000
O	0.881000	-2.185000	-1.041000
C	1.055000	1.942000	-0.468000
C	2.042000	2.001000	0.539000
C	2.821000	3.154000	0.634000
H	3.628000	3.155000	1.360000
C	2.654000	4.264000	-0.180000
C	1.624000	4.203000	-1.112000
H	1.453000	5.060000	-1.746000
C	0.818000	3.076000	-1.290000
C	2.426000	0.902000	1.562000
C	1.504000	-0.329000	1.638000
H	1.844000	-0.979000	2.450000
H	0.482000	-0.013000	1.897000
H	1.516000	-0.924000	0.730000
C	2.293000	1.539000	2.969000
H	2.997000	2.354000	3.141000
H	1.282000	1.939000	3.082000
H	2.444000	0.792000	3.755000
C	3.595000	5.464000	-0.034000
C	5.043000	5.001000	-0.287000
H	5.354000	4.234000	0.428000
H	5.144000	4.580000	-1.292000
H	5.737000	5.845000	-0.196000
C	3.270000	6.585000	-1.031000
H	3.974000	7.412000	-0.895000
H	3.358000	6.241000	-2.067000
H	2.260000	6.980000	-0.883000
C	3.482000	6.038000	1.391000
H	4.155000	6.894000	1.514000
H	2.459000	6.372000	1.593000
H	3.748000	5.292000	2.146000
C	-0.298000	3.119000	-2.355000
C	-1.655000	3.000000	-1.647000
H	-1.862000	3.896000	-1.054000
H	-2.470000	2.878000	-2.369000
H	-1.675000	2.154000	-0.966000
C	-0.133000	1.997000	-3.397000
H	-0.875000	2.116000	-4.194000
H	0.860000	2.047000	-3.862000
H	-0.272000	1.008000	-2.969000
C	-0.312000	4.440000	-3.145000
H	-0.478000	5.307000	-2.499000
H	0.614000	4.596000	-3.707000
H	-1.136000	4.409000	-3.865000
C	4.262000	0.112000	-0.064000
C	3.872000	0.450000	1.265000
C	4.820000	0.382000	2.281000
H	4.514000	0.615000	3.295000
C	6.152000	0.034000	2.055000
C	6.527000	-0.200000	0.734000
H	7.564000	-0.426000	0.525000
C	5.630000	-0.155000	-0.335000
C	7.131000	-0.046000	3.233000
C	6.618000	-1.076000	4.258000
H	5.638000	-0.796000	4.656000
H	7.312000	-1.156000	5.103000
H	6.522000	-2.064000	3.796000
C	8.537000	-0.475000	2.792000
H	8.978000	0.242000	2.092000
H	8.526000	-1.460000	2.312000
H	9.196000	-0.536000	3.664000
C	7.242000	1.334000	3.909000
H	7.600000	2.084000	3.196000
H	7.944000	1.297000	4.750000
H	6.275000	1.673000	4.294000
C	6.116000	-0.350000	-1.784000
C	5.470000	-1.591000	-2.430000
H	5.803000	-2.507000	-1.932000
H	4.383000	-1.552000	-2.359000
H	5.754000	-1.657000	-3.488000
C	7.640000	-0.541000	-1.869000
H	7.929000	-0.653000	-2.919000
H	8.183000	0.319000	-1.464000
H	7.971000	-1.441000	-1.339000
C	5.770000	0.910000	-2.603000
H	4.695000	1.092000	-2.600000
H	6.268000	1.789000	-2.180000
H	6.108000	0.794000	-3.640000
C	1.104000	-3.324000	-0.224000
H	0.834000	-3.061000	0.803000
H	0.404000	-4.109000	-0.529000
H	-1.713000	-2.671000	-1.261000
C	2.505000	-3.890000	-0.190000
C	2.725000	-5.238000	-0.483000
C	3.580000	-3.113000	0.240000
C	3.996000	-5.795000	-0.361000
H	1.892000	-5.862000	-0.801000
C	4.851000	-3.664000	0.364000
H	3.432000	-2.069000	0.483000
C	5.063000	-5.007000	0.063000
H	4.150000	-6.844000	-0.592000
H	5.669000	-3.030000	0.693000
H	6.053000	-5.440000	0.162000
C	0.514000	-2.455000	-2.793000
O	0.515000	-1.237000	-3.159000
O	-0.732000	-3.055000	-2.695000
C	-0.953000	-4.329000	-3.314000
H	-0.478000	-5.138000	-2.753000
H	-2.033000	-4.472000	-3.307000
H	-0.591000	-4.325000	-4.344000
C	1.629000	-3.357000	-3.225000
C	2.520000	-2.959000	-4.128000
H	1.698000	-4.339000	-2.773000
H	3.338000	-3.604000	-4.429000
H	2.449000	-1.979000	-4.588000

[Mg(PBTP)]2-1a-MA-Int3

Mg	-1.229000	0.041000	0.262000
O	-1.571000	-1.898000	-0.146000
O	-2.883000	0.728000	0.803000
C	-2.842000	-2.335000	0.261000
C	-3.965000	-1.701000	-0.281000
C	-5.203000	-2.025000	0.277000
H	-6.074000	-1.489000	-0.086000
C	-5.362000	-2.948000	1.300000
C	-4.215000	-3.581000	1.773000
H	-4.315000	-4.309000	2.563000
C	-2.937000	-3.290000	1.292000
C	-4.034000	-0.640000	-1.414000
C	-2.737000	-0.233000	-2.145000
H	-3.018000	0.285000	-3.066000
H	-2.087000	-1.062000	-2.422000
H	-2.153000	0.521000	-1.616000
C	-4.906000	-1.267000	-2.528000
H	-5.895000	-1.574000	-2.183000
H	-4.399000	-2.156000	-2.918000
H	-5.037000	-0.569000	-3.360000
C	-6.759000	-3.200000	1.879000
C	-7.299000	-1.881000	2.466000
H	-7.378000	-1.100000	1.704000
H	-6.638000	-1.511000	3.256000
H	-8.295000	-2.036000	2.895000
C	-6.746000	-4.257000	2.991000
H	-7.762000	-4.404000	3.368000
H	-6.121000	-3.950000	3.835000
H	-6.383000	-5.223000	2.626000
C	-7.699000	-3.685000	0.759000
H	-8.701000	-3.869000	1.161000
H	-7.330000	-4.617000	0.318000
H	-7.791000	-2.945000	-0.041000
C	-1.715000	-4.023000	1.885000
C	-1.142000	-4.982000	0.825000
H	-1.884000	-5.745000	0.567000
H	-0.254000	-5.491000	1.216000
H	-0.861000	-4.466000	-0.094000
C	-0.633000	-3.032000	2.357000
H	0.164000	-3.571000	2.880000
H	-1.052000	-2.298000	3.053000
H	-0.183000	-2.501000	1.521000
C	-2.091000	-4.873000	3.112000
H	-2.797000	-5.670000	2.863000
H	-2.519000	-4.265000	3.915000
H	-1.187000	-5.351000	3.500000
C	-4.033000	1.207000	0.349000
C	-4.656000	0.620000	-0.788000
C	-5.843000	1.157000	-1.271000
H	-6.311000	0.698000	-2.135000
C	-6.468000	2.252000	-0.673000
C	-5.865000	2.779000	0.466000
H	-6.346000	3.611000	0.962000
C	-4.676000	2.283000	1.009000
C	-7.785000	2.787000	-1.250000
C	-7.592000	3.160000	-2.732000
H	-7.290000	2.297000	-3.332000
H	-8.525000	3.550000	-3.154000
H	-6.820000	3.929000	-2.838000
C	-8.281000	4.035000	-0.507000
H	-8.496000	3.824000	0.545000
H	-7.547000	4.846000	-0.550000
H	-9.206000	4.396000	-0.968000
C	-8.869000	1.697000	-1.135000
H	-9.033000	1.427000	-0.087000
H	-9.819000	2.052000	-1.551000
H	-8.584000	0.789000	-1.676000
C	-4.110000	2.857000	2.322000
C	-2.717000	3.476000	2.100000
H	-2.775000	4.311000	1.395000
H	-2.015000	2.743000	1.701000
H	-2.320000	3.861000	3.047000
C	-5.005000	3.960000	2.909000
H	-4.566000	4.319000	3.845000
H	-6.013000	3.594000	3.133000
H	-5.092000	4.820000	2.236000
C	-4.021000	1.735000	3.376000
H	-3.364000	0.934000	3.036000
H	-5.012000	1.309000	3.567000
H	-3.634000	2.135000	4.321000
Mg	1.600000	-0.257000	-1.536000
O	0.369000	0.879000	-0.425000
O	3.328000	0.231000	-1.047000
O	1.436000	-2.481000	-1.185000
C	1.042000	2.057000	-0.183000
C	2.106000	2.072000	0.744000
C	2.859000	3.241000	0.854000
H	3.717000	3.225000	1.517000
C	2.599000	4.394000	0.128000
C	1.533000	4.347000	-0.763000
H	1.314000	5.229000	-1.346000
C	0.753000	3.206000	-0.965000
C	2.616000	0.915000	1.648000
C	1.772000	-0.371000	1.729000
H	2.251000	-1.048000	2.444000
H	0.781000	-0.152000	2.139000
H	1.671000	-0.928000	0.798000
C	2.575000	1.450000	3.103000
H	3.246000	2.293000	3.274000
H	1.558000	1.784000	3.331000
H	2.835000	0.665000	3.820000
C	3.492000	5.626000	0.315000

C	4.943000	5.261000	-0.051000
H	5.328000	4.451000	0.576000
H	5.009000	4.934000	-1.094000
H	5.600000	6.128000	0.080000
C	3.053000	6.804000	-0.565000
H	3.713000	7.659000	-0.389000
H	3.109000	6.556000	-1.630000
H	2.030000	7.120000	-0.338000
C	3.434000	6.078000	1.787000
H	4.069000	6.958000	1.942000
H	2.410000	6.339000	2.071000
H	3.781000	5.292000	2.465000
C	-0.361000	3.250000	-2.038000
C	-1.742000	3.193000	-1.363000
H	-1.924000	4.116000	-0.806000
H	-2.538000	3.086000	-2.109000
H	-1.841000	2.376000	-0.651000
C	-0.200000	2.118000	-3.073000
H	-0.945000	2.230000	-3.868000
H	0.791000	2.166000	-3.540000
H	-0.338000	1.127000	-2.645000
C	-0.333000	4.557000	-2.855000
H	-0.516000	5.440000	-2.237000
H	0.617000	4.691000	-3.382000
H	-1.128000	4.518000	-3.605000
C	4.311000	0.271000	-0.174000
C	4.047000	0.557000	1.196000
C	5.096000	0.519000	2.108000
H	4.888000	0.717000	3.154000
C	6.414000	0.255000	1.734000
C	6.656000	0.053000	0.376000
H	7.674000	-0.128000	0.057000
C	5.651000	0.057000	-0.591000
C	7.519000	0.227000	2.798000
C	7.194000	-0.844000	3.856000
H	6.236000	-0.650000	4.348000
H	7.969000	-0.868000	4.630000
H	7.140000	-1.837000	3.398000
C	8.894000	-0.100000	2.200000
H	9.207000	0.651000	1.467000
H	8.898000	-1.079000	1.710000
H	9.647000	-0.121000	2.994000
C	7.610000	1.605000	3.483000
H	7.847000	2.383000	2.750000
H	8.394000	1.604000	4.249000
H	6.667000	1.875000	3.967000
C	5.984000	-0.145000	-2.081000
C	5.277000	-1.388000	-2.655000
H	5.588000	-2.293000	-2.126000
H	4.194000	-1.307000	-2.574000
H	5.535000	-1.507000	-3.715000
C	7.490000	-0.344000	-2.316000
H	7.673000	-0.469000	-3.388000
H	8.078000	0.516000	-1.978000
H	7.866000	-1.240000	-1.811000
C	5.557000	1.110000	-2.870000
H	4.489000	1.295000	-2.747000
H	6.102000	1.991000	-2.515000
H	5.774000	0.981000	-3.937000
C	1.872000	-3.641000	-0.431000
H	1.490000	-3.479000	0.579000
H	1.374000	-4.521000	-0.836000
H	-1.154000	-2.451000	-0.879000
C	3.367000	-3.809000	-0.399000
C	4.001000	-4.778000	-1.180000
C	4.136000	-3.034000	0.470000
C	5.377000	-4.968000	-1.092000
H	3.414000	-5.401000	-1.849000
C	5.512000	-3.217000	0.558000
H	3.664000	-2.276000	1.085000
C	6.134000	-4.187000	-0.222000
H	5.856000	-5.729000	-1.700000
H	6.091000	-2.588000	1.225000
H	7.207000	-4.336000	-0.152000
C	0.831000	-2.586000	-2.343000
O	0.594000	-1.351000	-2.791000
O	-0.450000	-3.273000	-2.015000
C	-1.294000	-3.553000	-3.124000
H	-0.923000	-4.413000	-3.688000
H	-2.281000	-3.786000	-2.717000
H	-1.363000	-2.686000	-3.787000
C	1.565000	-3.482000	-3.338000
C	2.117000	-3.010000	-4.448000
H	1.628000	-4.540000	-3.096000
H	2.660000	-3.656000	-5.130000
H	2.036000	-1.956000	-4.695000

[Mg(PBTP)]2-1a-MA-TS3

Mg	-1.293000	-0.005000	0.274000
O	-1.490000	-1.890000	-0.194000
O	-2.904000	0.811000	0.770000
C	-2.703000	-2.318000	0.278000
C	-3.890000	-1.741000	-0.224000
C	-5.099000	-2.089000	0.378000
H	-5.995000	-1.584000	0.033000
C	-5.205000	-3.002000	1.416000
C	-4.022000	-3.590000	1.856000
H	-4.075000	-4.310000	2.660000
C	-2.768000	-3.270000	1.331000
C	-4.044000	-0.703000	-1.375000
C	-2.787000	-0.250000	-2.150000
H	-3.114000	0.252000	-3.065000
H	-2.124000	-1.066000	-2.430000
H	-2.212000	0.518000	-1.633000
C	-4.915000	-1.391000	-2.453000
H	-5.879000	-1.733000	-2.073000
H	-4.381000	-2.266000	-2.835000
H	-5.100000	-0.721000	-3.298000
C	-6.575000	-3.286000	2.043000
C	-7.134000	-1.978000	2.636000
H	-7.251000	-1.205000	1.870000
H	-6.462000	-1.586000	3.405000
H	-8.115000	-2.153000	3.092000
C	-6.494000	-4.330000	3.164000
H	-7.491000	-4.501000	3.582000
H	-5.845000	-3.998000	3.981000
H	-6.119000	-5.291000	2.795000
C	-7.540000	-3.810000	0.963000
H	-8.524000	-4.016000	1.399000
H	-7.161000	-4.737000	0.520000
H	-7.678000	-3.082000	0.158000
C	-1.518000	-3.966000	1.912000
C	-0.967000	-4.967000	0.879000
H	-1.707000	-5.750000	0.681000
H	-0.058000	-5.448000	1.260000
H	-0.730000	-4.484000	-0.068000
C	-0.429000	-2.948000	2.294000
H	0.400000	-3.452000	2.806000
H	-0.826000	-2.187000	2.976000
H	-0.038000	-2.451000	1.410000
C	-1.834000	-4.764000	3.190000
H	-2.530000	-5.589000	3.007000
H	-2.251000	-4.127000	3.977000
H	-0.908000	-5.204000	3.572000
C	-4.088000	1.205000	0.330000
C	-4.709000	0.548000	-0.770000
C	-5.929000	1.016000	-1.243000
H	-6.393000	0.507000	-2.082000
C	-6.591000	2.103000	-0.672000
C	-5.992000	2.696000	0.436000
H	-6.500000	3.523000	0.913000
C	-4.770000	2.273000	0.968000
C	-7.935000	2.566000	-1.250000
C	-7.763000	2.920000	-2.740000
H	-7.428000	2.057000	-3.324000
H	-8.713000	3.262000	-3.166000
H	-7.024000	3.717000	-2.864000
C	-8.485000	3.805000	-0.529000
H	-8.678000	3.605000	0.530000
H	-7.793000	4.651000	-0.597000
H	-9.431000	4.108000	-0.988000
C	-8.969000	1.433000	-1.112000
H	-9.121000	1.177000	-0.058000
H	-9.934000	1.737000	-1.534000
H	-8.645000	0.527000	-1.634000
C	-4.206000	2.917000	2.249000
C	-2.846000	3.588000	1.983000
H	-2.952000	4.396000	1.251000
H	-2.121000	2.872000	1.597000
H	-2.451000	4.023000	2.909000
C	-5.139000	3.998000	2.818000
H	-4.699000	4.408000	3.733000
H	-6.124000	3.595000	3.076000
H	-5.279000	4.829000	2.118000
C	-4.048000	1.834000	3.336000
H	-3.363000	1.053000	3.006000
H	-5.016000	1.372000	3.558000
H	-3.661000	2.279000	4.261000
Mg	1.612000	-0.196000	-1.534000
O	0.313000	0.845000	-0.450000
O	3.334000	0.304000	-1.056000
O	1.699000	-2.406000	-1.297000
C	0.961000	2.046000	-0.220000
C	2.021000	2.096000	0.712000
C	2.744000	3.284000	0.816000
H	3.596000	3.295000	1.488000
C	2.465000	4.422000	0.075000
C	1.413000	4.338000	-0.829000
H	1.182000	5.206000	-1.426000
C	0.661000	3.176000	-1.026000
C	2.561000	0.964000	1.630000
C	1.770000	-0.354000	1.703000
H	2.273000	-1.015000	2.417000
H	0.767000	-0.181000	2.105000
H	1.696000	-0.909000	0.769000
C	2.479000	1.504000	3.081000
H	3.114000	2.374000	3.254000
H	1.447000	1.798000	3.293000
H	2.760000	0.734000	3.805000
C	3.321000	5.680000	0.258000
C	4.789000	5.348000	-0.072000
H	5.185000	4.567000	0.583000
H	4.885000	4.998000	-1.105000
H	5.417000	6.238000	0.050000
C	2.868000	6.829000	-0.652000
H	3.499000	7.707000	-0.476000
H	2.954000	6.566000	-1.711000
H	1.832000	7.120000	-0.452000
C	3.220000	6.154000	1.720000
H	3.826000	7.055000	1.873000
H	2.183000	6.391000	1.978000
H	3.574000	5.390000	2.418000
C	-0.438000	3.186000	-2.114000
C	-1.825000	3.163000	-1.450000
H	-2.005000	4.110000	-0.933000
H	-2.615000	3.029000	-2.198000
H	-1.933000	2.376000	-0.705000
C	-0.270000	2.018000	-3.107000
H	-1.002000	2.107000	-3.916000
H	0.728000	2.045000	-3.561000
H	-0.426000	1.044000	-2.647000
C	-0.392000	4.461000	-2.981000
H	-0.584000	5.368000	-2.401000
H	0.567000	4.573000	-3.497000
H	-1.176000	4.395000	-3.741000
C	4.300000	0.357000	-0.163000
C	4.008000	0.647000	1.200000
C	5.041000	0.630000	2.131000
H	4.813000	0.832000	3.172000
C	6.369000	0.375000	1.782000
C	6.636000	0.159000	0.431000
H	7.660000	-0.019000	0.131000
C	5.648000	0.146000	-0.553000
C	7.454000	0.368000	2.866000
C	7.127000	-0.707000	3.920000
H	6.157000	-0.527000	4.393000
H	7.888000	-0.717000	4.708000
H	7.097000	-1.702000	3.463000
C	8.845000	0.063000	2.293000
H	9.156000	0.815000	1.561000

H	8.876000	-0.919000	1.809000
H	9.585000	0.059000	3.100000
C	7.510000	1.747000	3.550000
H	7.743000	2.530000	2.821000
H	8.283000	1.761000	4.327000
H	6.556000	2.001000	4.022000
C	6.007000	-0.076000	-2.033000
C	5.328000	-1.344000	-2.590000
H	5.711000	-2.238000	-2.090000
H	4.249000	-1.316000	-2.446000
H	5.537000	-1.439000	-3.663000
C	7.519000	-0.258000	-2.244000
H	7.718000	-0.400000	-3.312000
H	8.089000	0.617000	-1.915000
H	7.901000	-1.139000	-1.717000
C	5.575000	1.158000	-2.851000
H	4.503000	1.330000	-2.754000
H	6.101000	2.052000	-2.500000
H	5.817000	1.016000	-3.912000
C	2.061000	-3.555000	-0.484000
H	1.643000	-3.337000	0.499000
H	1.544000	-4.432000	-0.874000
C	3.548000	-3.754000	-0.403000
C	4.184000	-4.735000	-1.167000
C	4.305000	-2.977000	0.475000
C	5.556000	-4.937000	-1.052000
H	3.604000	-5.356000	-1.843000
C	5.677000	-3.174000	0.589000
H	3.828000	-2.206000	1.070000
C	6.304000	-4.157000	-0.172000
H	6.040000	-5.707000	-1.644000
H	6.251000	-2.545000	1.260000
H	7.373000	-4.315000	-0.080000
C	1.122000	-2.510000	-2.546000
O	0.853000	-1.363000	-3.002000
C	1.556000	-3.616000	-3.441000
C	1.779000	-3.385000	-4.730000
H	1.672000	-4.603000	-3.011000
H	2.106000	-4.179000	-5.392000
H	1.644000	-2.394000	-5.151000
H	-0.887000	-2.660000	-1.227000
O	-0.464000	-3.274000	-1.970000
C	-1.421000	-3.555000	-2.982000
H	-1.155000	-4.494000	-3.469000
H	-2.404000	-3.655000	-2.514000
H	-1.448000	-2.754000	-3.728000

[Mg(PBTP)]2-1a-MA-Int4

Mg	-1.126000	-0.337000	-0.498000
O	-1.422000	-2.231000	-0.674000
O	-2.458000	0.609000	0.405000
C	-2.541000	-2.621000	-0.016000
C	-3.775000	-1.962000	-0.228000
C	-4.835000	-2.248000	0.634000
H	-5.745000	-1.667000	0.517000
C	-4.779000	-3.204000	1.637000
C	-3.589000	-3.919000	1.748000
H	-3.520000	-4.694000	2.499000
C	-2.469000	-3.657000	0.959000
C	-4.138000	-0.929000	-1.338000
C	-3.078000	-0.605000	-2.420000
H	-3.590000	-0.153000	-3.274000
H	-2.547000	-1.490000	-2.771000
H	-2.360000	0.172000	-2.143000
C	-5.272000	-1.596000	-2.158000
H	-6.133000	-1.878000	-1.549000
H	-4.881000	-2.508000	-2.620000
H	-5.622000	-0.938000	-2.960000
C	-5.986000	-3.414000	2.558000
C	-6.290000	-2.098000	3.300000
H	-6.516000	-1.285000	2.603000
H	-5.432000	-1.789000	3.905000
H	-7.153000	-2.223000	3.964000
C	-5.736000	-4.510000	3.603000
H	-6.619000	-4.621000	4.240000
H	-4.888000	-4.263000	4.250000
H	-5.539000	-5.479000	3.134000
C	-7.214000	-3.820000	1.720000
H	-8.086000	-3.971000	2.365000
H	-7.023000	-4.752000	1.178000
H	-7.471000	-3.051000	0.985000
C	-1.171000	-4.451000	1.199000
C	-0.700000	-5.116000	-0.109000
H	-1.449000	-5.837000	-0.453000
H	0.238000	-5.659000	0.058000
H	-0.541000	-4.387000	-0.901000
C	-0.095000	-3.505000	1.763000
H	0.865000	-4.023000	1.878000
H	-0.397000	-3.129000	2.746000
H	0.040000	-2.648000	1.106000
C	-1.347000	-5.586000	2.223000
H	-2.110000	-6.306000	1.909000
H	-1.611000	-5.212000	3.217000
H	-0.400000	-6.127000	2.319000
C	-3.696000	1.042000	0.242000
C	-4.588000	0.372000	-0.645000
C	-5.876000	0.868000	-0.809000
H	-6.553000	0.350000	-1.480000
C	-6.347000	1.991000	-0.127000
C	-5.464000	2.613000	0.753000
H	-5.810000	3.475000	1.306000
C	-4.155000	2.172000	0.965000
C	-7.792000	2.459000	-0.339000
C	-8.017000	2.794000	-1.826000
H	-7.835000	1.927000	-2.467000
H	-9.049000	3.124000	-1.994000
H	-7.345000	3.596000	-2.147000
C	-8.128000	3.709000	0.486000
H	-8.028000	3.524000	1.560000
H	-7.482000	4.553000	0.222000
H	-9.163000	4.010000	0.296000
C	-8.761000	1.336000	0.081000
H	-8.619000	1.080000	1.136000
H	-9.801000	1.650000	-0.060000
H	-8.602000	0.427000	-0.508000
C	-3.239000	2.876000	1.985000
C	-2.000000	3.467000	1.287000
H	-2.292000	4.234000	0.562000
H	-1.437000	2.697000	0.760000
H	-1.336000	3.938000	2.023000
C	-3.950000	4.032000	2.707000
H	-3.258000	4.486000	3.424000
H	-4.828000	3.690000	3.265000
H	-4.266000	4.817000	2.013000
C	-2.791000	1.871000	3.067000
H	-2.239000	1.043000	2.622000
H	-3.660000	1.463000	3.595000
H	-2.150000	2.371000	3.803000
Mg	1.924000	0.073000	-2.084000
O	0.270000	0.785000	-1.272000
O	3.381000	0.532000	-1.037000
O	2.217000	-2.227000	-1.891000
C	0.665000	2.052000	-0.881000
C	1.490000	2.203000	0.253000
C	2.054000	3.457000	0.484000
H	2.747000	3.550000	1.314000
C	1.797000	4.568000	-0.307000
C	0.916000	4.396000	-1.371000
H	0.680000	5.251000	-1.985000
C	0.340000	3.165000	-1.695000
C	1.849000	1.139000	1.320000
C	1.137000	-0.225000	1.239000
H	1.474000	-0.842000	2.077000
H	0.057000	-0.098000	1.403000
H	1.347000	-0.793000	0.331000
C	1.346000	1.716000	2.670000
H	1.884000	2.615000	2.976000
H	0.288000	1.975000	2.572000
H	1.435000	0.980000	3.474000
C	2.467000	5.907000	0.021000
C	3.996000	5.739000	-0.049000
H	4.355000	4.985000	0.658000
H	4.306000	5.431000	-1.053000
H	4.494000	6.686000	0.189000
C	2.058000	7.018000	-0.955000
H	2.564000	7.950000	-0.683000
H	2.340000	6.776000	-1.985000
H	0.980000	7.206000	-0.928000
C	2.062000	6.342000	1.443000
H	2.527000	7.302000	1.695000
H	0.976000	6.457000	1.518000
H	2.376000	5.611000	2.193000
C	-0.664000	3.090000	-2.868000
C	-2.076000	2.888000	-2.285000
H	-2.411000	3.796000	-1.776000
H	-2.795000	2.658000	-3.079000
H	-2.106000	2.090000	-1.544000
C	-0.333000	1.967000	-3.872000
H	-0.961000	2.072000	-4.763000
H	0.712000	2.033000	-4.203000
H	-0.520000	0.976000	-3.460000
C	-0.695000	4.392000	-3.690000
H	-1.011000	5.254000	-3.095000
H	0.278000	4.617000	-4.139000
H	-1.421000	4.280000	-4.501000
C	4.046000	0.593000	0.098000
C	3.368000	0.880000	1.316000
C	4.086000	0.876000	2.508000
H	3.561000	1.082000	3.434000
C	5.457000	0.624000	2.564000
C	6.107000	0.399000	1.352000
H	7.173000	0.219000	1.365000
C	5.450000	0.382000	0.121000
C	6.180000	0.627000	3.917000
C	5.540000	-0.418000	4.850000
H	4.478000	-0.214000	5.019000
H	6.039000	-0.418000	5.826000
H	5.625000	-1.424000	4.425000
C	7.671000	0.289000	3.780000
H	8.199000	1.023000	3.163000
H	7.821000	-0.702000	3.338000
H	8.141000	0.288000	4.769000
C	6.060000	2.022000	4.561000
H	6.511000	2.784000	3.917000
H	6.571000	2.045000	5.530000
H	5.014000	2.299000	4.727000
C	6.232000	0.147000	-1.185000
C	5.744000	-1.129000	-1.898000
H	5.931000	-2.013000	-1.282000
H	4.675000	-1.076000	-2.100000
H	6.276000	-1.254000	-2.849000
C	7.739000	-0.032000	-0.939000
H	8.243000	-0.181000	-1.899000
H	8.186000	0.847000	-0.463000
H	7.949000	-0.909000	-0.317000
C	6.060000	1.368000	-2.111000
H	5.007000	1.535000	-2.342000
H	6.455000	2.270000	-1.632000
H	6.608000	1.214000	-3.049000
C	2.171000	-3.395000	-1.014000
H	1.405000	-3.128000	-0.290000
H	1.805000	-4.248000	-1.583000
C	3.505000	-3.620000	-0.370000
C	4.374000	-4.606000	-0.841000
C	3.897000	-2.817000	0.702000
C	5.622000	-4.781000	-0.251000
H	4.075000	-5.248000	-1.665000
C	5.145000	-2.985000	1.289000
H	3.236000	-2.040000	1.071000
C	6.009000	-3.968000	0.813000
H	6.291000	-5.550000	-0.620000
H	5.444000	-2.332000	2.102000
H	6.985000	-4.101000	1.269000
C	2.311000	-2.256000	-3.215000
O	2.237000	-1.137000	-3.740000
C	2.556000	-3.489000	-3.962000
C	2.651000	-3.443000	-5.291000
H	2.660000	-4.421000	-3.423000
H	2.837000	-4.343000	-5.866000
H	2.544000	-2.507000	-5.829000

H	-0.776000	-2.759000	-2.118000
O	-0.281000	-2.920000	-2.956000
C	-1.031000	-3.797000	-3.766000
H	-0.445000	-4.007000	-4.665000
H	-1.235000	-4.749000	-3.258000
H	-1.990000	-3.360000	-4.075000

[Mg(PBTP)]2-2a-MeOH

Mg	1.374000	0.655000	-1.229000
O	1.056000	-1.158000	-0.471000
O	3.189000	1.062000	-0.951000
C	2.190000	-1.917000	-0.557000
C	3.332000	-1.579000	0.223000
C	4.548000	-2.195000	-0.059000
H	5.420000	-1.848000	0.487000
C	4.712000	-3.191000	-1.010000
C	3.566000	-3.573000	-1.685000
H	3.639000	-4.370000	-2.414000
C	2.313000	-2.966000	-1.511000
C	3.445000	-0.569000	1.396000
C	2.163000	0.107000	1.889000
H	2.411000	0.722000	2.759000
H	1.432000	-0.637000	2.218000
H	1.717000	0.781000	1.168000
C	3.909000	-1.393000	2.625000
H	4.881000	-1.872000	2.490000
H	3.174000	-2.183000	2.813000
H	3.961000	-0.767000	3.522000
C	6.097000	-3.792000	-1.265000
C	7.046000	-2.677000	-1.748000
H	7.136000	-1.877000	-1.008000
H	6.676000	-2.232000	-2.678000
H	8.047000	-3.082000	-1.934000
C	6.062000	-4.895000	-2.330000
H	7.069000	-5.298000	-2.480000
H	5.710000	-4.513000	-3.294000
H	5.414000	-5.725000	-2.031000
C	6.646000	-4.396000	0.041000
H	7.637000	-4.833000	-0.125000
H	5.982000	-5.184000	0.412000
H	6.742000	-3.639000	0.826000
C	1.211000	-3.577000	-2.411000
C	1.026000	-5.053000	-1.997000
H	1.922000	-5.649000	-2.188000
H	0.199000	-5.508000	-2.554000
H	0.809000	-5.123000	-0.926000
C	-0.152000	-2.894000	-2.345000
H	-0.865000	-3.448000	-2.966000
H	-0.089000	-1.881000	-2.739000
H	-0.541000	-2.848000	-1.330000
C	1.640000	-3.516000	-3.894000
H	2.557000	-4.072000	-4.098000
H	1.801000	-2.478000	-4.202000
H	0.851000	-3.937000	-4.527000
C	4.259000	1.259000	-0.206000
C	4.456000	0.521000	0.996000
C	5.579000	0.778000	1.773000
H	5.713000	0.219000	2.693000
C	6.552000	1.713000	1.417000
C	6.363000	2.391000	0.216000
H	7.111000	3.107000	-0.097000
C	5.254000	2.189000	-0.609000
C	7.764000	1.936000	2.331000
C	7.282000	2.443000	3.704000
H	6.597000	1.731000	4.176000
H	8.130000	2.593000	4.381000
H	6.755000	3.397000	3.599000
C	8.746000	2.968000	1.759000
H	9.151000	2.648000	0.793000
H	8.274000	3.947000	1.627000
H	9.588000	3.095000	2.448000
C	8.523000	0.608000	2.519000
H	8.872000	0.223000	1.555000
H	9.395000	0.752000	3.167000
H	7.891000	-0.158000	2.977000
C	5.120000	2.947000	-1.942000
C	3.863000	3.837000	-1.918000
H	3.956000	4.612000	-1.150000
H	2.977000	3.248000	-1.683000
H	3.723000	4.335000	-2.886000
C	6.317000	3.868000	-2.228000
H	6.167000	4.363000	-3.193000
H	7.258000	3.312000	-2.284000
H	6.423000	4.650000	-1.469000
C	5.040000	1.940000	-3.108000
H	4.252000	1.205000	-2.939000
H	5.984000	1.393000	-3.204000
H	4.859000	2.462000	-4.056000
Mg	-0.601000	-0.614000	0.579000
O	-0.238000	1.219000	-0.231000
O	-2.493000	-0.414000	0.693000
O	-0.962000	-3.673000	0.772000
C	-1.173000	2.213000	-0.242000
C	-2.360000	2.083000	-1.005000
C	-3.319000	3.095000	-0.913000
H	-4.267000	2.934000	-1.411000
C	-3.163000	4.253000	-0.175000
C	-1.974000	4.374000	0.533000
H	-1.822000	5.262000	1.126000
C	-0.989000	3.385000	0.552000
C	-2.850000	0.877000	-1.863000
C	-1.828000	-0.188000	-2.262000
H	-2.288000	-0.859000	-2.995000
H	-0.949000	0.253000	-2.743000
H	-1.523000	-0.827000	-1.445000
C	-3.324000	1.418000	-3.237000
H	-4.089000	2.193000	-3.184000
H	-2.466000	1.843000	-3.767000
H	-3.720000	0.603000	-3.851000
C	-4.298000	5.281000	-0.120000
C	-5.533000	4.625000	0.527000
H	-5.856000	3.738000	-0.027000
H	-5.311000	4.312000	1.552000
H	-6.371000	5.332000	0.557000
C	-3.918000	6.520000	0.702000
H	-4.747000	7.236000	0.696000
H	-3.708000	6.267000	1.746000
H	-3.039000	7.024000	0.287000
C	-4.653000	5.741000	-1.547000
H	-5.460000	6.481000	-1.520000
H	-3.785000	6.198000	-2.034000
H	-4.988000	4.905000	-2.169000
C	0.184000	3.569000	1.540000
C	1.550000	3.513000	0.837000
H	1.632000	4.337000	0.120000
H	2.363000	3.618000	1.564000
H	1.732000	2.590000	0.297000
C	0.041000	2.514000	2.653000
H	0.867000	2.584000	3.369000
H	-0.898000	2.672000	3.192000
H	0.028000	1.501000	2.257000
C	0.157000	4.935000	2.255000
H	0.227000	5.770000	1.551000
H	-0.739000	5.070000	2.868000
H	1.021000	4.995000	2.925000
C	-3.726000	-0.183000	0.296000
C	-3.995000	0.269000	-1.031000
C	-5.310000	0.346000	-1.473000
H	-5.498000	0.656000	-2.496000
C	-6.404000	0.090000	-0.643000
C	-6.121000	-0.196000	0.690000
H	-6.948000	-0.332000	1.374000
C	-4.823000	-0.323000	1.190000
C	-7.827000	0.176000	-1.205000
C	-7.997000	-0.874000	-2.320000
H	-7.270000	-0.725000	-3.124000
H	-9.001000	-0.818000	-2.758000
H	-7.853000	-1.884000	-1.921000
C	-8.894000	-0.088000	-0.134000
H	-8.847000	0.651000	0.672000
H	-8.784000	-1.085000	0.307000
H	-9.891000	-0.029000	-0.583000
C	-8.075000	1.581000	-1.787000
H	-7.974000	2.344000	-1.008000
H	-9.085000	1.654000	-2.207000
H	-7.365000	1.821000	-2.584000
C	-4.584000	-0.574000	2.688000
C	-3.904000	-1.936000	2.896000
H	-4.550000	-2.749000	2.552000
H	-2.977000	-1.970000	2.330000
H	-3.681000	-2.097000	3.958000
C	-5.888000	-0.582000	3.502000
H	-5.650000	-0.740000	4.559000
H	-6.429000	0.367000	3.420000
H	-6.559000	-1.391000	3.192000
C	-3.697000	0.551000	3.260000
H	-2.739000	0.596000	2.740000
H	-4.191000	1.522000	3.148000
H	-3.513000	0.384000	4.328000
C	-1.731000	-4.857000	0.439000
H	-1.371000	-5.100000	-0.561000
H	-1.472000	-5.685000	1.101000
H	2.206000	1.875000	-3.297000
C	-3.202000	-4.557000	0.429000
C	-4.089000	-5.303000	1.203000
C	-3.688000	-3.530000	-0.383000
C	-5.456000	-5.029000	1.157000
H	-3.716000	-6.099000	1.841000
C	-5.046000	-3.244000	-0.415000
H	-2.999000	-2.935000	-0.976000
C	-5.932000	-3.999000	0.352000
H	-6.142000	-5.615000	1.760000
H	-5.409000	-2.421000	-1.021000
H	-6.994000	-3.773000	0.328000
C	-0.801000	-3.208000	1.998000
O	-0.422000	-2.038000	2.103000
O	1.294000	1.695000	-3.031000
C	0.499000	2.876000	-3.235000
H	-0.476000	2.685000	-2.788000
H	0.956000	3.734000	-2.736000
H	0.389000	3.069000	-4.303000
C	-1.036000	-4.063000	3.172000
C	-1.047000	-3.523000	4.390000
H	-1.208000	-5.121000	3.028000
H	-1.220000	-4.133000	5.269000
H	-0.894000	-2.458000	4.532000

Na2(PBTP)•2(MMA)•2(1a)

Na	2.207000	0.135000	-1.060000
O	1.279000	-1.453000	0.190000
C	0.089000	-1.759000	0.623000
C	-0.632000	-0.865000	1.476000
C	-1.926000	-1.184000	1.880000
H	-2.463000	-0.469000	2.487000
C	-2.581000	-2.354000	1.493000
C	-1.862000	-3.233000	0.678000
H	-2.343000	-4.156000	0.373000
C	-0.566000	-2.974000	0.225000
C	0.057000	0.388000	2.037000
C	1.069000	-0.144000	3.076000
H	0.545000	-0.812000	3.766000
H	1.509000	0.659000	3.676000
H	1.873000	-0.706000	2.598000
C	-4.019000	-2.682000	1.915000
C	-4.018000	-3.917000	2.835000
H	-3.432000	-3.725000	3.739000
H	-3.585000	-4.787000	2.332000
H	-5.040000	-4.175000	3.137000
C	-4.677000	-1.510000	2.658000
H	-5.720000	-1.755000	2.886000
H	-4.660000	-0.603000	2.045000
H	-4.173000	-1.294000	3.606000
C	-4.874000	-2.979000	0.670000
H	-5.906000	-3.211000	0.956000
H	-4.489000	-3.832000	0.102000
H	-4.897000	-2.114000	0.001000
C	0.144000	-3.965000	-0.714000
C	1.453000	-4.463000	-0.071000
H	1.243000	-5.008000	0.855000

H	2.106000	-3.623000	0.166000
H	1.981000	-5.141000	-0.752000
C	-0.711000	-5.204000	-1.022000
H	-0.148000	-5.873000	-1.681000
H	-1.643000	-4.943000	-1.535000
H	-0.962000	-5.767000	-0.116000
C	0.450000	-3.275000	-2.056000
H	0.923000	-3.980000	-2.750000
H	1.117000	-2.425000	-1.916000
H	-0.477000	-2.922000	-2.525000
O	-1.158000	1.200000	-0.502000
C	0.035000	1.658000	-0.221000
C	0.728000	1.272000	0.971000
C	2.005000	1.773000	1.218000
H	2.512000	1.443000	2.114000
C	2.680000	2.639000	0.356000
C	2.012000	2.987000	-0.819000
H	2.512000	3.639000	-1.523000
C	0.727000	2.528000	-1.134000
C	-0.917000	1.316000	2.791000
H	-0.370000	2.197000	3.139000
H	-1.348000	0.829000	3.672000
H	-1.732000	1.659000	2.151000
C	4.112000	3.106000	0.652000
C	4.365000	4.520000	0.101000
H	3.647000	5.237000	0.513000
H	4.294000	4.559000	-0.990000
H	5.373000	4.852000	0.370000
C	4.390000	3.141000	2.164000
H	5.388000	3.553000	2.348000
H	4.363000	2.145000	2.615000
H	3.660000	3.768000	2.686000
C	5.102000	2.132000	-0.016000
H	6.138000	2.371000	0.254000
H	5.012000	2.190000	-1.104000
H	4.895000	1.098000	0.279000
C	0.060000	2.957000	-2.451000
C	-1.243000	3.718000	-2.137000
H	-1.015000	4.655000	-1.617000
H	-1.890000	3.117000	-1.500000
H	-1.777000	3.968000	-3.062000
C	0.938000	3.896000	-3.292000
H	0.402000	4.160000	-4.210000
H	1.882000	3.426000	-3.587000
H	1.169000	4.828000	-2.765000
C	-0.223000	1.712000	-3.315000
H	-0.762000	1.988000	-4.229000
H	-0.813000	0.984000	-2.760000
H	0.718000	1.236000	-3.616000
Na	-2.201000	-0.791000	-0.886000
C	3.930000	-1.400000	4.819000
C	4.652000	-0.448000	4.102000
C	4.954000	-0.671000	2.762000
C	4.538000	-1.840000	2.122000
C	3.817000	-2.788000	2.850000
C	3.515000	-2.571000	4.192000
C	4.792000	-2.042000	0.647000
O	3.796000	-1.432000	-0.147000
H	3.694000	-1.228000	5.865000
H	4.983000	0.465000	4.586000
H	5.525000	0.068000	2.206000
H	3.483000	-3.699000	2.360000
H	2.951000	-3.315000	4.746000
H	4.852000	-3.118000	0.425000
H	5.747000	-1.591000	0.360000
H	2.894000	-1.669000	0.192000
C	-3.123000	4.211000	3.759000
C	-4.035000	3.164000	3.873000
C	-4.501000	2.520000	2.732000
C	-4.063000	2.913000	1.465000
C	-3.156000	3.968000	1.360000
C	-2.686000	4.615000	2.500000
C	-4.459000	2.121000	0.241000
O	-3.641000	0.978000	0.097000
H	-2.753000	4.710000	4.649000
H	-4.381000	2.847000	4.852000
H	-5.203000	1.695000	2.820000
H	-2.800000	4.273000	0.380000
H	-1.973000	5.428000	2.406000
H	-4.402000	2.761000	-0.653000
H	-5.490000	1.765000	0.329000
H	-2.690000	1.264000	0.075000
C	-4.909000	-0.432000	-2.628000
O	-3.871000	-1.071000	-2.525000
O	-4.938000	0.858000	-2.936000
C	-3.672000	1.490000	-3.156000
H	-3.899000	2.527000	-3.394000
H	-3.061000	1.435000	-2.255000
H	-3.152000	1.014000	-3.989000
C	-6.278000	-0.999000	-2.456000
C	-6.386000	-2.324000	-2.351000
H	-7.353000	-2.801000	-2.232000
H	-5.507000	-2.958000	-2.377000
C	-7.446000	-0.053000	-2.435000
H	-8.375000	-0.598000	-2.261000
H	-7.329000	0.698000	-1.648000
H	-7.530000	0.487000	-3.383000
C	4.019000	-0.960000	-3.114000
O	2.796000	-0.947000	-3.111000
O	4.736000	-2.070000	-3.038000
C	3.999000	-3.282000	-2.825000
H	4.745000	-4.074000	-2.797000
H	3.464000	-3.211000	-1.876000
H	3.290000	-3.446000	-3.638000
C	4.861000	0.270000	-3.200000
C	4.256000	1.392000	-3.600000
H	4.799000	2.328000	-3.679000
H	3.203000	1.393000	-3.860000
C	6.309000	0.178000	-2.816000
H	6.795000	1.150000	-2.917000
H	6.408000	-0.155000	-1.778000
H	6.838000	-0.547000	-3.441000

Na2(PBTP)•2(MMA)•2(1a)-TS4

Na	2.209000	0.329000	-1.004000
O	1.411000	-1.160000	0.684000
C	0.166000	-1.582000	1.047000
C	-0.623000	-0.617000	1.702000
C	-1.922000	-0.968000	2.068000
H	-2.541000	-0.215000	2.530000
C	-2.463000	-2.226000	1.816000
C	-1.636000	-3.159000	1.190000
H	-2.034000	-4.148000	1.002000
C	-0.323000	-2.883000	0.793000
C	-0.044000	0.743000	2.127000
C	0.940000	0.416000	3.275000
H	0.421000	-0.195000	4.020000
H	1.282000	1.323000	3.783000
H	1.810000	-0.138000	2.917000
C	-3.900000	-2.600000	2.199000
C	-3.871000	-3.725000	3.249000
H	-3.338000	-3.402000	4.149000
H	-3.374000	-4.621000	2.865000
H	-4.891000	-4.003000	3.536000
C	-4.666000	-1.401000	2.773000
H	-5.698000	-1.693000	2.990000
H	-4.684000	-0.577000	2.052000
H	-4.221000	-1.037000	3.705000
C	-4.657000	-3.080000	0.948000
H	-5.687000	-3.351000	1.206000
H	-4.188000	-3.958000	0.492000
H	-4.696000	-2.289000	0.194000
C	0.519000	-3.964000	0.091000
C	1.803000	-4.255000	0.898000
H	1.548000	-4.733000	1.849000
H	2.391000	-3.369000	1.141000
H	2.449000	-4.938000	0.336000
C	-0.234000	-5.301000	-0.018000
H	0.427000	-6.039000	-0.483000
H	-1.128000	-5.220000	-0.646000
H	-0.527000	-5.692000	0.961000
C	0.841000	-3.524000	-1.352000
H	1.306000	-4.356000	-1.892000
H	1.525000	-2.677000	-1.442000
H	-0.085000	-3.268000	-1.878000
O	-1.192000	1.100000	-0.513000
C	-0.065000	1.715000	-0.259000
C	0.613000	1.537000	0.987000
C	1.827000	2.186000	1.219000
H	2.320000	2.023000	2.168000
C	2.435000	3.025000	0.287000
C	1.775000	3.181000	-0.935000
H	2.229000	3.824000	-1.680000
C	0.568000	2.551000	-1.244000
C	-1.122000	1.678000	2.713000
H	-0.651000	2.628000	2.977000
H	-1.572000	1.269000	3.624000
H	-1.915000	1.886000	1.993000
C	3.719000	3.813000	0.579000
C	3.379000	5.316000	0.619000
H	2.642000	5.524000	1.402000
H	2.961000	5.655000	-0.334000
H	4.277000	5.909000	0.826000
C	4.349000	3.425000	1.923000
H	5.257000	4.013000	2.087000
H	4.633000	2.369000	1.939000
H	3.674000	3.617000	2.763000
C	4.767000	3.562000	-0.519000
H	5.688000	4.114000	-0.303000
H	4.409000	3.884000	-1.501000
H	5.010000	2.497000	-0.586000
C	-0.078000	2.757000	-2.624000
C	-1.456000	3.422000	-2.443000
H	-1.337000	4.424000	-2.015000
H	-2.076000	2.831000	-1.770000
H	-1.966000	3.524000	-3.408000
C	0.755000	3.667000	-3.540000
H	0.245000	3.770000	-4.504000
H	1.748000	3.250000	-3.736000
H	0.877000	4.672000	-3.123000
C	-0.215000	1.401000	-3.343000
H	-0.710000	1.529000	-4.313000
H	-0.797000	0.705000	-2.741000
H	0.769000	0.956000	-3.527000
Na	-2.066000	-0.956000	-0.828000
C	5.053000	-1.235000	4.024000
C	4.611000	-0.276000	3.117000
C	4.467000	-0.596000	1.769000
C	4.760000	-1.880000	1.308000
C	5.196000	-2.837000	2.228000
C	5.348000	-2.520000	3.574000
C	4.617000	-2.247000	-0.156000
O	3.662000	-1.465000	-0.800000
H	5.160000	-0.986000	5.075000
H	4.365000	0.724000	3.463000
H	4.104000	0.150000	1.069000
H	5.409000	-3.847000	1.884000
H	5.685000	-3.278000	4.274000
H	4.363000	-3.320000	-0.215000
H	5.598000	-2.158000	-0.644000
H	1.970000	-1.792000	0.202000
C	-3.579000	4.473000	3.166000
C	-4.358000	3.351000	3.448000
C	-4.741000	2.495000	2.420000
C	-4.353000	2.748000	1.103000
C	-3.582000	3.879000	0.830000
C	-3.195000	4.738000	1.855000
C	-4.651000	1.753000	0.007000
O	-3.682000	0.722000	-0.019000
H	-3.276000	5.140000	3.967000
H	-4.663000	3.144000	4.468000
H	-5.341000	1.617000	2.642000
H	-3.271000	4.081000	-0.191000
H	-2.591000	5.611000	1.629000
H	-4.697000	2.269000	-0.964000
H	-5.620000	1.272000	0.172000
H	-2.775000	1.122000	-0.036000
C	-4.773000	-1.072000	-2.587000
O	-3.697000	-1.613000	-2.369000
O	-4.880000	0.162000	-3.062000

C	-3.654000	0.856000	-3.318000
H	-3.941000	1.806000	-3.764000
H	-3.123000	1.026000	-2.380000
H	-3.028000	0.284000	-4.004000
C	-6.105000	-1.711000	-2.383000
C	-6.127000	-3.025000	-2.149000
H	-7.064000	-3.552000	-2.001000
H	-5.208000	-3.597000	-2.101000
C	-7.332000	-0.846000	-2.463000
H	-8.228000	-1.438000	-2.268000
H	-7.285000	-0.035000	-1.730000
H	-7.425000	-0.383000	-3.449000
C	3.814000	-1.151000	-2.523000
O	2.613000	-1.077000	-2.899000
O	4.626000	-2.183000	-2.965000
C	3.958000	-3.408000	-3.203000
H	4.703000	-4.091000	-3.612000
H	3.557000	-3.821000	-2.271000
H	3.136000	-3.281000	-3.912000
C	4.660000	0.127000	-2.519000
C	4.139000	1.208000	-3.103000
H	4.682000	2.147000	-3.149000
H	3.156000	1.163000	-3.560000
C	6.025000	0.129000	-1.893000
H	6.556000	1.057000	-2.121000
H	5.950000	0.040000	-0.804000
H	6.621000	-0.714000	-2.253000

Na2(PBTP)•2(MMA)•2(1a)-Int5

Na	2.242000	0.401000	-0.957000
O	1.405000	-1.082000	0.691000
C	0.157000	-1.457000	1.100000
C	-0.594000	-0.456000	1.745000
C	-1.891000	-0.770000	2.152000
H	-2.484000	0.009000	2.603000
C	-2.464000	-2.023000	1.952000
C	-1.673000	-2.992000	1.332000
H	-2.094000	-3.977000	1.184000
C	-0.369000	-2.752000	0.887000
C	0.016000	0.912000	2.100000
C	1.062000	0.622000	3.202000
H	0.589000	0.027000	3.989000
H	1.422000	1.545000	3.666000
H	1.918000	0.064000	2.816000
C	-3.893000	-2.358000	2.397000
C	-3.830000	-3.378000	3.550000
H	-3.276000	-2.968000	4.400000
H	-3.334000	-4.302000	3.238000
H	-4.840000	-3.634000	3.889000
C	-4.648000	-1.109000	2.874000
H	-5.679000	-1.377000	3.125000
H	-4.666000	-0.345000	2.090000
H	-4.194000	-0.675000	3.771000
C	-4.685000	-2.964000	1.225000
H	-5.706000	-3.202000	1.543000
H	-4.234000	-3.890000	0.854000
H	-4.750000	-2.264000	0.387000
C	0.427000	-3.866000	0.182000
C	1.708000	-4.192000	0.980000
H	1.444000	-4.638000	1.944000
H	2.335000	-3.325000	1.198000
H	2.320000	-4.913000	0.427000
C	-0.372000	-5.177000	0.096000
H	0.250000	-5.937000	-0.386000
H	-1.280000	-5.065000	-0.507000
H	-0.652000	-5.557000	1.083000
C	0.744000	-3.456000	-1.272000
H	1.201000	-4.301000	-1.798000
H	1.430000	-2.614000	-1.392000
H	-0.184000	-3.206000	-1.798000
O	-1.247000	1.124000	-0.496000
C	-0.117000	1.758000	-0.333000
C	0.610000	1.664000	0.898000
C	1.818000	2.342000	1.040000
H	2.356000	2.250000	1.976000
C	2.386000	3.120000	0.026000
C	1.683000	3.184000	-1.177000
H	2.104000	3.761000	-1.989000
C	0.469000	2.523000	-1.395000
C	-1.028000	1.867000	2.713000
H	-0.542000	2.823000	2.927000
H	-1.432000	1.484000	3.655000
H	-1.855000	2.060000	2.027000
C	3.719000	3.841000	0.262000
C	3.572000	4.815000	1.447000
H	3.291000	4.293000	2.366000
H	2.804000	5.566000	1.237000
H	4.518000	5.336000	1.634000
C	4.815000	2.810000	0.587000
H	5.782000	3.305000	0.730000
H	4.917000	2.086000	-0.230000
H	4.588000	2.261000	1.506000
C	4.167000	4.645000	-0.965000
H	5.118000	5.144000	-0.751000
H	3.438000	5.417000	-1.232000
H	4.319000	4.000000	-1.836000
C	-0.218000	2.600000	-2.770000
C	-1.617000	3.225000	-2.620000
H	-1.536000	4.262000	-2.278000
H	-2.208000	2.664000	-1.894000
H	-2.142000	3.228000	-3.583000
C	0.565000	3.459000	-3.776000
H	0.024000	3.477000	-4.727000
H	1.562000	3.051000	-3.973000
H	0.674000	4.495000	-3.439000
C	-0.322000	1.187000	-3.374000
H	-0.797000	1.227000	-4.361000
H	-0.916000	0.541000	-2.728000
H	0.671000	0.738000	-3.492000
Na	-2.133000	-0.911000	-0.724000
C	5.046000	-1.334000	4.019000
C	4.726000	-0.367000	3.070000
C	4.581000	-0.721000	1.732000
C	4.757000	-2.043000	1.321000
C	5.074000	-3.007000	2.280000
C	5.221000	-2.657000	3.619000
C	4.613000	-2.430000	-0.133000
O	3.692000	-1.585000	-0.776000
H	5.152000	-1.061000	5.065000
H	4.578000	0.666000	3.373000
H	4.319000	0.030000	0.996000
H	5.194000	-4.044000	1.976000
H	5.462000	-3.420000	4.353000
H	4.279000	-3.478000	-0.192000
H	5.588000	-2.398000	-0.630000
H	1.922000	-1.767000	0.242000
C	-3.375000	4.699000	3.093000
C	-4.220000	3.633000	3.395000
C	-4.656000	2.782000	2.384000
C	-4.255000	2.986000	1.061000
C	-3.414000	4.060000	0.768000
C	-2.974000	4.913000	1.777000
C	-4.623000	1.991000	-0.014000
O	-3.740000	0.886000	-0.004000
H	-3.031000	5.361000	3.881000
H	-4.538000	3.464000	4.419000
H	-5.308000	1.946000	2.621000
H	-3.088000	4.220000	-0.256000
H	-2.315000	5.741000	1.536000
H	-4.618000	2.485000	-0.997000
H	-5.630000	1.595000	0.155000
H	-2.807000	1.224000	-0.037000
C	-4.802000	-1.377000	-2.548000
O	-3.683000	-1.753000	-2.227000
O	-5.021000	-0.201000	-3.115000
C	-3.858000	0.603000	-3.340000
H	-4.220000	1.510000	-3.820000
H	-3.382000	0.847000	-2.389000
H	-3.156000	0.084000	-3.995000
C	-6.052000	-2.170000	-2.375000
C	-5.925000	-3.435000	-1.971000
H	-6.794000	-4.070000	-1.832000
H	-4.948000	-3.860000	-1.769000
C	-7.366000	-1.506000	-2.677000
H	-8.192000	-2.197000	-2.495000
H	-7.510000	-0.619000	-2.054000
H	-7.410000	-1.177000	-3.719000
C	3.856000	-1.224000	-2.291000
O	2.668000	-1.001000	-2.720000
O	4.586000	-2.290000	-2.873000
C	3.810000	-3.431000	-3.175000
H	4.410000	-4.057000	-3.838000
H	3.568000	-4.003000	-2.268000
H	2.875000	-3.149000	-3.665000
C	4.824000	-0.015000	-2.308000
C	4.393000	1.129000	-2.845000
H	5.028000	2.010000	-2.882000
H	3.398000	1.194000	-3.276000
C	6.209000	-0.141000	-1.734000
H	6.805000	0.749000	-1.955000
H	6.179000	-0.259000	-0.645000
H	6.721000	-1.015000	-2.146000

Mg(PBTP)•MA•1a

O	-2.320000	-0.199000	-1.273000
O	0.083000	-0.752000	0.867000
C	1.289000	-0.227000	0.689000
C	2.249000	-0.304000	1.732000
C	1.642000	0.415000	-0.532000
C	3.548000	0.152000	1.484000
C	2.948000	0.857000	-0.702000
C	3.935000	0.723000	0.276000
H	4.282000	0.071000	2.274000
H	3.215000	1.335000	-1.638000
C	-1.955000	1.069000	-1.041000
C	-0.594000	1.454000	-1.060000
C	-2.940000	2.055000	-0.716000
C	-0.242000	2.717000	-0.568000
C	-2.517000	3.307000	-0.285000
C	-1.170000	3.660000	-0.155000
H	0.817000	2.946000	-0.506000
H	-3.265000	4.043000	-0.012000
C	0.591000	0.632000	-1.635000
C	-4.442000	1.731000	-0.803000
C	-4.785000	1.185000	-2.203000
C	-4.819000	0.708000	0.284000
C	-5.327000	2.970000	-0.582000
H	-4.162000	0.326000	-2.452000
H	-5.840000	0.887000	-2.247000
H	-4.622000	1.959000	-2.960000
H	-4.640000	1.129000	1.280000
H	-5.881000	0.441000	0.214000
H	-4.227000	-0.200000	0.185000
H	-6.376000	2.689000	-0.715000
H	-5.224000	3.377000	0.430000
H	-5.100000	3.766000	-1.299000
C	1.858000	-0.818000	3.134000
C	0.727000	0.066000	3.697000
C	1.391000	-2.286000	3.105000
C	3.031000	-0.747000	4.126000
H	1.067000	1.102000	3.797000
H	-0.140000	0.050000	3.035000
H	0.423000	-0.290000	4.689000
H	2.151000	-2.933000	2.651000
H	1.221000	-2.648000	4.125000
H	0.455000	-2.393000	2.557000
H	2.690000	-1.085000	5.110000
H	3.864000	-1.391000	3.826000
H	3.409000	0.274000	4.241000
C	-0.782000	5.031000	0.411000
C	-1.332000	5.166000	1.843000
C	0.740000	5.226000	0.464000
C	-1.378000	6.146000	-0.469000
H	-2.422000	5.076000	1.865000
H	-0.918000	4.385000	2.490000
H	-1.067000	6.141000	2.268000
H	1.190000	5.171000	-0.533000
H	0.971000	6.212000	0.881000
H	1.222000	4.474000	1.097000

H	-1.111000	7.132000	-0.074000
H	-0.999000	6.073000	-1.494000
H	-2.470000	6.087000	-0.511000
C	5.352000	1.246000	0.005000
C	6.295000	1.017000	1.193000
C	5.949000	0.530000	-1.222000
C	5.292000	2.760000	-0.275000
H	5.954000	1.547000	2.088000
H	6.386000	-0.046000	1.438000
H	7.295000	1.389000	0.948000
H	5.315000	0.644000	-2.106000
H	6.938000	0.938000	-1.462000
H	6.066000	-0.542000	-1.027000
H	6.296000	3.158000	-0.460000
H	4.677000	2.984000	-1.152000
H	4.863000	3.293000	0.580000
C	1.137000	1.484000	-2.810000
C	0.266000	-0.721000	-2.301000
H	1.481000	2.473000	-2.499000
H	1.963000	0.979000	-3.322000
H	0.333000	1.629000	-3.537000
H	-0.577000	-0.643000	-2.988000
H	1.152000	-1.050000	-2.854000
H	0.075000	-1.530000	-1.598000
C	3.560000	-2.827000	-2.829000
C	2.546000	-3.555000	-3.446000
C	1.481000	-4.046000	-2.694000
C	1.432000	-3.832000	-1.317000
C	2.468000	-3.123000	-0.703000
C	3.517000	-2.609000	-1.454000
C	0.258000	-4.302000	-0.493000
O	-0.398000	-3.216000	0.177000
H	4.378000	-2.426000	-3.418000
H	2.573000	-3.728000	-4.517000
H	0.678000	-4.591000	-3.183000
H	2.452000	-2.939000	0.368000
H	4.287000	-2.026000	-0.962000
H	0.579000	-5.023000	0.268000
H	-0.496000	-4.780000	-1.119000
H	0.266000	-2.646000	0.612000
C	-4.029000	-2.985000	0.946000
O	-3.050000	-2.239000	1.023000
O	-4.481000	-3.632000	1.996000
C	-3.776000	-3.441000	3.236000
H	-4.292000	-4.067000	3.959000
H	-2.736000	-3.753000	3.126000
H	-3.818000	-2.392000	3.532000
C	-4.814000	-3.249000	-0.270000
C	-4.649000	-2.533000	-1.383000
H	-5.259000	-2.740000	-2.256000
H	-3.935000	-1.714000	-1.455000
Mg	-1.519000	-1.372000	0.019000
H	-5.557000	-4.035000	-0.190000

Mg(PBTP)•MA•1a-TS5

O	-1.370000	-2.540000	-0.727000
O	0.731000	-0.568000	1.022000
C	0.704000	0.747000	0.740000
C	1.148000	1.675000	1.712000
C	0.259000	1.207000	-0.527000
C	1.230000	3.025000	1.352000
C	0.369000	2.564000	-0.811000
C	0.865000	3.498000	0.098000
H	1.582000	3.733000	2.090000
H	0.043000	2.916000	-1.782000
C	-2.225000	-1.508000	-0.688000
C	-1.785000	-0.182000	-0.910000
C	-3.598000	-1.734000	-0.348000
C	-2.658000	0.873000	-0.603000
C	-4.413000	-0.638000	-0.101000
C	-3.961000	0.686000	-0.178000
H	-2.270000	1.881000	-0.697000
H	-5.445000	-0.810000	0.184000
C	-0.424000	0.256000	-1.530000
C	-4.154000	-3.167000	-0.253000
C	-3.907000	-3.908000	-1.582000
C	-3.489000	-3.942000	0.902000
C	-5.670000	-3.184000	0.006000
H	-2.841000	-3.935000	-1.814000
H	-4.281000	-4.936000	-1.518000
H	-4.433000	-3.406000	-2.401000
H	-3.603000	-3.399000	1.847000
H	-3.960000	-4.924000	1.021000
H	-2.428000	-4.096000	0.702000
H	-6.022000	-4.221000	0.009000
H	-5.928000	-2.747000	0.977000
H	-6.223000	-2.648000	-0.772000
C	1.480000	1.240000	3.155000
C	0.253000	0.549000	3.782000
C	2.692000	0.291000	3.193000
C	1.827000	2.438000	4.056000
H	-0.601000	1.234000	3.803000
H	-0.032000	-0.338000	3.214000
H	0.473000	0.248000	4.812000
H	3.567000	0.769000	2.740000
H	2.946000	0.045000	4.231000
H	2.488000	-0.639000	2.664000
H	2.016000	2.077000	5.072000
H	2.729000	2.960000	3.720000
H	1.008000	3.162000	4.110000
C	-4.895000	1.845000	0.191000
C	-5.346000	1.690000	1.656000
C	-4.207000	3.210000	0.046000
C	-6.132000	1.829000	-0.727000
H	-5.879000	0.748000	1.816000
H	-4.482000	1.707000	2.329000
H	-6.018000	2.508000	1.940000
H	-3.893000	3.398000	-0.986000
H	-4.903000	4.005000	0.332000
H	-3.325000	3.289000	0.690000
H	-6.810000	2.651000	-0.471000
H	-5.837000	1.941000	-1.775000
H	-6.691000	0.893000	-0.633000
C	0.922000	4.981000	-0.291000
C	1.491000	5.857000	0.833000
C	1.814000	5.161000	-1.533000
C	-0.503000	5.476000	-0.612000
H	0.870000	5.814000	1.734000
H	2.509000	5.558000	1.102000
H	1.526000	6.901000	0.505000
H	1.445000	4.579000	-2.384000
H	1.842000	6.213000	-1.838000
H	2.840000	4.842000	-1.321000
H	-0.489000	6.537000	-0.885000
H	-0.945000	4.921000	-1.444000
H	-1.157000	5.354000	0.257000
C	-0.792000	0.972000	-2.855000
C	0.545000	-0.853000	-1.994000
H	-1.504000	1.790000	-2.725000
H	0.103000	1.364000	-3.349000
H	-1.255000	0.241000	-3.524000
H	0.020000	-1.611000	-2.577000
H	1.315000	-0.392000	-2.620000
H	1.084000	-1.351000	-1.194000
C	2.476000	-3.564000	0.554000
O	1.314000	-3.481000	1.052000
O	3.483000	-4.060000	1.286000
C	3.370000	-3.904000	2.701000
H	4.280000	-4.331000	3.117000
H	3.302000	-2.843000	2.955000
H	2.495000	-4.433000	3.080000
C	2.693000	-3.878000	-0.889000
C	1.690000	-4.061000	-1.739000
H	1.884000	-4.298000	-2.780000
H	0.650000	-3.966000	-1.440000
Mg	-0.163000	-2.233000	0.717000
H	3.729000	-3.980000	-1.194000
C	3.648000	0.999000	-3.499000
C	4.095000	-0.321000	-3.537000
C	4.280000	-1.025000	-2.352000
C	4.021000	-0.422000	-1.119000
C	3.580000	0.901000	-1.090000
C	3.391000	1.608000	-2.274000
C	4.173000	-1.196000	0.165000
O	2.954000	-1.810000	0.590000
H	3.501000	1.550000	-4.422000
H	4.301000	-0.800000	-4.489000
H	4.632000	-2.052000	-2.385000
H	3.360000	1.381000	-0.139000
H	3.031000	2.629000	-2.235000
H	4.520000	-0.545000	0.974000
H	4.891000	-2.014000	0.058000
H	2.172000	-1.184000	0.714000

Mg(PBTP)•MA•1a-Int6

Mg	-1.094000	-1.577000	1.482000
O	-1.699000	0.136000	0.639000
O	0.749000	-1.538000	1.222000
C	1.884000	-1.417000	0.555000
C	3.073000	-2.013000	1.055000
C	1.944000	-0.678000	-0.662000
C	4.269000	-1.815000	0.362000
C	3.171000	-0.526000	-1.300000
C	4.358000	-1.070000	-0.810000
H	5.171000	-2.260000	0.760000
H	3.210000	0.051000	-2.217000
C	-0.911000	1.259000	0.443000
C	0.259000	1.144000	-0.308000
C	-1.251000	2.424000	1.163000
C	1.161000	2.215000	-0.229000
C	-0.334000	3.469000	1.135000
C	0.898000	3.376000	0.477000
H	2.114000	2.102000	-0.731000
H	-0.560000	4.380000	1.673000
C	0.679000	-0.021000	-1.244000
C	-2.559000	2.538000	1.975000
C	-3.792000	2.316000	1.076000
C	-2.578000	1.515000	3.130000
C	-2.709000	3.935000	2.604000
H	-3.850000	1.296000	0.694000
H	-4.707000	2.493000	1.651000
H	-3.786000	3.014000	0.232000
H	-1.663000	1.585000	3.728000
H	-3.430000	1.714000	3.789000
H	-2.687000	0.496000	2.757000
H	-3.659000	3.983000	3.143000
H	-1.912000	4.148000	3.323000
H	-2.716000	4.725000	1.847000
C	3.046000	-2.862000	2.340000
C	2.579000	-2.007000	3.534000
C	2.108000	-4.069000	2.145000
C	4.430000	-3.424000	2.705000
H	3.276000	-1.180000	3.704000
H	1.590000	-1.587000	3.349000
H	2.545000	-2.614000	4.446000
H	2.489000	-4.722000	1.353000
H	2.045000	-4.658000	3.068000
H	1.105000	-3.745000	1.866000
H	4.344000	-4.023000	3.618000
H	4.831000	-4.074000	1.920000
H	5.158000	-2.629000	2.901000
C	1.895000	4.539000	0.561000
C	2.257000	4.793000	2.037000
C	3.192000	4.248000	-0.207000
C	1.253000	5.805000	-0.036000
H	1.378000	5.057000	2.631000
H	2.712000	3.903000	2.482000
H	2.973000	5.619000	2.115000
H	3.004000	4.090000	-1.275000
H	3.872000	5.101000	-0.113000
H	3.708000	3.366000	0.185000
H	1.954000	6.646000	0.015000
H	0.986000	5.646000	-1.085000
H	0.347000	6.094000	0.504000
C	5.675000	-0.817000	-1.554000
C	6.870000	-1.492000	-0.866000
C	5.577000	-1.366000	-2.990000
C	5.947000	0.699000	-1.607000
H	7.014000	-1.118000	0.153000

H	6.749000	-2.579000	-0.819000
H	7.786000	-1.283000	-1.430000
H	4.767000	-0.889000	-3.550000
H	6.511000	-1.187000	-3.535000
H	5.388000	-2.444000	-2.979000
H	6.886000	0.904000	-2.135000
H	5.147000	1.234000	-2.127000
H	6.025000	1.113000	-0.596000
C	0.926000	0.630000	-2.630000
C	-0.379000	-1.101000	-1.562000
H	1.649000	1.448000	-2.616000
H	1.275000	-0.118000	-3.348000
H	-0.021000	1.033000	-2.998000
H	-1.344000	-0.667000	-1.826000
H	-0.028000	-1.668000	-2.429000
H	-0.519000	-1.837000	-0.772000
C	-2.382000	0.678000	-4.630000
C	-2.756000	1.518000	-3.584000
C	-3.521000	1.021000	-2.533000
C	-3.915000	-0.319000	-2.513000
C	-3.541000	-1.151000	-3.569000
C	-2.779000	-0.657000	-4.623000
C	-4.631000	-0.877000	-1.312000
O	-3.634000	-1.165000	-0.333000
H	-1.782000	1.063000	-5.448000
H	-2.450000	2.560000	-3.585000
H	-3.811000	1.677000	-1.717000
H	-3.843000	-2.195000	-3.559000
H	-2.492000	-1.313000	-5.438000
H	-5.163000	-1.799000	-1.566000
H	-5.350000	-0.152000	-0.911000
C	-3.911000	-2.220000	0.676000
O	-2.816000	-2.370000	1.400000
O	-4.288000	-3.371000	-0.042000
C	-3.235000	-3.963000	-0.782000
H	-3.681000	-4.776000	-1.356000
H	-2.778000	-3.241000	-1.471000
H	-2.459000	-4.365000	-0.124000
C	-5.147000	-1.799000	1.449000
C	-5.112000	-1.404000	2.715000
H	-6.082000	-1.820000	0.895000
H	-6.009000	-1.085000	3.236000
H	-4.177000	-1.398000	3.266000
H	-2.473000	-0.060000	0.055000

Na(BHT)•2(MMA)•1a

C	-3.050000	-2.197000	1.282000
O	-1.989000	-2.547000	1.779000
O	0.319000	-0.723000	-0.592000
O	-1.824000	0.196000	0.561000
C	1.563000	-0.563000	-0.986000
C	2.448000	-1.692000	-1.089000
C	2.087000	0.724000	-1.349000
C	3.803000	-1.474000	-1.345000
C	3.450000	0.858000	-1.607000
C	4.340000	-0.211000	-1.573000
H	4.483000	-2.318000	-1.380000
H	3.854000	1.838000	-1.843000
H	-1.107000	0.167000	-0.119000
C	-2.570000	1.389000	0.537000
H	-3.370000	1.254000	1.276000
O	-3.356000	-2.402000	0.008000
C	-2.296000	-2.885000	-0.829000
H	-1.916000	-3.838000	-0.456000
H	-2.738000	-3.012000	-1.816000
H	-1.489000	-2.146000	-0.857000
C	-4.152000	-1.511000	2.021000
C	-3.979000	-1.308000	3.328000
H	-4.734000	-0.806000	3.924000
H	-3.078000	-1.647000	3.828000
H	-1.967000	2.244000	0.872000
C	-3.164000	1.707000	-0.816000
C	-3.540000	0.685000	-1.688000
C	-3.343000	3.034000	-1.206000
C	-4.083000	0.987000	-2.933000
H	-3.397000	-0.347000	-1.385000
C	-3.893000	3.338000	-2.448000
H	-3.039000	3.836000	-0.538000
C	-4.261000	2.314000	-3.317000
H	-4.365000	0.184000	-3.607000
H	-4.025000	4.375000	-2.741000
H	-4.682000	2.548000	-4.290000
C	5.821000	-0.010000	-1.770000
H	6.342000	0.155000	-0.817000
H	6.286000	-0.882000	-2.240000
H	6.028000	0.860000	-2.402000
C	1.910000	-3.136000	-1.027000
C	1.220000	-3.463000	0.311000
C	0.908000	-3.331000	-2.183000
C	3.021000	-4.185000	-1.212000
H	1.829000	-3.127000	1.158000
H	0.232000	-3.011000	0.365000
H	1.080000	-4.546000	0.415000
H	1.425000	-3.282000	-3.147000
H	0.416000	-4.309000	-2.111000
H	0.147000	-2.550000	-2.164000
H	2.572000	-5.184000	-1.214000
H	3.550000	-4.061000	-2.161000
H	3.756000	-4.154000	-0.400000
C	1.167000	1.952000	-1.465000
C	-0.009000	1.639000	-2.412000
C	0.678000	2.376000	-0.069000
C	1.881000	3.179000	-2.061000
H	-0.535000	0.730000	-2.120000
H	-0.727000	2.466000	-2.429000
H	0.369000	1.494000	-3.430000
H	1.518000	2.760000	0.519000
H	-0.072000	3.172000	-0.143000
H	0.245000	1.536000	0.475000
H	1.156000	3.992000	-2.171000
H	2.687000	3.545000	-1.417000
H	2.299000	2.968000	-3.050000
Na	-0.135000	-1.090000	1.631000
C	1.957000	1.215000	2.807000
O	1.414000	0.124000	2.717000
O	1.326000	2.285000	3.285000
C	-0.050000	2.106000	3.632000
H	-0.627000	1.816000	2.750000
H	-0.155000	1.342000	4.405000
H	-0.388000	3.071000	4.003000
C	3.356000	1.507000	2.406000
C	3.969000	0.607000	1.634000
H	4.981000	0.772000	1.280000
H	3.467000	-0.296000	1.301000
C	-5.367000	-1.078000	1.251000
C	3.965000	2.816000	2.829000
H	-5.094000	-0.388000	0.447000
H	-5.861000	-1.933000	0.782000
H	-6.080000	-0.580000	1.911000
H	3.430000	3.658000	2.379000
H	3.917000	2.947000	3.914000
H	5.010000	2.866000	2.517000

Na(BHT)•2(MMA)•1a-TS6

C	-2.474000	-2.401000	-0.592000
O	-1.348000	-2.570000	-1.101000
O	-0.252000	0.208000	-0.168000
O	-2.174000	-1.113000	0.604000
C	0.695000	1.063000	0.188000
C	0.934000	2.213000	-0.634000
C	1.512000	0.861000	1.341000
C	1.943000	3.104000	-0.275000
C	2.504000	1.801000	1.633000
C	2.741000	2.924000	0.852000
H	2.131000	3.980000	-0.887000
H	3.135000	1.661000	2.503000
H	-1.367000	-0.472000	0.382000
C	-3.207000	-0.584000	1.423000
H	-4.063000	-1.255000	1.310000
O	-3.476000	-1.813000	-1.324000
C	-3.026000	-0.890000	-2.304000
H	-2.390000	-1.382000	-3.045000
H	-3.920000	-0.495000	-2.786000
H	-2.472000	-0.074000	-1.829000
C	-3.071000	-3.465000	0.318000
C	-2.297000	-4.012000	1.253000
H	-2.663000	-4.803000	1.901000
H	-1.277000	-3.671000	1.398000
H	-2.891000	-0.631000	2.471000
C	-3.608000	0.825000	1.060000
C	-4.494000	1.052000	0.003000
C	-3.109000	1.917000	1.769000
C	-4.862000	2.346000	-0.347000
H	-4.889000	0.200000	-0.542000
C	-3.479000	3.215000	1.424000
H	-2.424000	1.754000	2.597000
C	-4.354000	3.432000	0.364000
H	-5.552000	2.509000	-1.170000
H	-3.079000	4.056000	1.981000
H	-4.641000	4.443000	0.094000
C	3.841000	3.902000	1.185000
H	4.654000	3.863000	0.449000
H	3.475000	4.934000	1.200000
H	4.277000	3.690000	2.166000
C	0.065000	2.493000	-1.877000
C	0.121000	1.318000	-2.877000
C	-1.394000	2.726000	-1.446000
C	0.527000	3.745000	-2.640000
H	1.156000	1.000000	-3.049000
H	-0.460000	0.479000	-2.501000
H	-0.307000	1.616000	-3.841000
H	-1.477000	3.632000	-0.838000
H	-2.041000	2.850000	-2.323000
H	-1.764000	1.887000	-0.855000
H	-0.132000	3.905000	-3.500000
H	0.479000	4.646000	-2.021000
H	1.550000	3.641000	-3.020000
C	1.281000	-0.316000	2.312000
C	-0.021000	-0.058000	3.089000
C	1.181000	-1.677000	1.597000
C	2.419000	-0.457000	3.340000
H	-0.846000	0.101000	2.396000
H	-0.272000	-0.908000	3.734000
H	0.075000	0.835000	3.714000
H	2.040000	-1.828000	0.935000
H	1.193000	-2.486000	2.336000
H	0.260000	-1.770000	1.024000
H	2.220000	-1.323000	3.981000
H	3.387000	-0.616000	2.851000
H	2.501000	0.414000	3.996000
Na	0.536000	-1.472000	-1.443000
C	3.837000	-1.727000	-0.996000
O	2.822000	-1.557000	-1.658000
O	4.196000	-2.925000	-0.545000
C	3.324000	-4.015000	-0.864000
H	2.345000	-3.865000	-0.401000
H	3.207000	-4.106000	-1.945000
H	3.801000	-4.902000	-0.454000
C	4.787000	-0.657000	-0.599000
C	4.390000	0.604000	-0.781000
H	5.025000	1.437000	-0.496000
H	3.413000	0.841000	-1.189000
C	-4.494000	-3.892000	0.076000
C	6.098000	-1.052000	0.023000
H	-5.189000	-3.056000	0.197000
H	-4.623000	-4.259000	-0.947000
H	-4.779000	-4.687000	0.770000
H	5.939000	-1.588000	0.964000
H	6.667000	-1.716000	-0.634000
H	6.701000	-0.165000	0.229000

Na(BHT)•2(MMA)•1a-Int7

C	-2.310000	-2.210000	-0.273000
O	-1.213000	-2.375000	-0.946000
O	-0.172000	0.608000	-0.278000

O	-2.224000	-0.903000	0.442000	C	-3.995000	3.768000	0.373000	H	0.665000	-2.469000	2.210000
C	0.941000	1.228000	0.220000	H	-4.922000	3.135000	-1.465000	H	0.285000	-1.678000	0.700000
C	1.364000	2.354000	-0.525000	H	-3.033000	4.086000	2.271000	H	1.756000	-1.452000	4.035000
C	1.651000	0.776000	1.353000	H	-4.153000	4.825000	0.184000	H	3.130000	-0.945000	3.049000
C	2.564000	2.960000	-0.157000	C	4.639000	3.171000	1.260000	H	2.278000	0.233000	4.075000
C	2.835000	1.454000	1.666000	H	5.444000	2.793000	0.619000	Na	0.055000	-0.970000	-2.001000
C	3.322000	2.519000	0.922000	H	4.595000	4.255000	1.117000	C	3.020000	-2.038000	-1.249000
H	2.929000	3.815000	-0.714000	H	4.926000	2.978000	2.297000	O	2.274000	-1.420000	-1.997000
H	3.417000	1.133000	2.521000	C	0.494000	2.966000	-1.644000	O	2.823000	-3.307000	-0.920000
H	-0.734000	0.065000	0.312000	C	0.187000	1.963000	-2.779000	C	1.629000	-3.933000	-1.417000
C	-3.379000	-0.436000	1.125000	C	-0.833000	3.458000	-1.034000	H	0.736000	-3.467000	-0.987000
H	-4.249000	-1.003000	0.785000	C	1.181000	4.178000	-2.298000	H	1.596000	-3.864000	-2.507000
O	-3.503000	-2.124000	-1.075000	H	1.072000	1.370000	-3.038000	H	1.702000	-4.974000	-1.110000
C	-3.321000	-1.421000	-2.279000	H	-0.638000	1.307000	-2.501000	C	4.229000	-1.462000	-0.601000
H	-2.672000	-1.965000	-2.976000	H	-0.124000	2.500000	-3.681000	C	4.431000	-0.151000	-0.743000
H	-4.310000	-1.305000	-2.732000	H	-0.648000	4.230000	-0.281000	H	5.280000	0.337000	-0.276000
H	-2.897000	-0.422000	-2.108000	H	-1.470000	3.891000	-1.814000	H	3.741000	0.467000	-1.307000
C	-2.577000	-3.341000	0.730000	H	-1.382000	2.641000	-0.564000	C	-3.097000	-4.617000	0.128000
C	-2.261000	-3.239000	2.020000	H	0.515000	4.596000	-3.058000	C	5.107000	-2.369000	0.217000
H	-2.371000	-4.082000	2.697000	H	1.389000	4.971000	-1.574000	H	-4.100000	-4.473000	-0.283000
H	-1.861000	-2.319000	2.433000	H	2.119000	3.903000	-2.792000	H	-2.455000	-4.928000	-0.702000
H	-3.264000	-0.604000	2.204000	C	1.161000	-0.362000	2.272000	H	-3.127000	-5.423000	0.867000
C	-3.589000	1.036000	0.863000	C	-0.172000	0.053000	2.927000	H	4.552000	-2.791000	1.060000
C	-4.223000	1.465000	-0.308000	C	1.008000	-1.694000	1.516000	H	5.475000	-3.210000	-0.378000
C	-3.168000	1.996000	1.784000	C	2.148000	-0.635000	3.422000	H	5.963000	-1.816000	0.608000
C	-4.424000	2.819000	-0.553000	H	-0.972000	0.190000	2.201000				
H	-4.577000	0.725000	-1.019000	H	-0.502000	-0.719000	3.631000				
C	-3.367000	3.353000	1.543000	H	-0.050000	0.991000	3.478000				
H	-2.687000	1.677000	2.705000	H	1.978000	-2.014000	1.125000				

9. References

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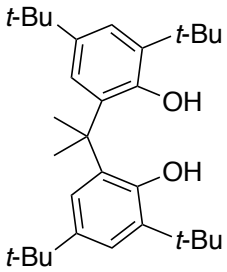
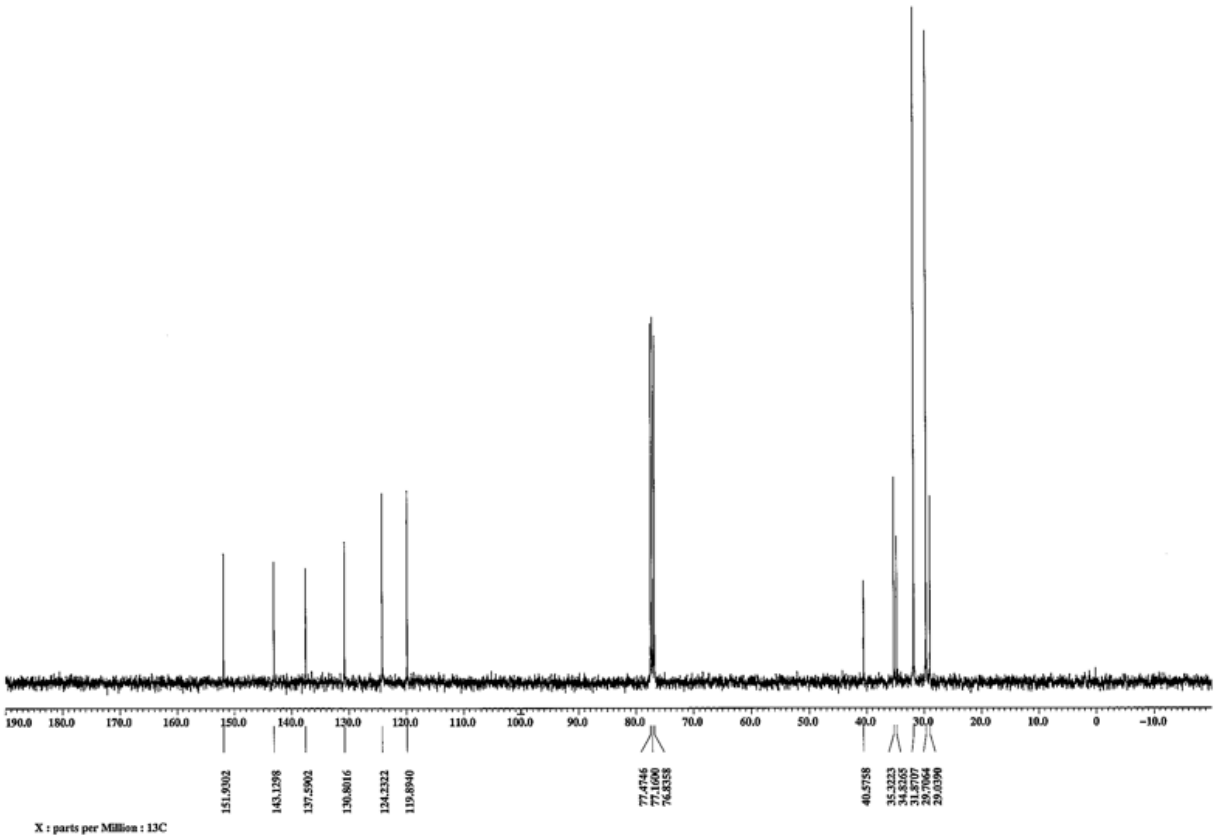
^{1}H and ^{13}C NMR spectra of PBTP-H$_2$





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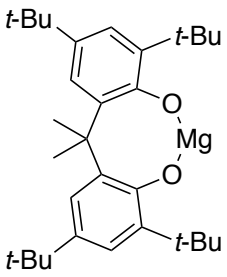
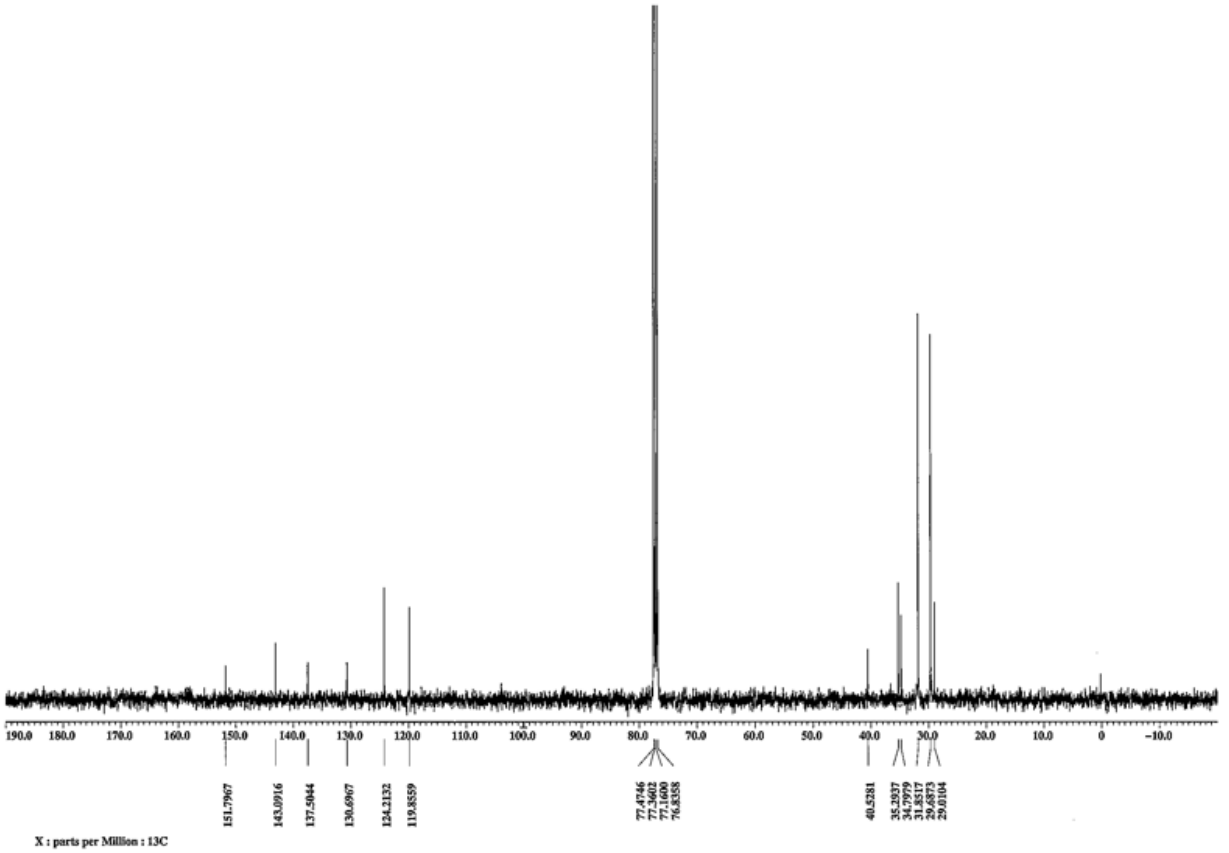
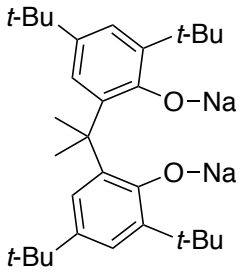
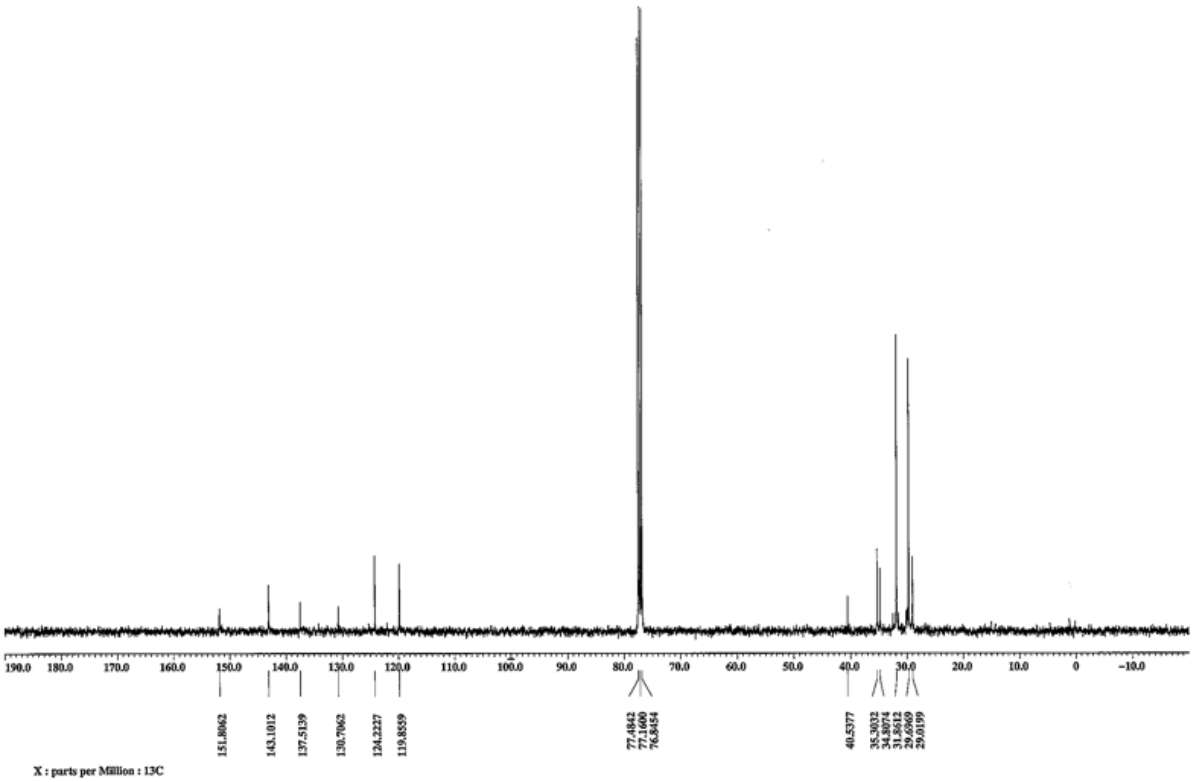


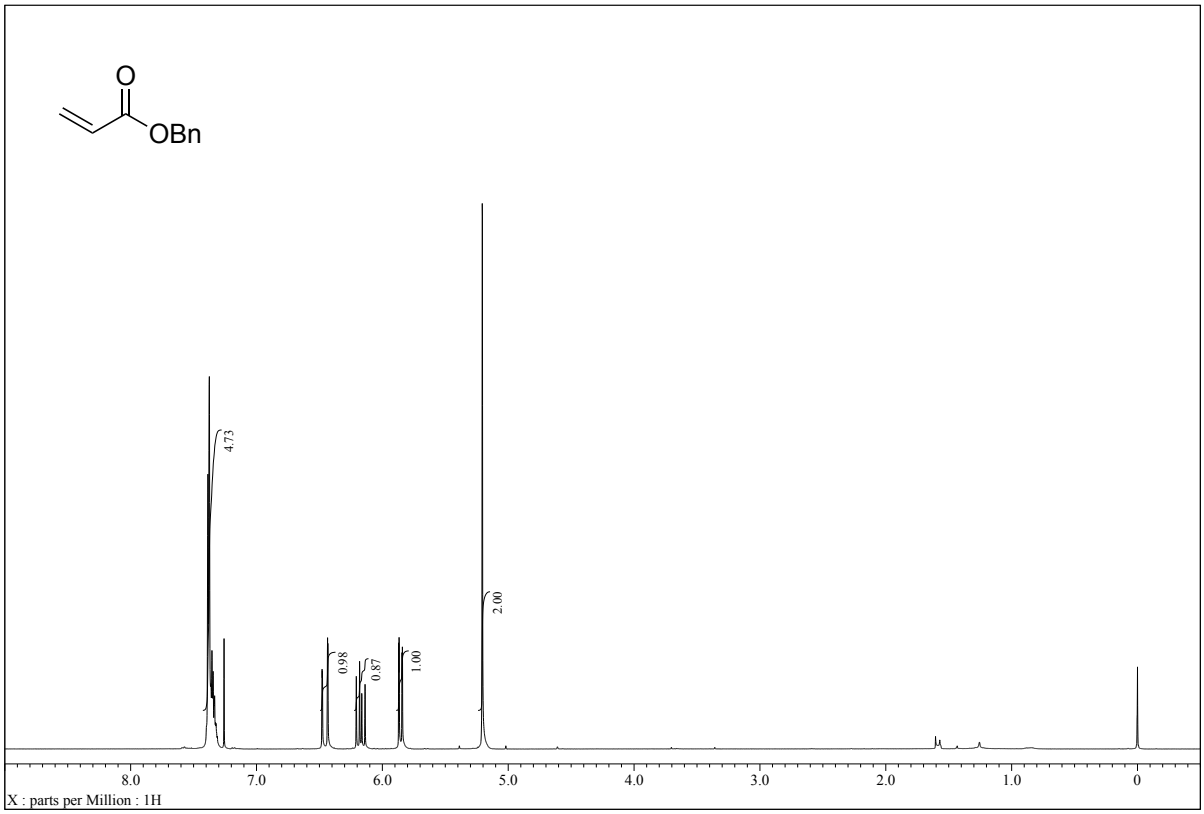


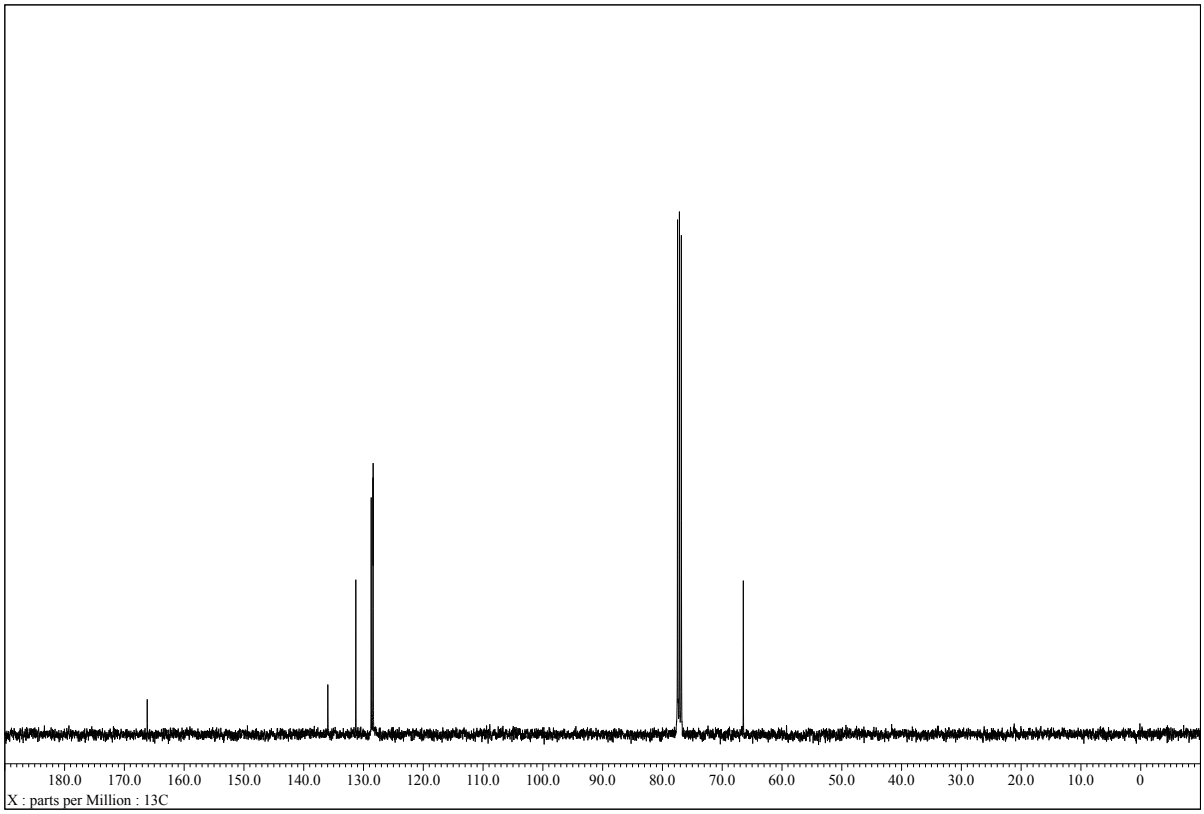
^{1}H and ^{13}C NMR spectra of Na_2(PBTP)



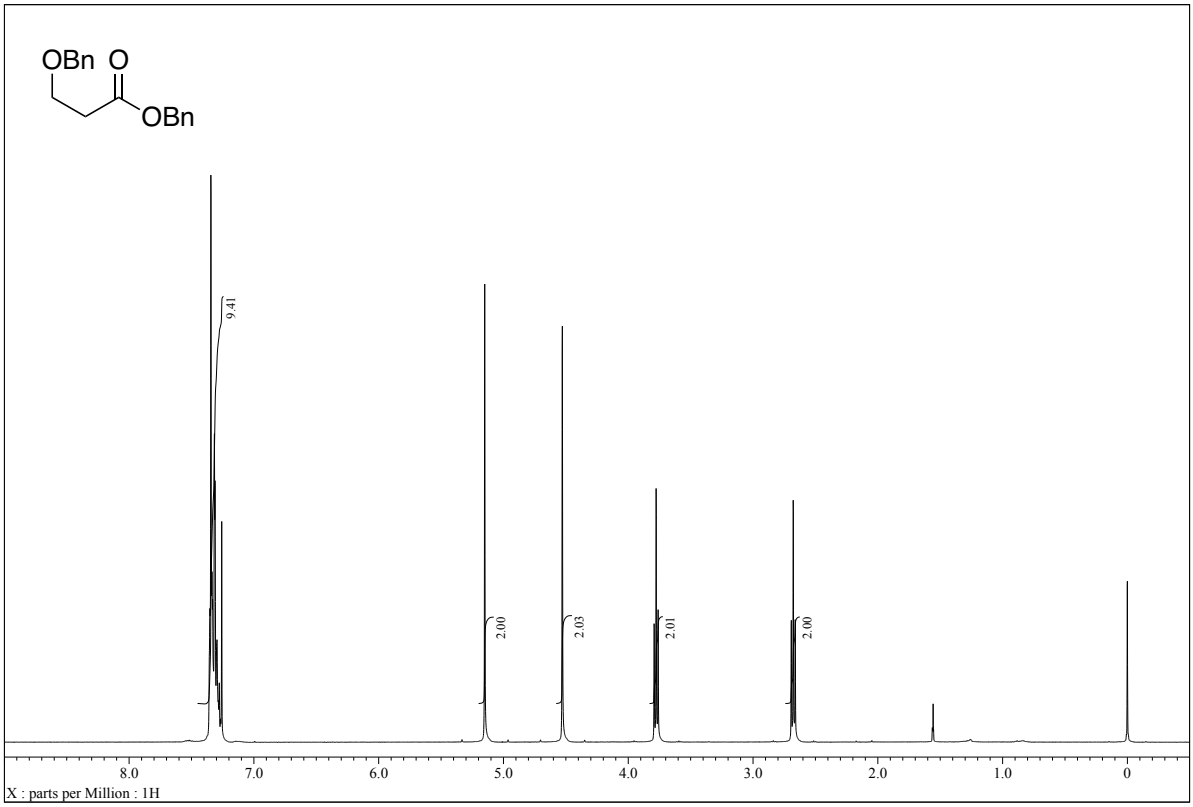


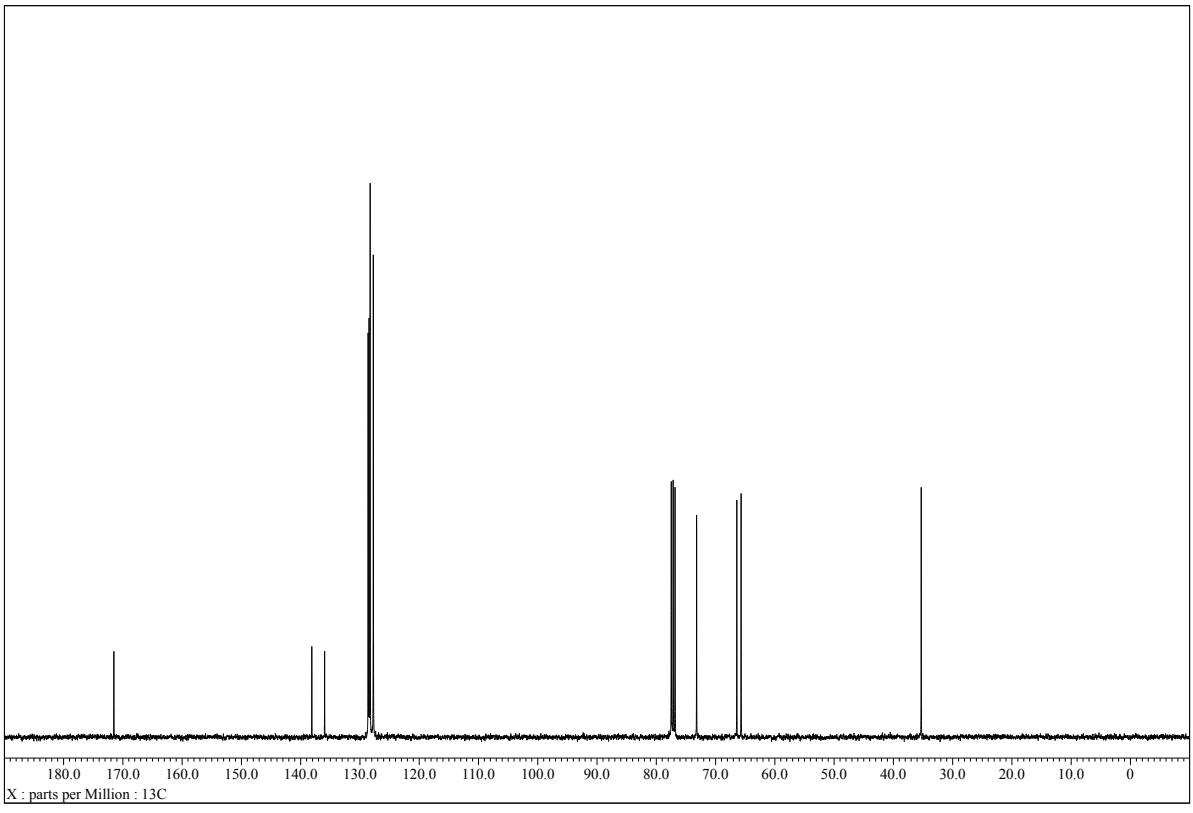
^{1}H and ^{13}C NMR spectra of benzyl acrylate (2a)



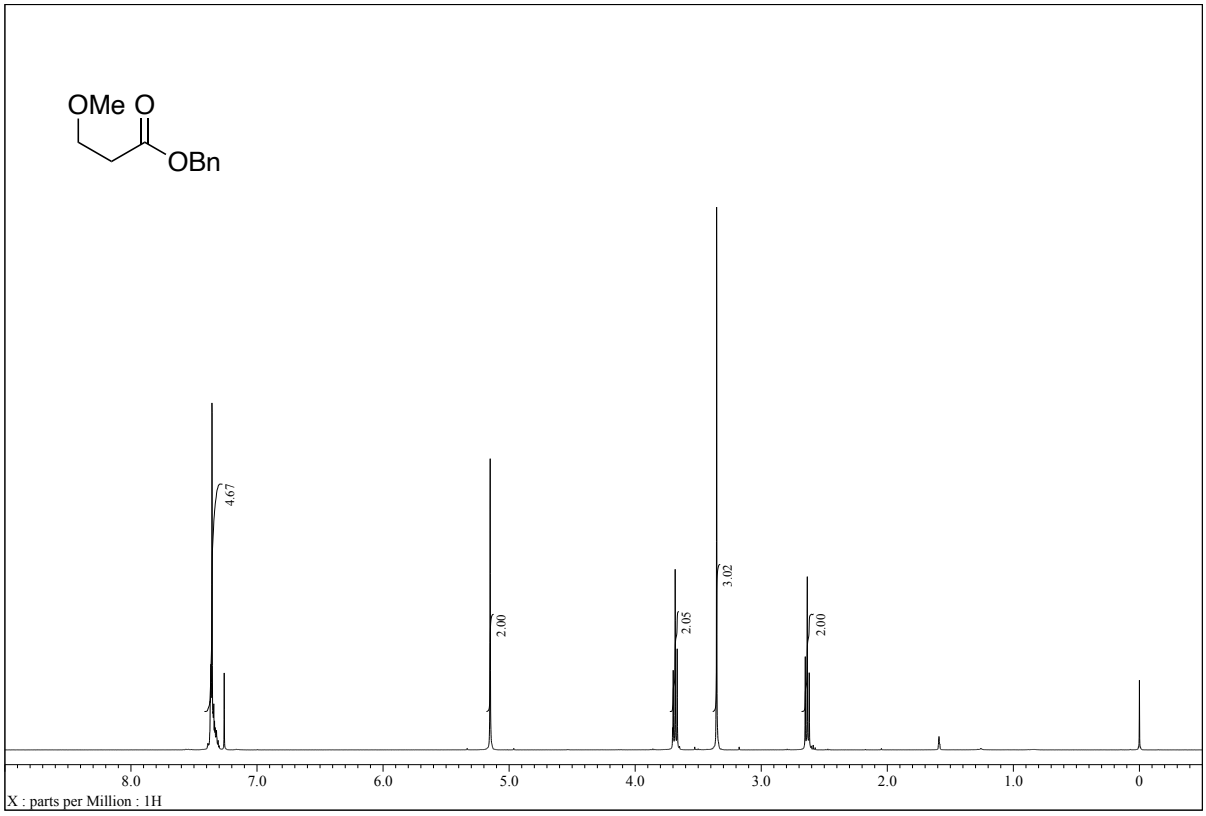


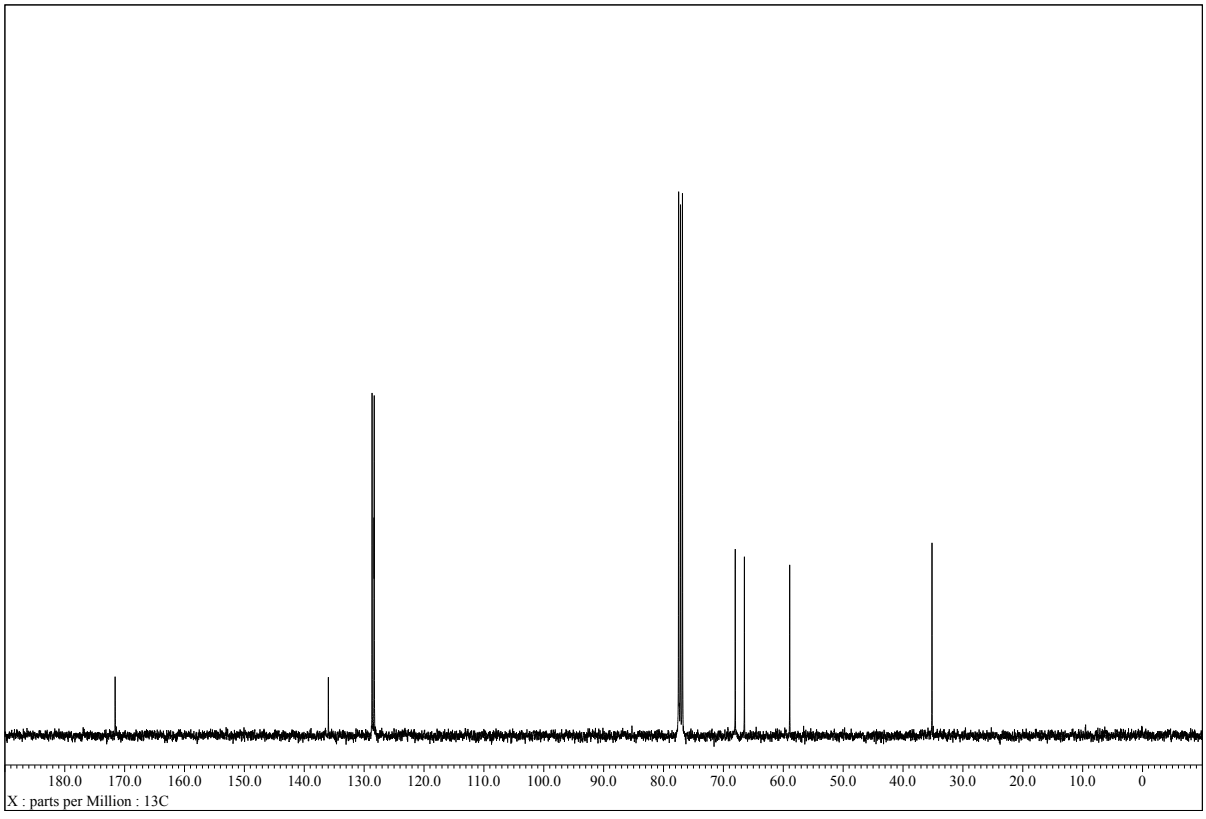
^{1}H and ^{13}C NMR spectra of benzyl 3-(benzyloxy)propanoate (3a)



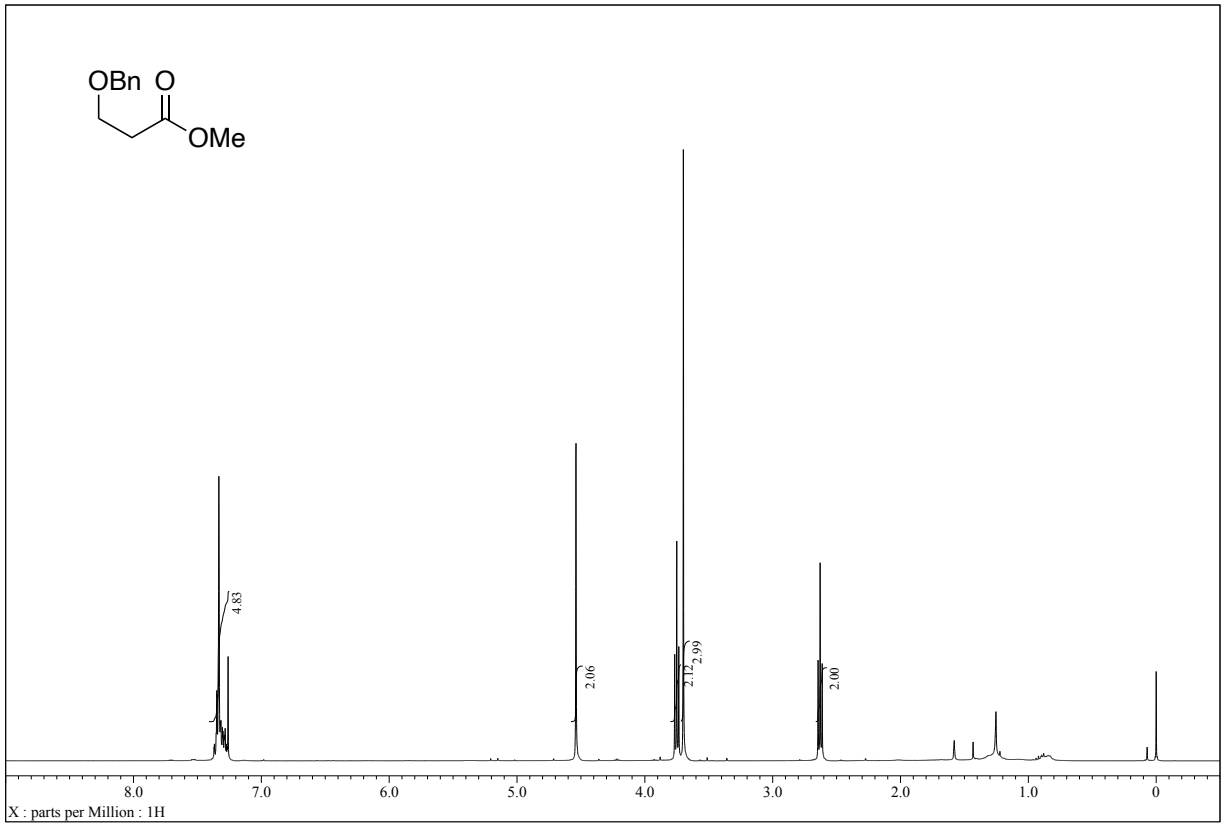


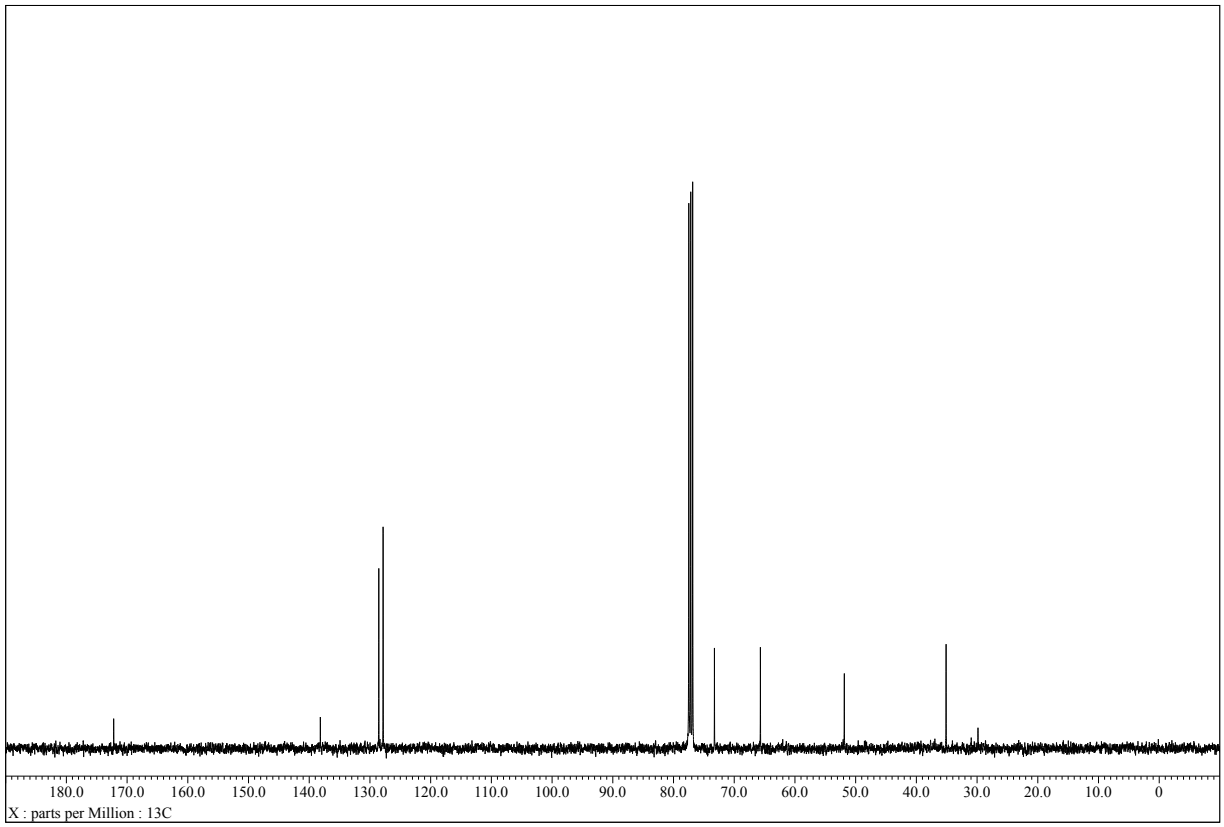
^{1}H and ^{13}C NMR spectra of Benzyl 3-methoxypropanoate (4a):



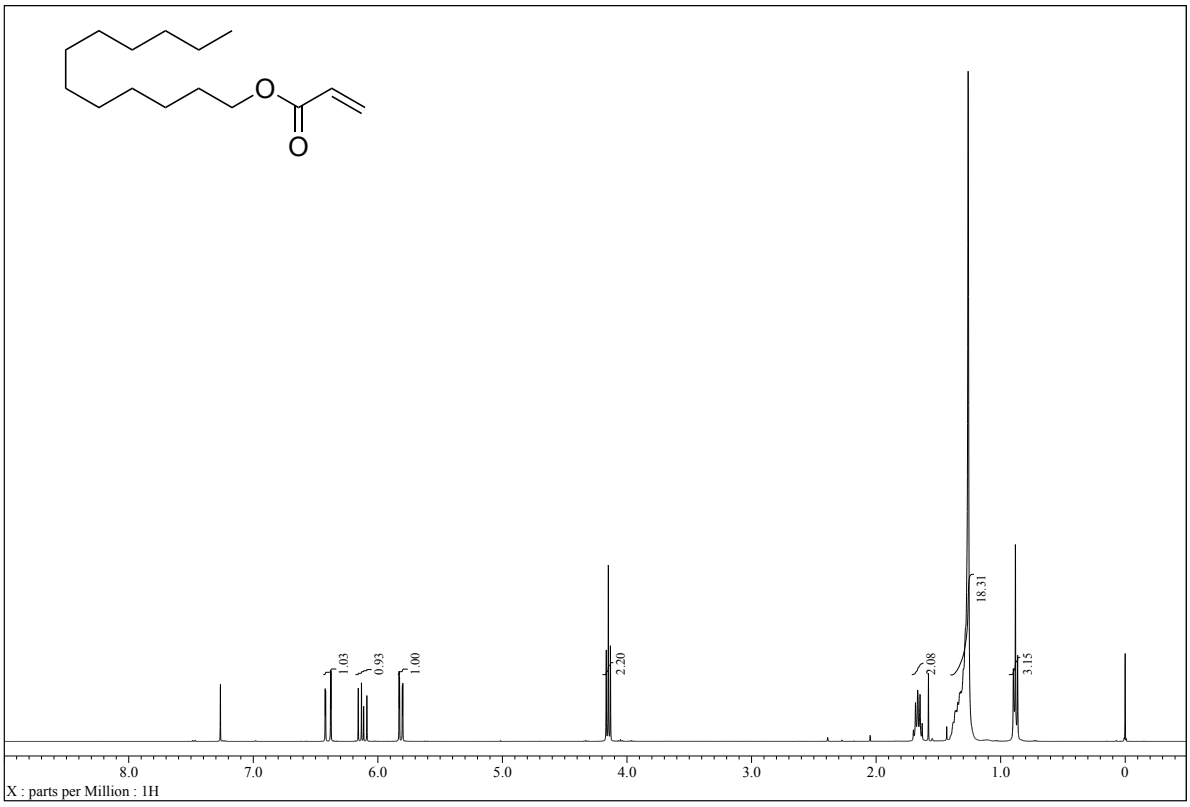


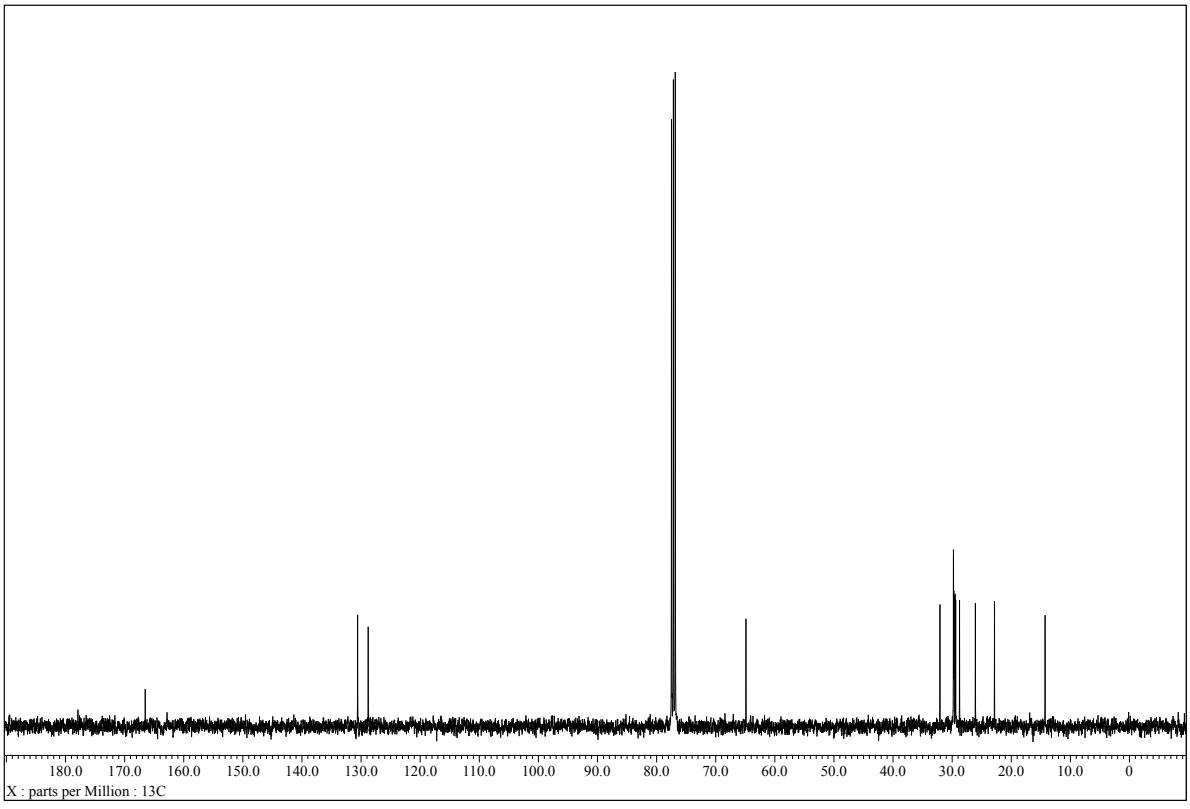
^{1}H and ^{13}C NMR spectra of Methyl 3-(benzyloxy)propanoate (5a)



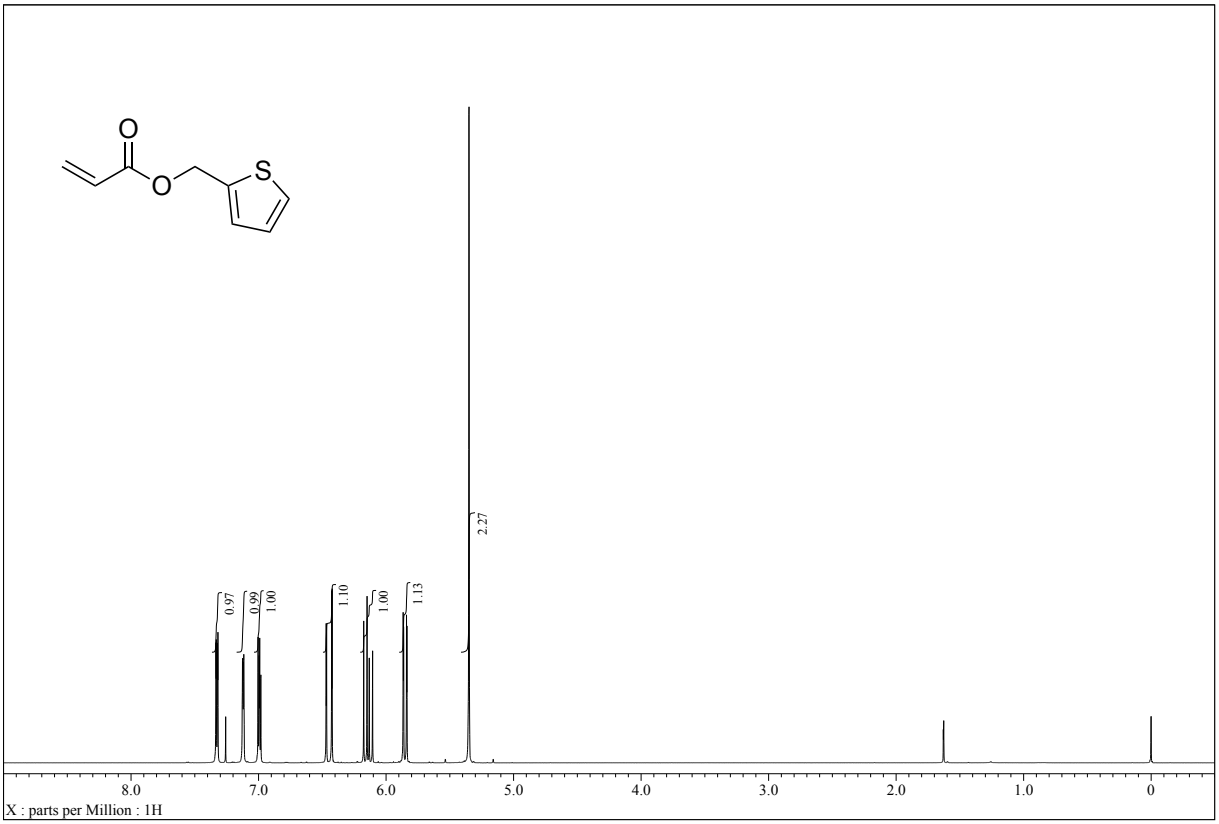


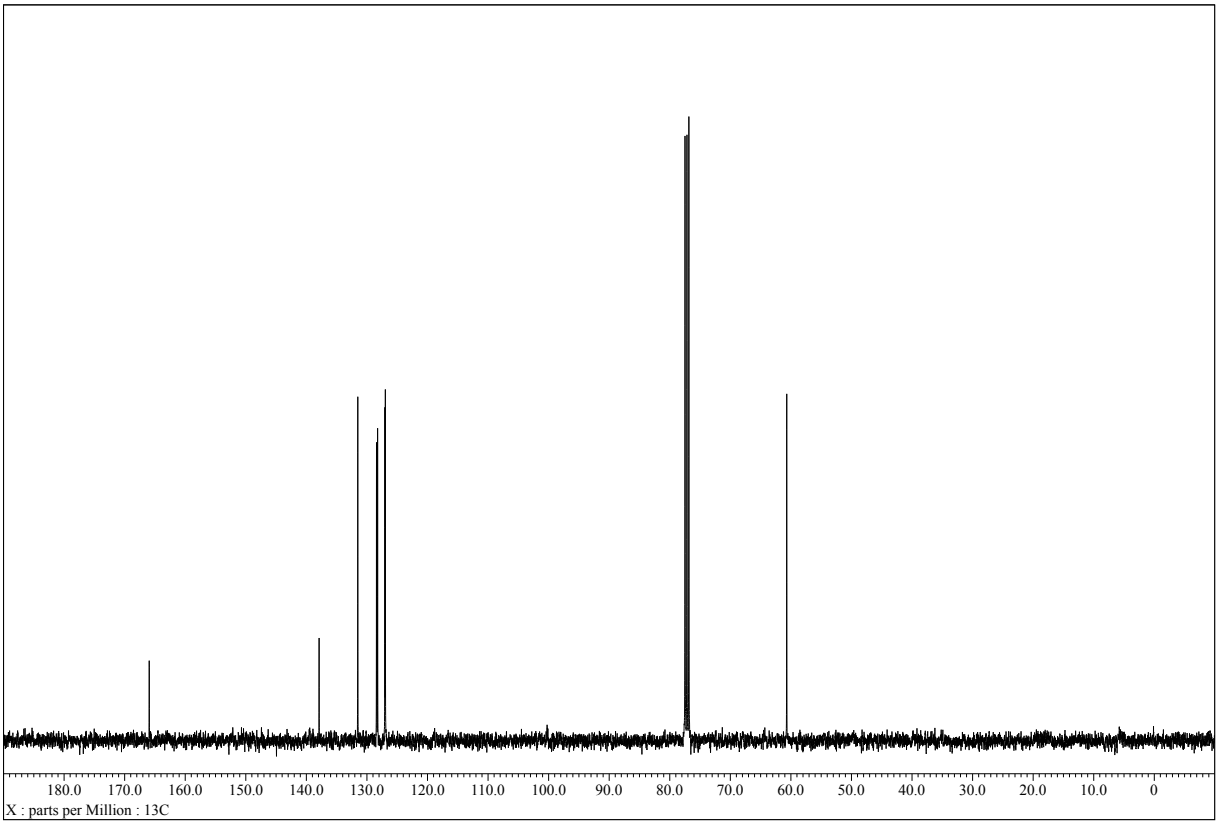
^{1}H and ^{13}C NMR spectra of Dodecyl acrylate (2c)



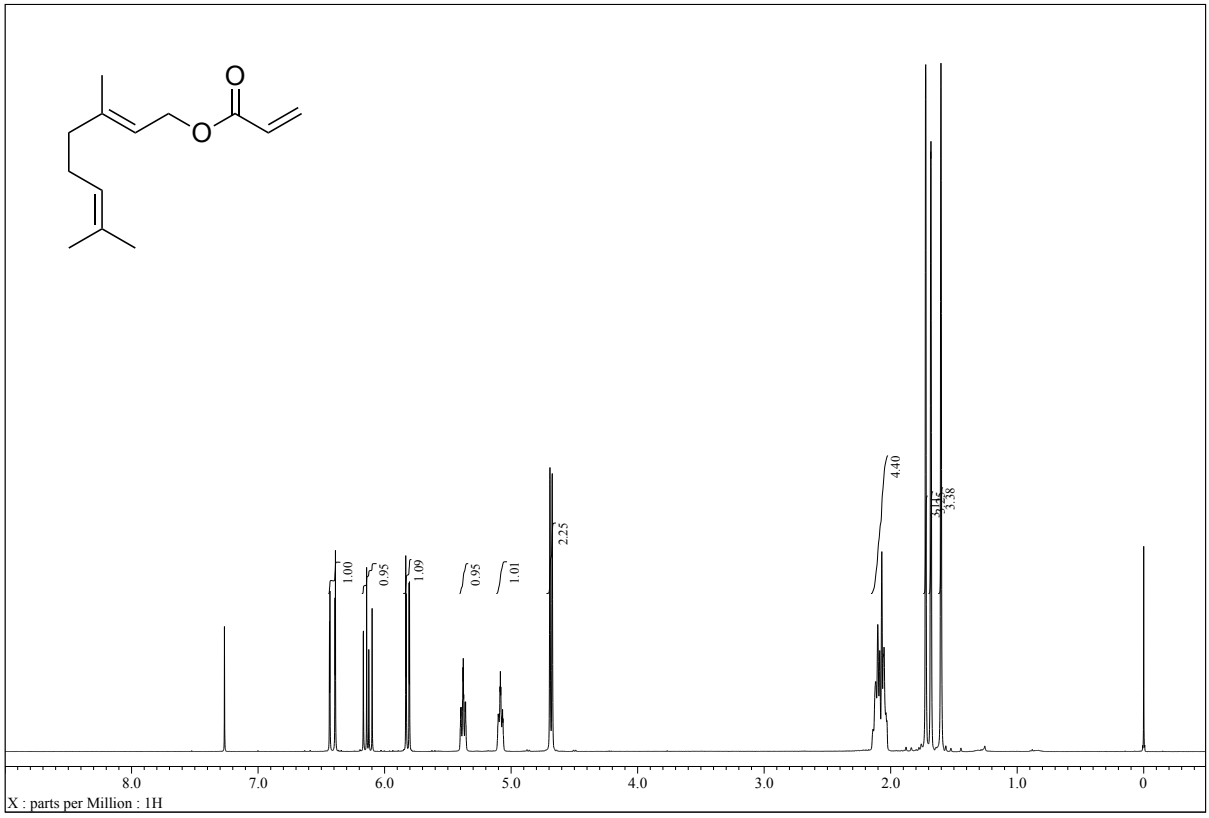


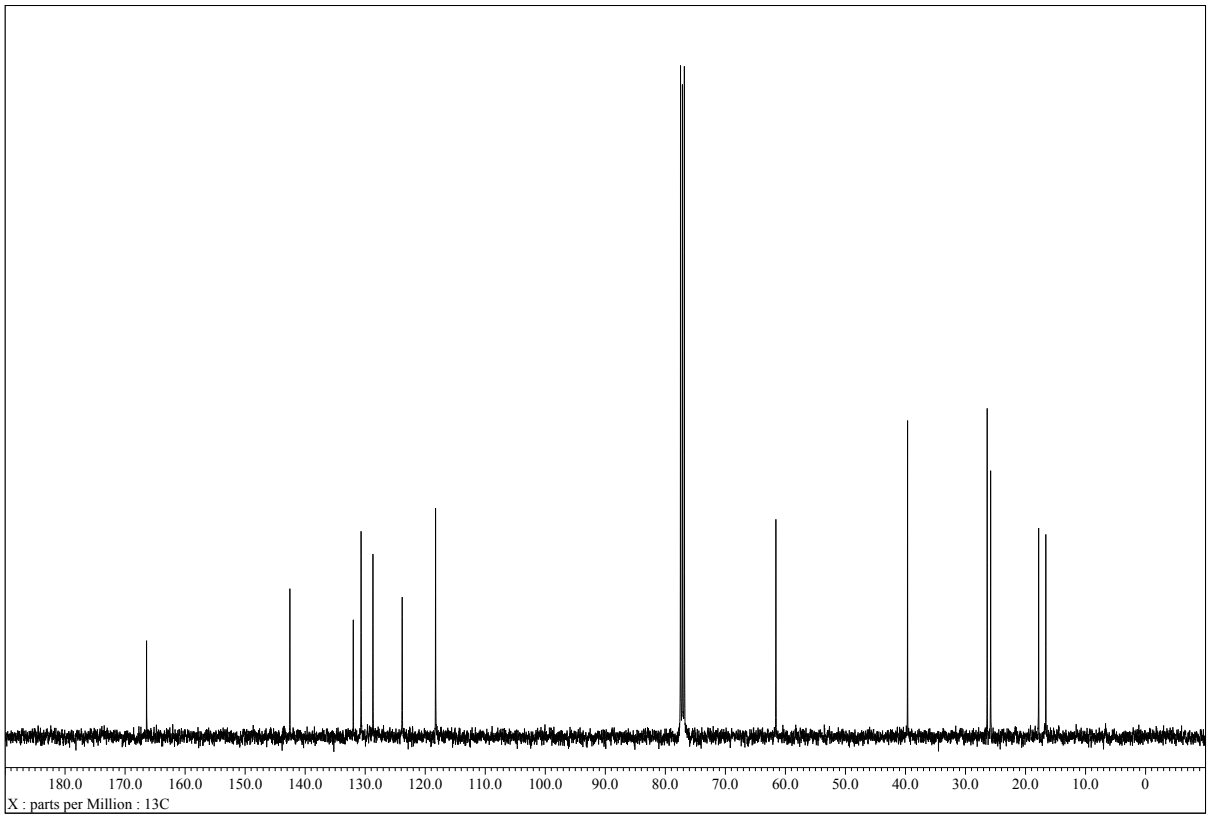
^{1}H and ^{13}C NMR spectra of Thiophen-2-ylmethyl acrylate (2d)



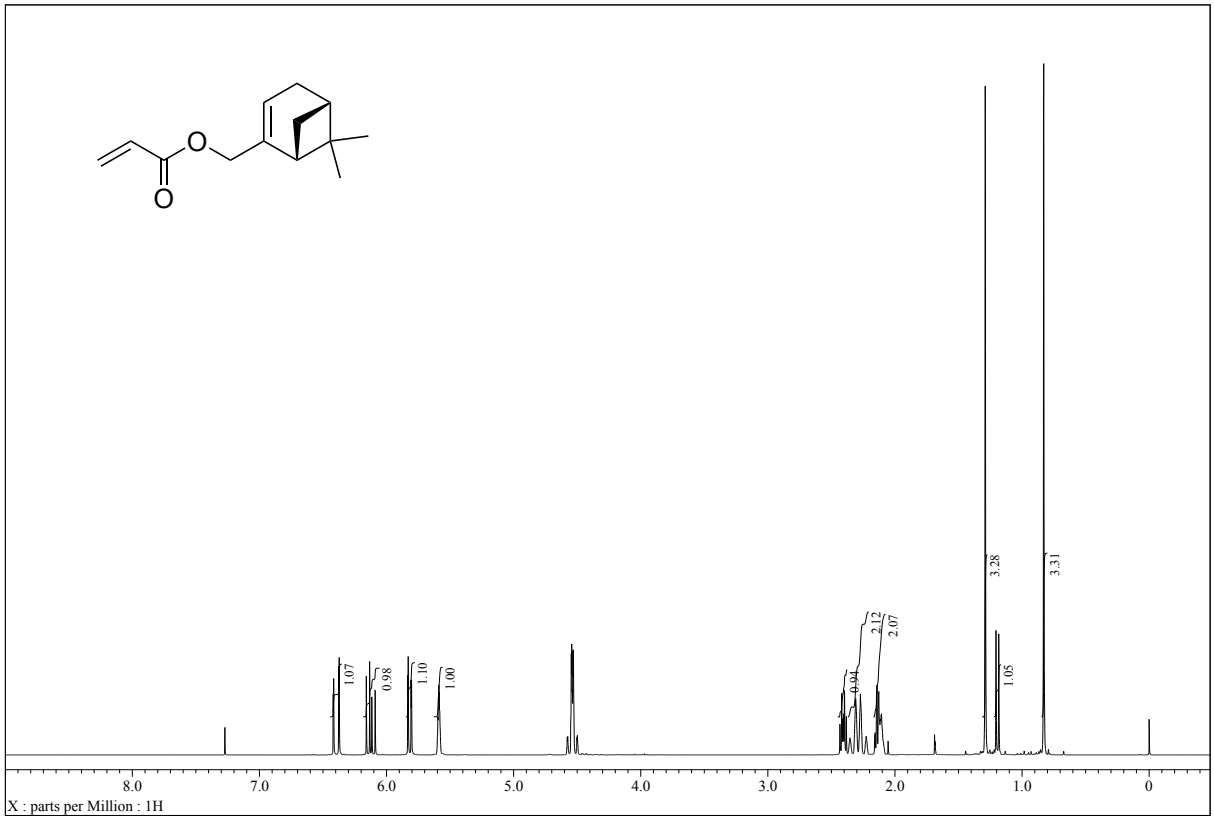


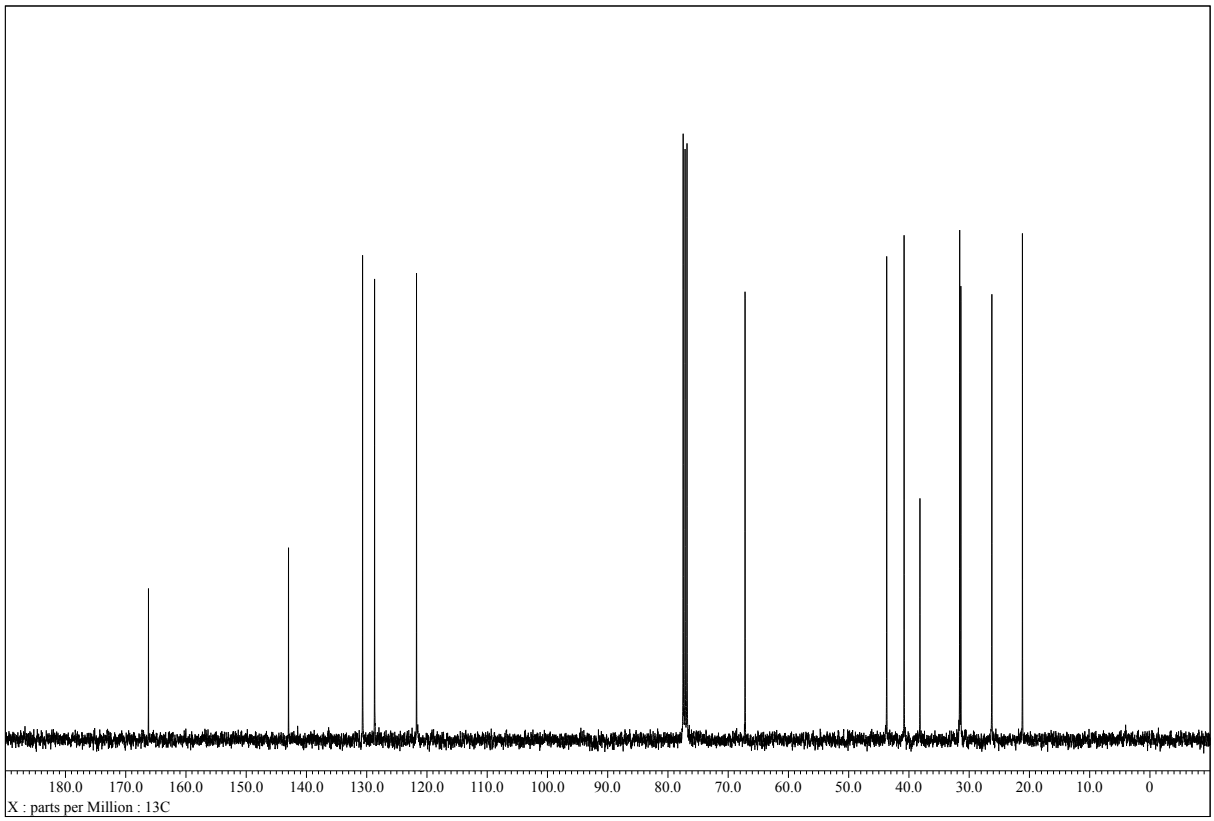
^{1}H and ^{13}C NMR spectra of Geranyl acrylate (2e)



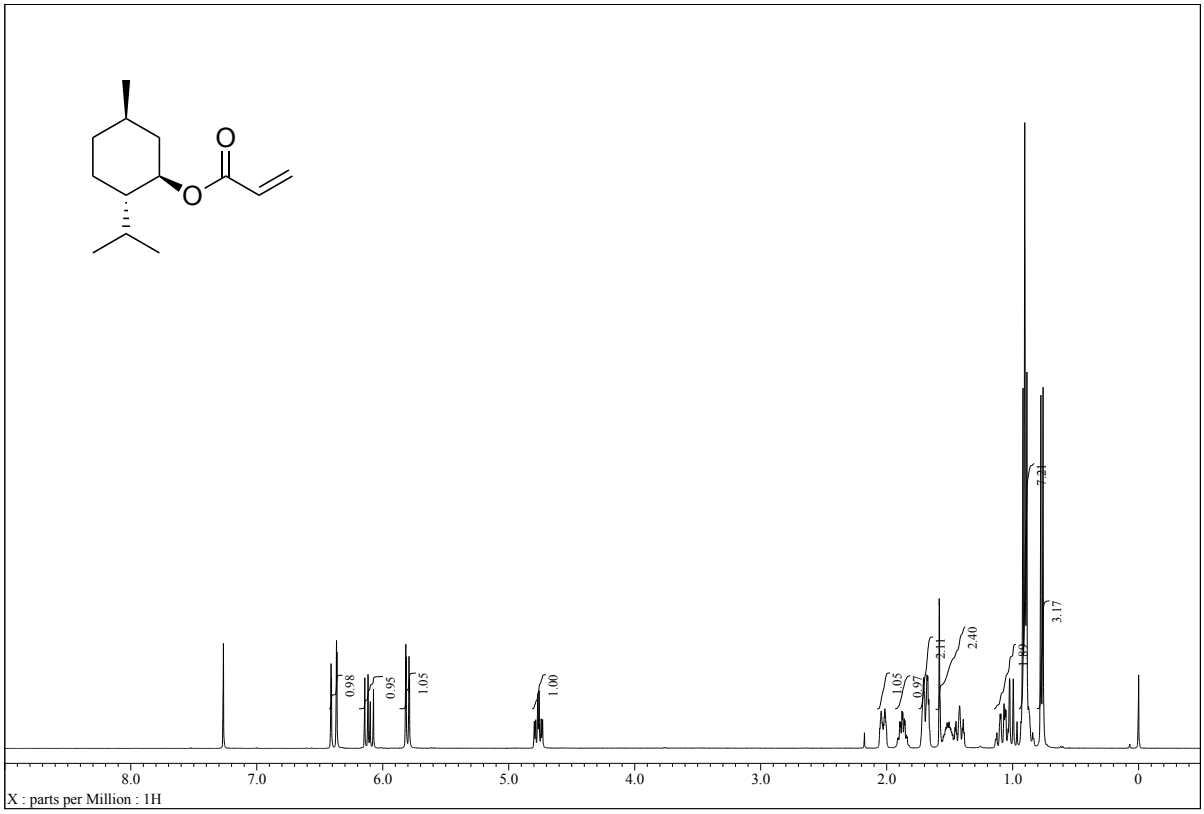


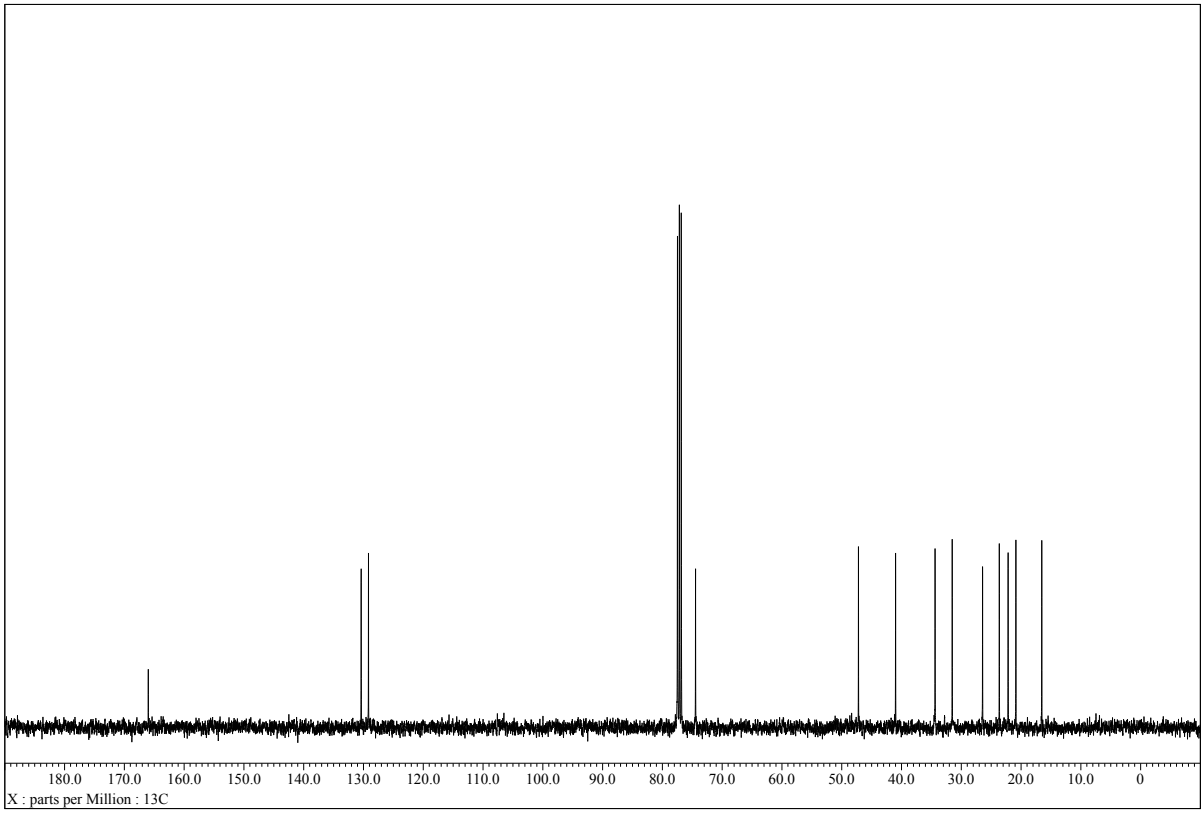
^{1}H and ^{13}C NMR spectra of (1*R*)-(–)-Myrtenyl acrylate (2f)



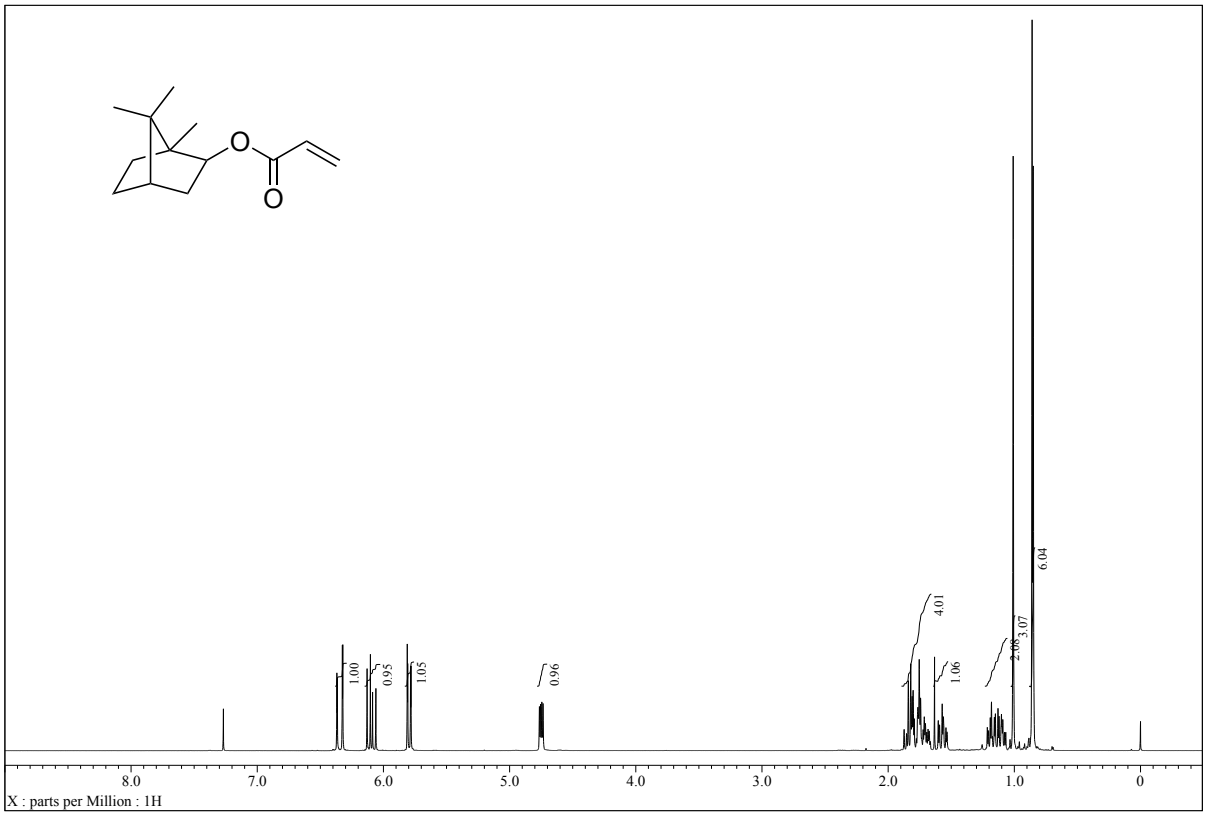


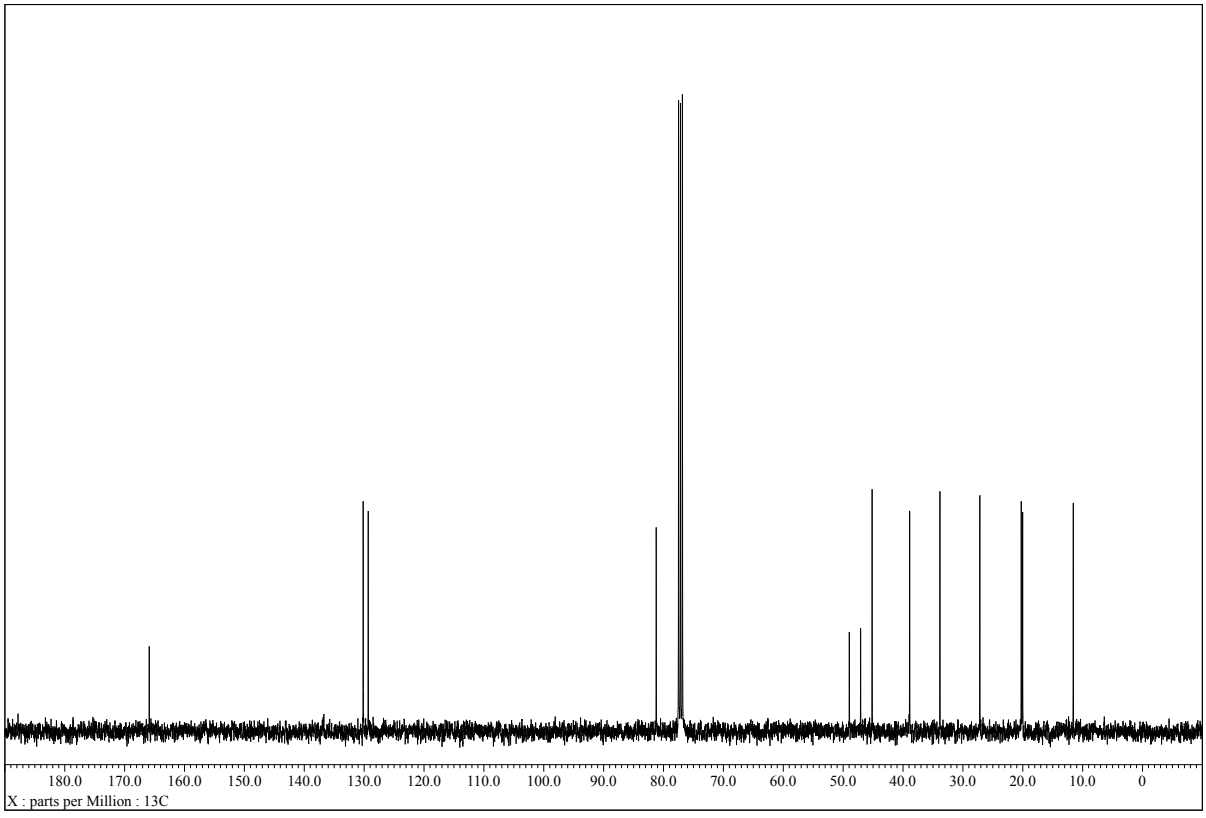
^{1}H and ^{13}C NMR spectra of L-Menthyl acrylate (2g)



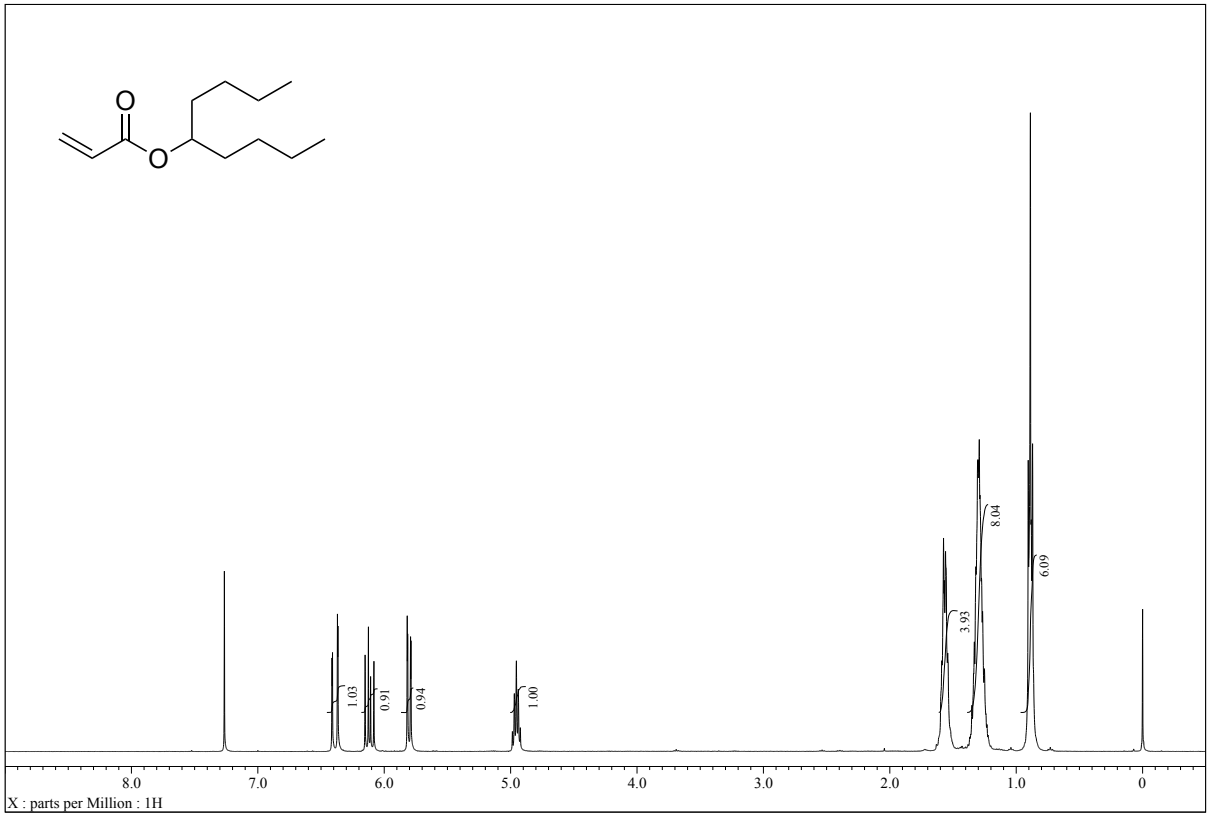


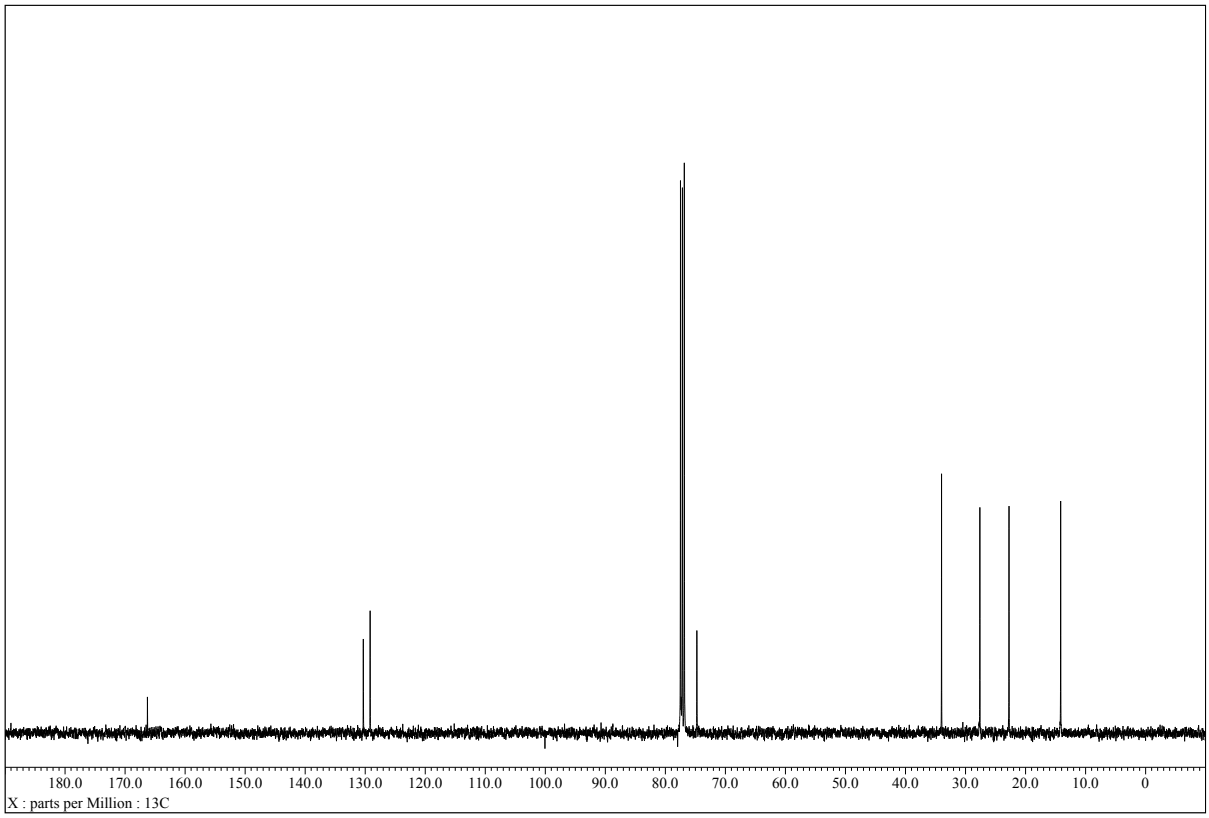
^{1}H and ^{13}C NMR spectra of Isobornyl acrylate (2b)



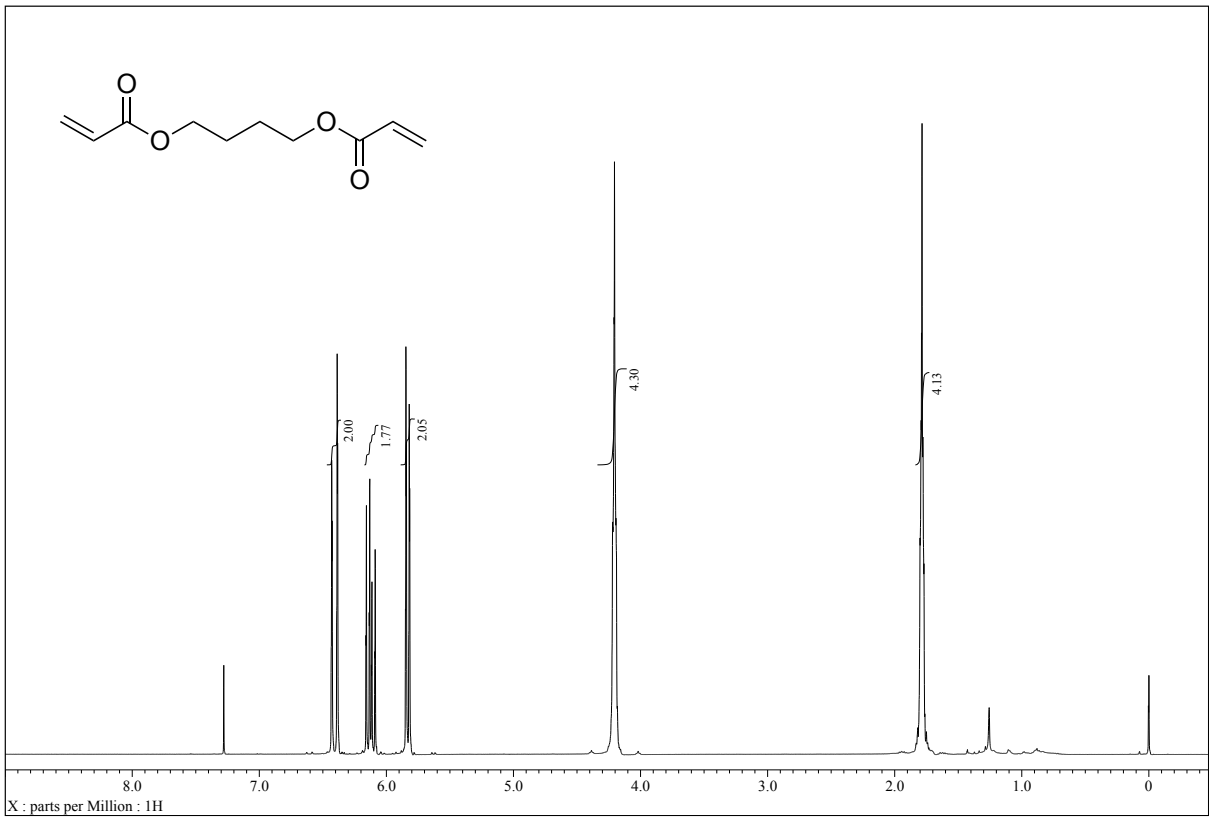


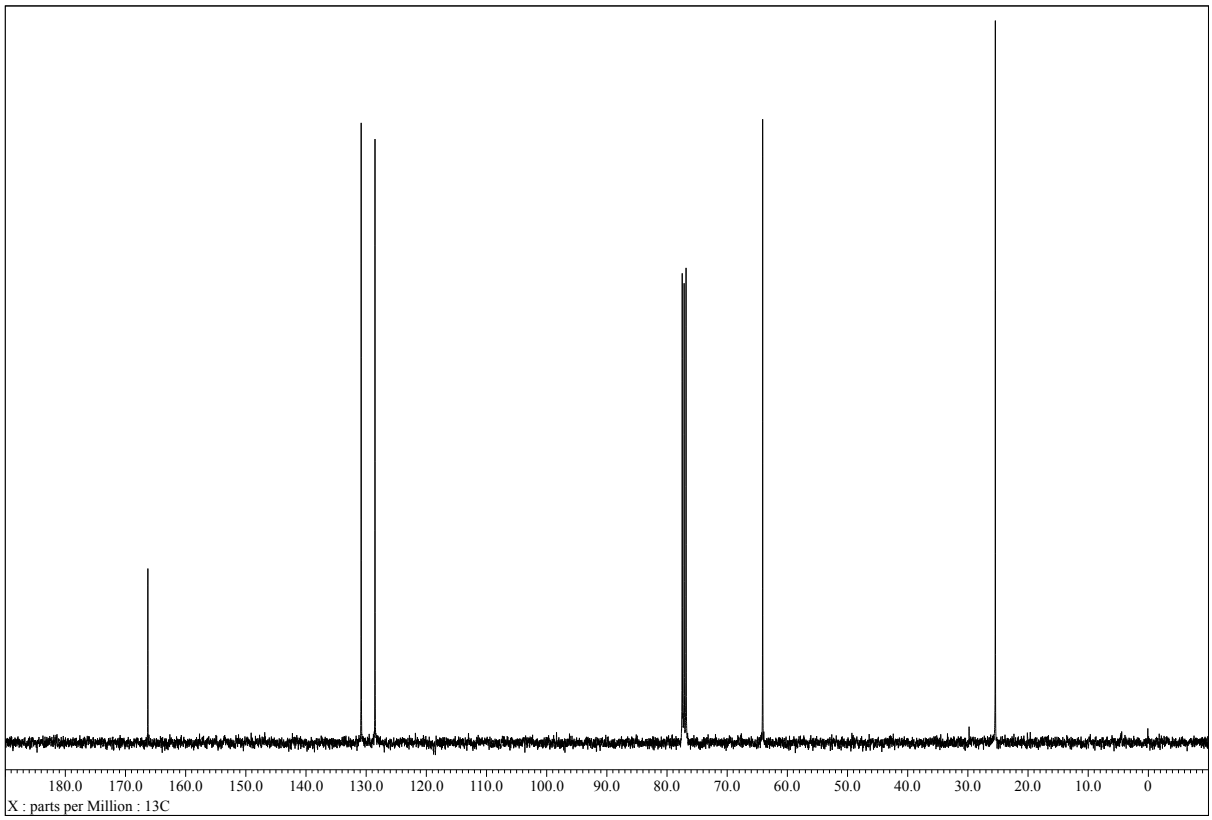
^{1}H and ^{13}C NMR spectra of Nonan-5-yl acrylate (2h)



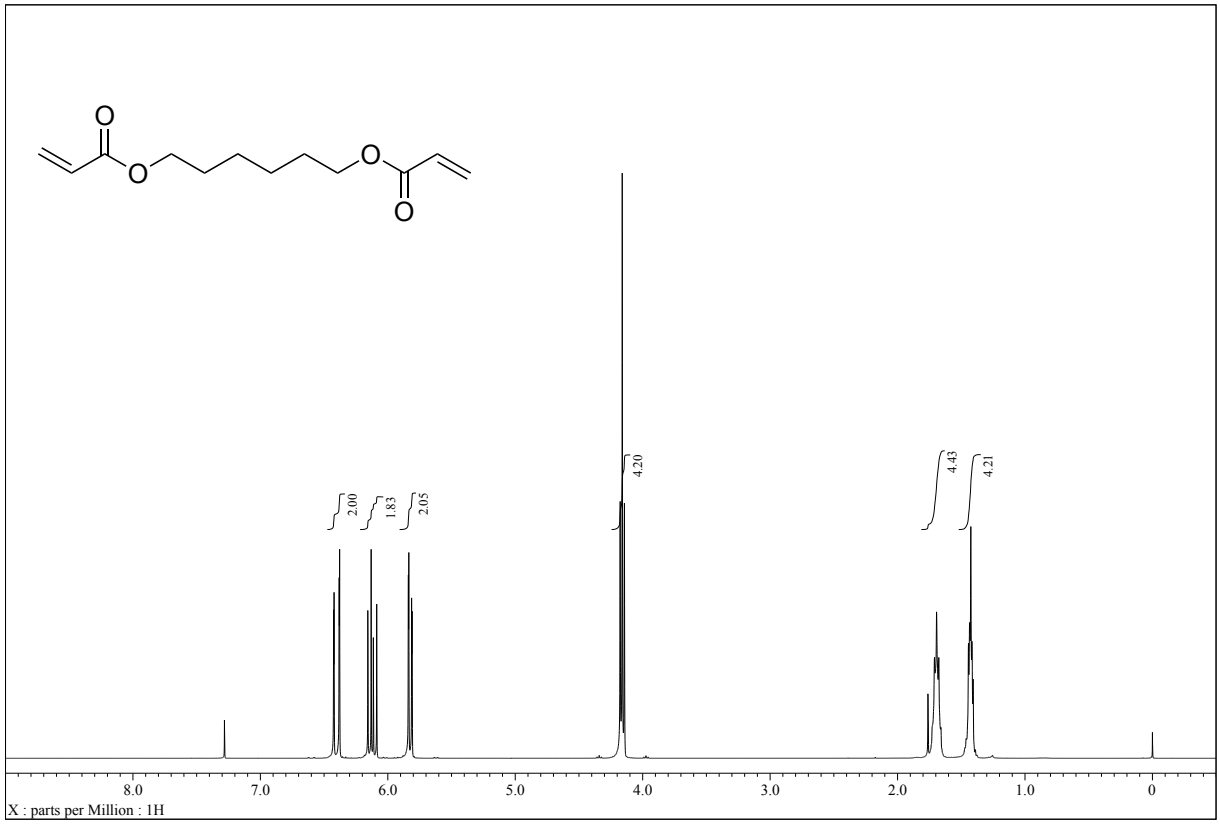


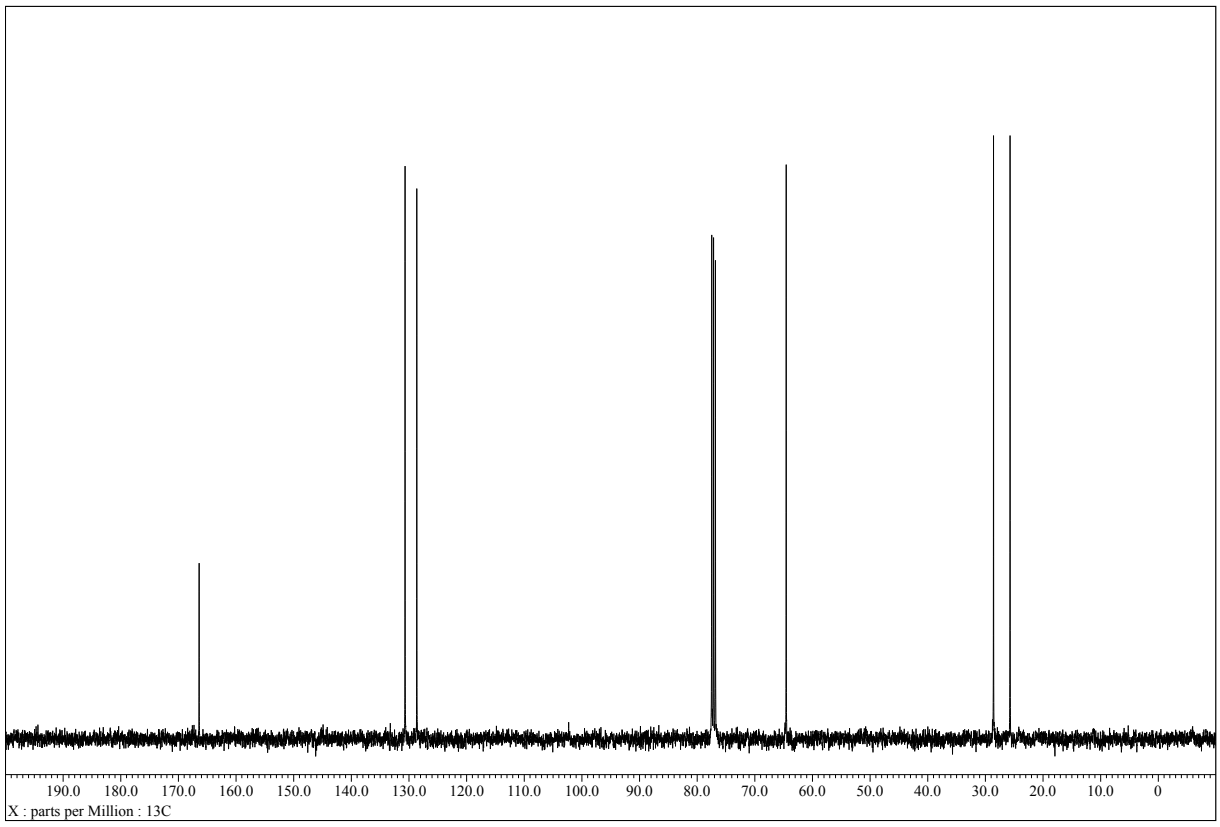
^{1}H and ^{13}C NMR spectra of Butane-1,4-diyl diacrylate (2i)



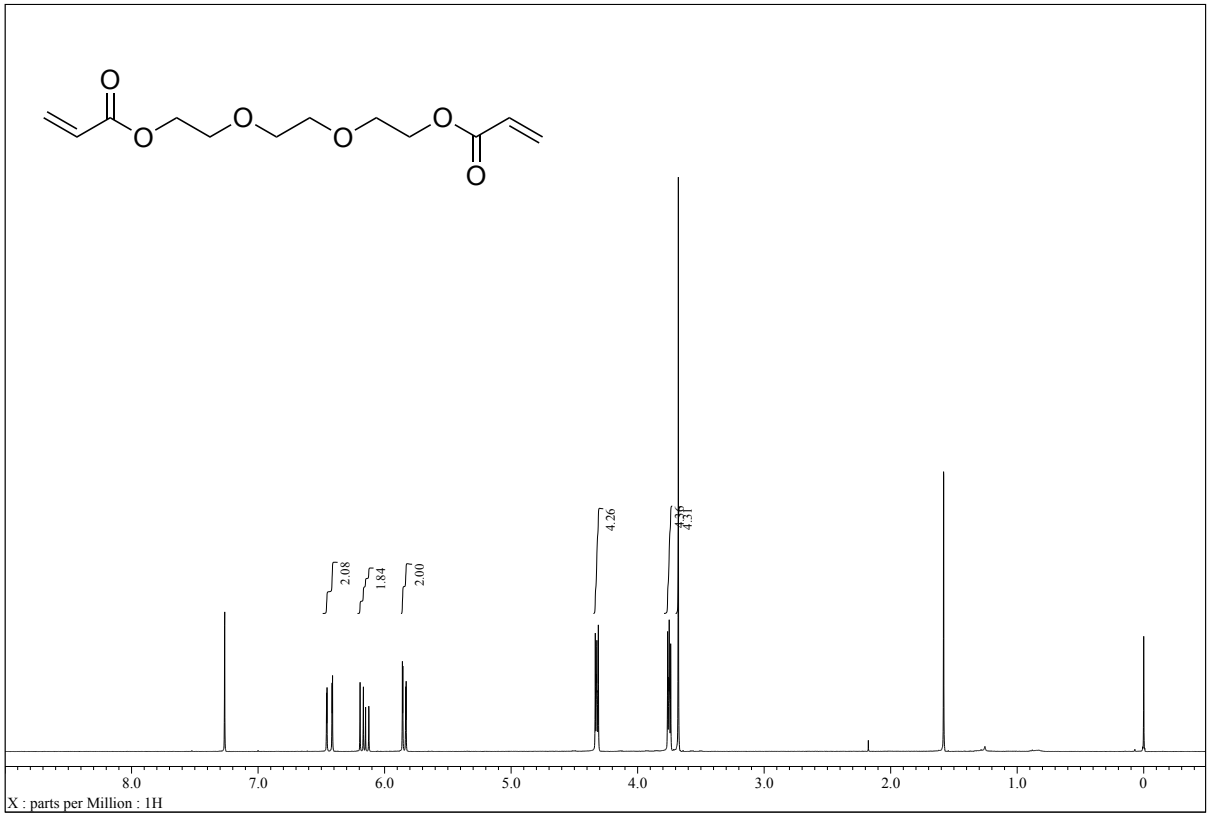


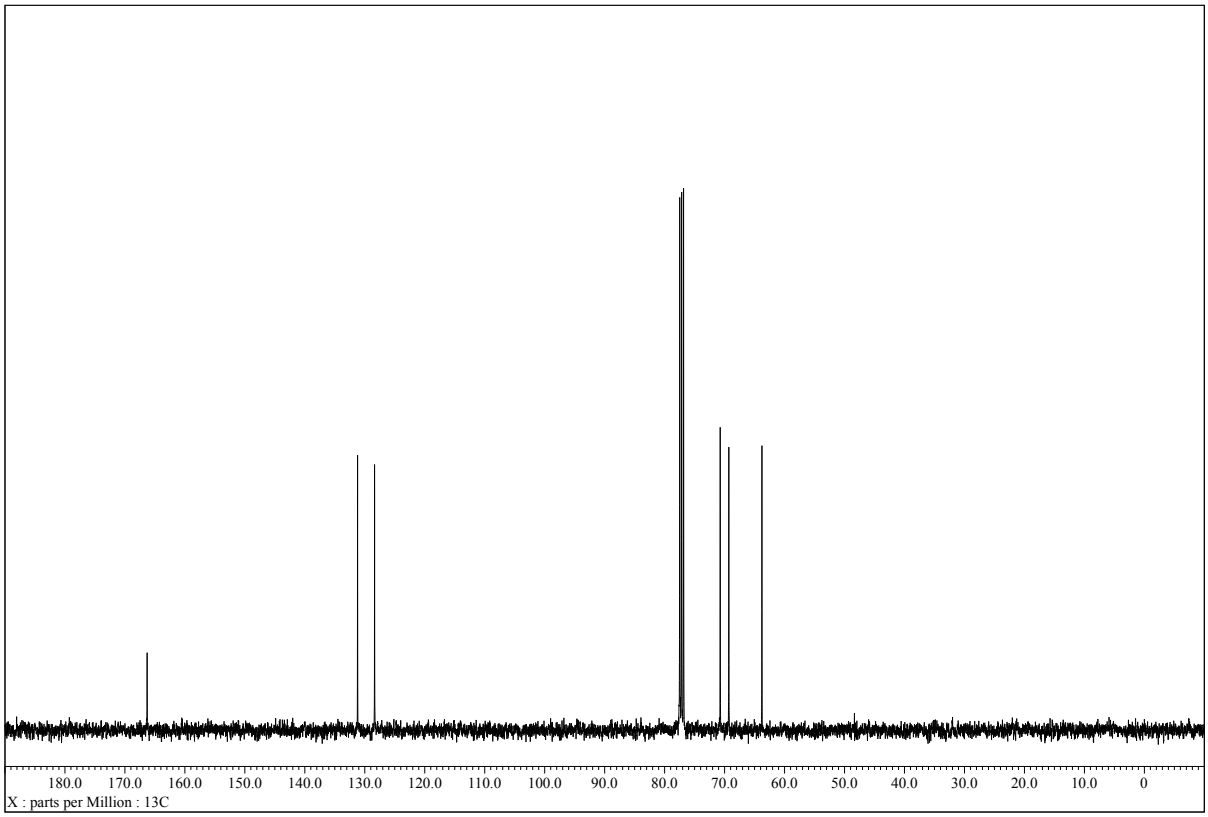
^{1}H and ^{13}C NMR spectra of hexane-1,6-diyl diacrylate (2j)



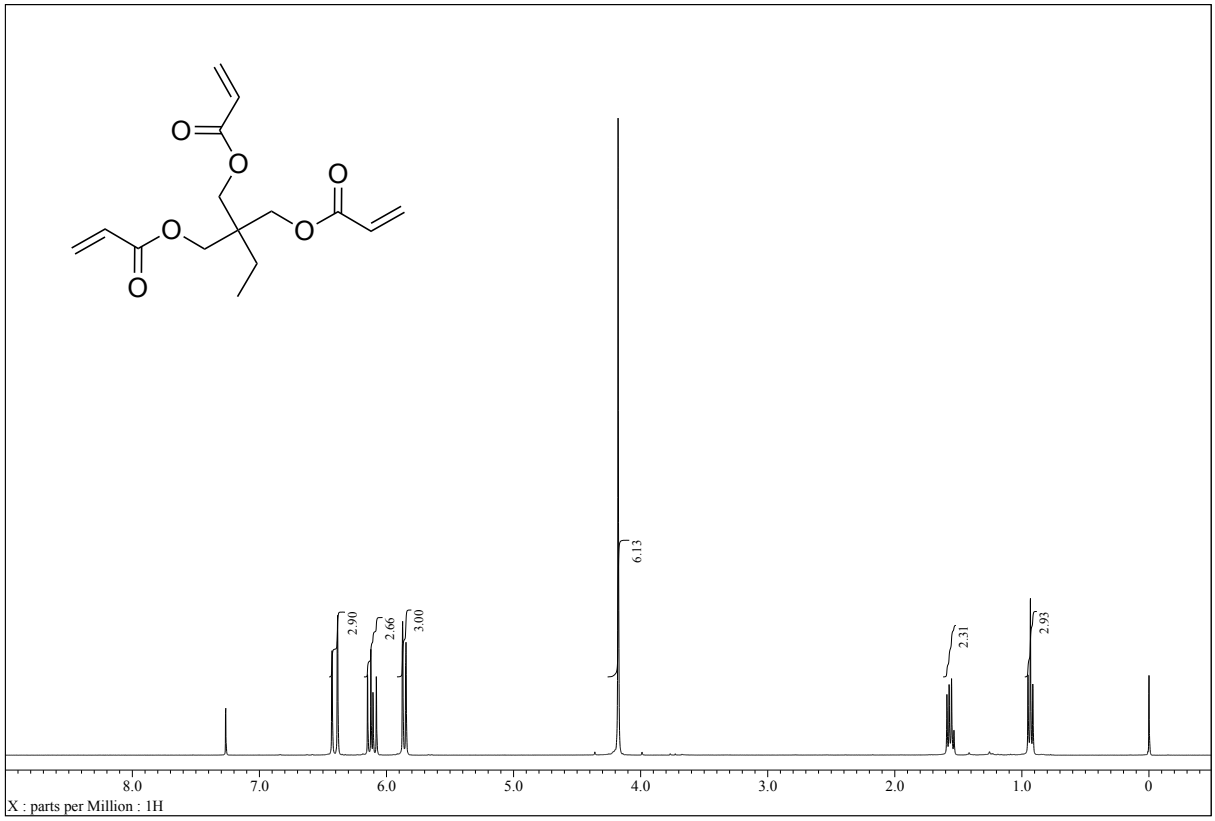


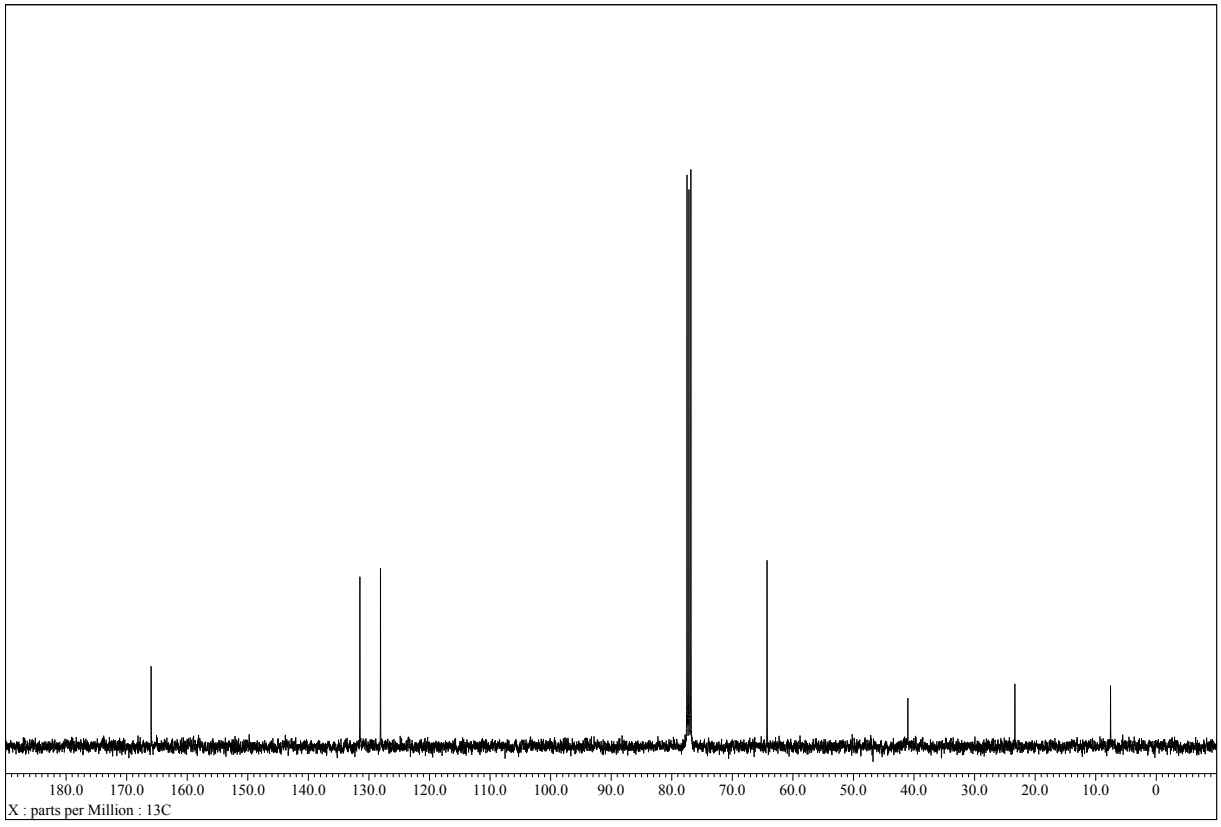
^{1}H and ^{13}C NMR spectra of (Ethane-1,2-diylbis(oxy))bis(ethane-2,1-diyl) diacrylate (2k)



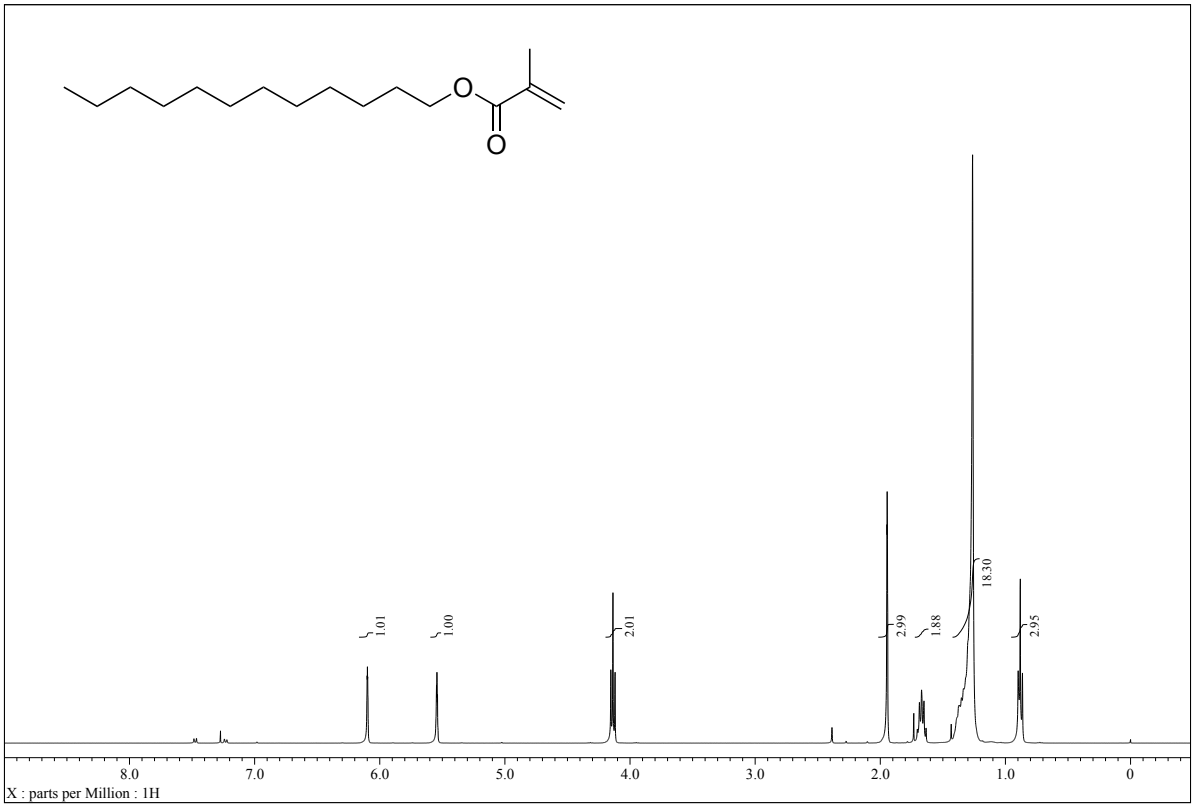


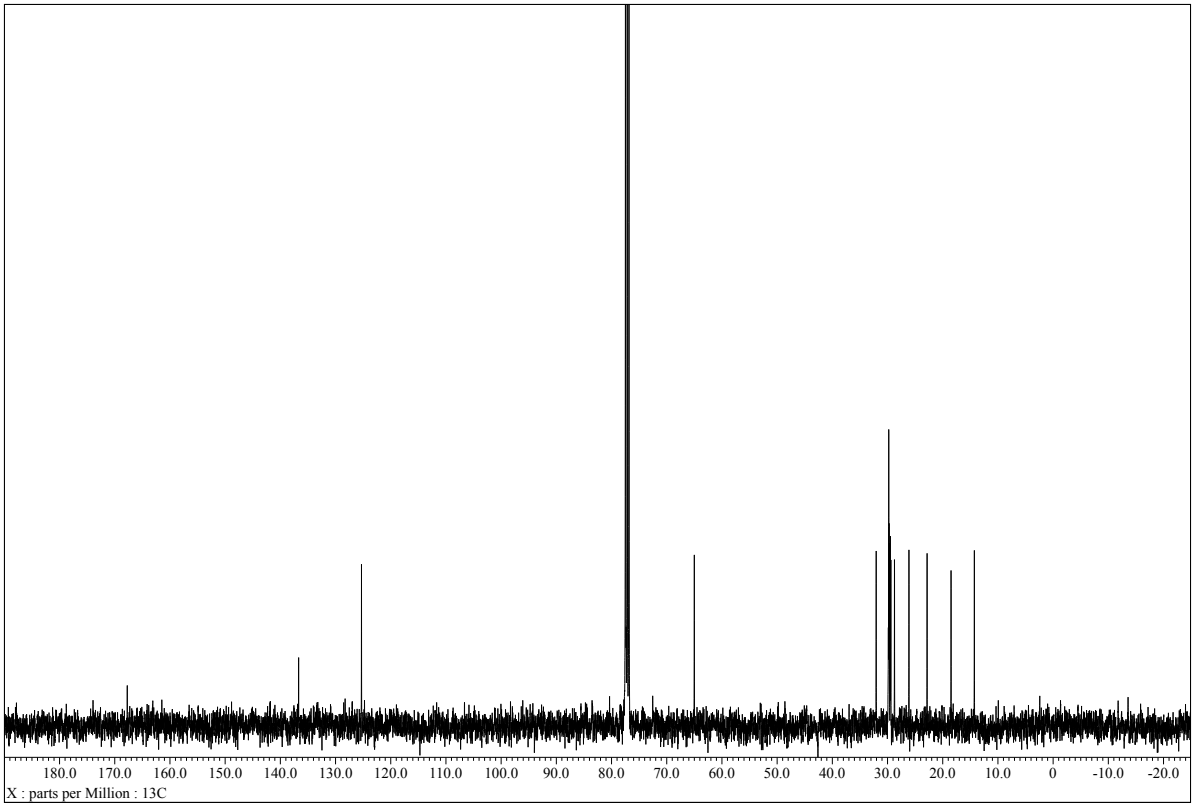
^{1}H and ^{13}C NMR spectra of 2-((Acryloyloxy)methyl)-2-ethylpropane-1,3-diyl diacrylate (2l)



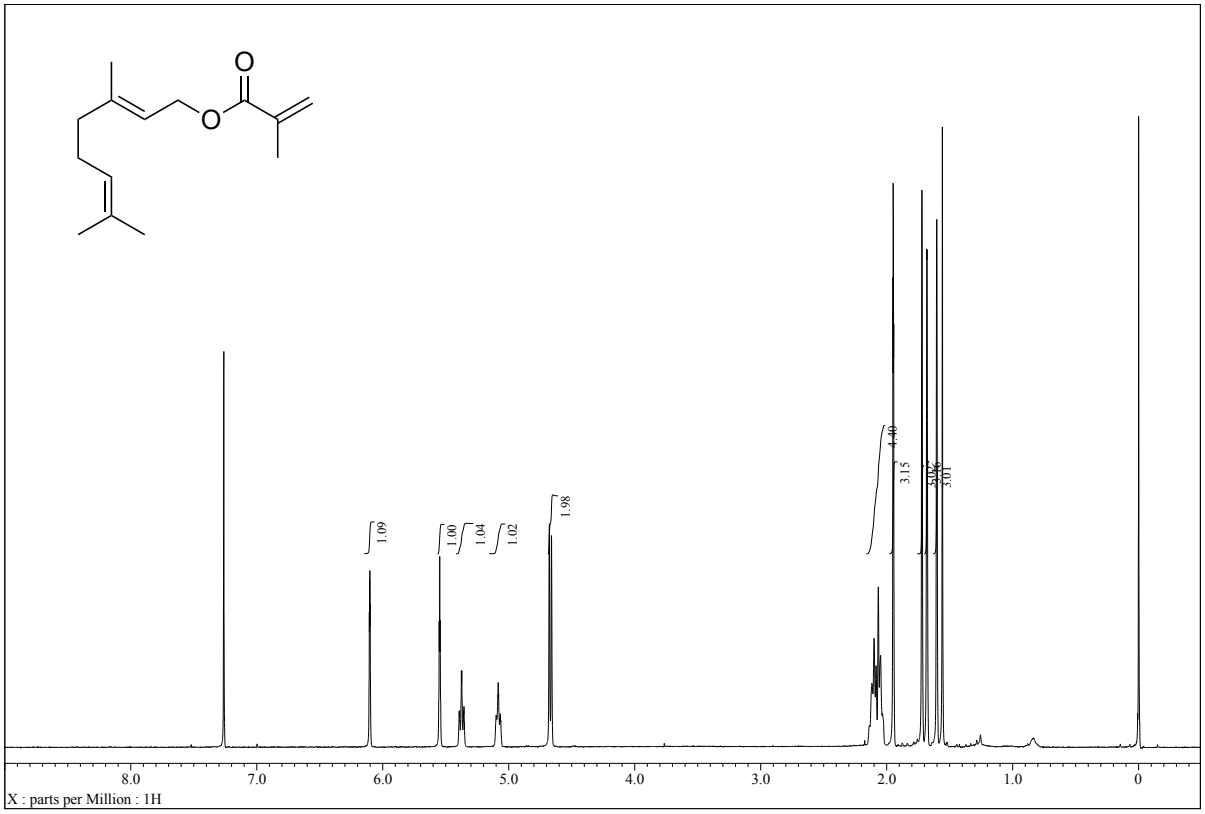


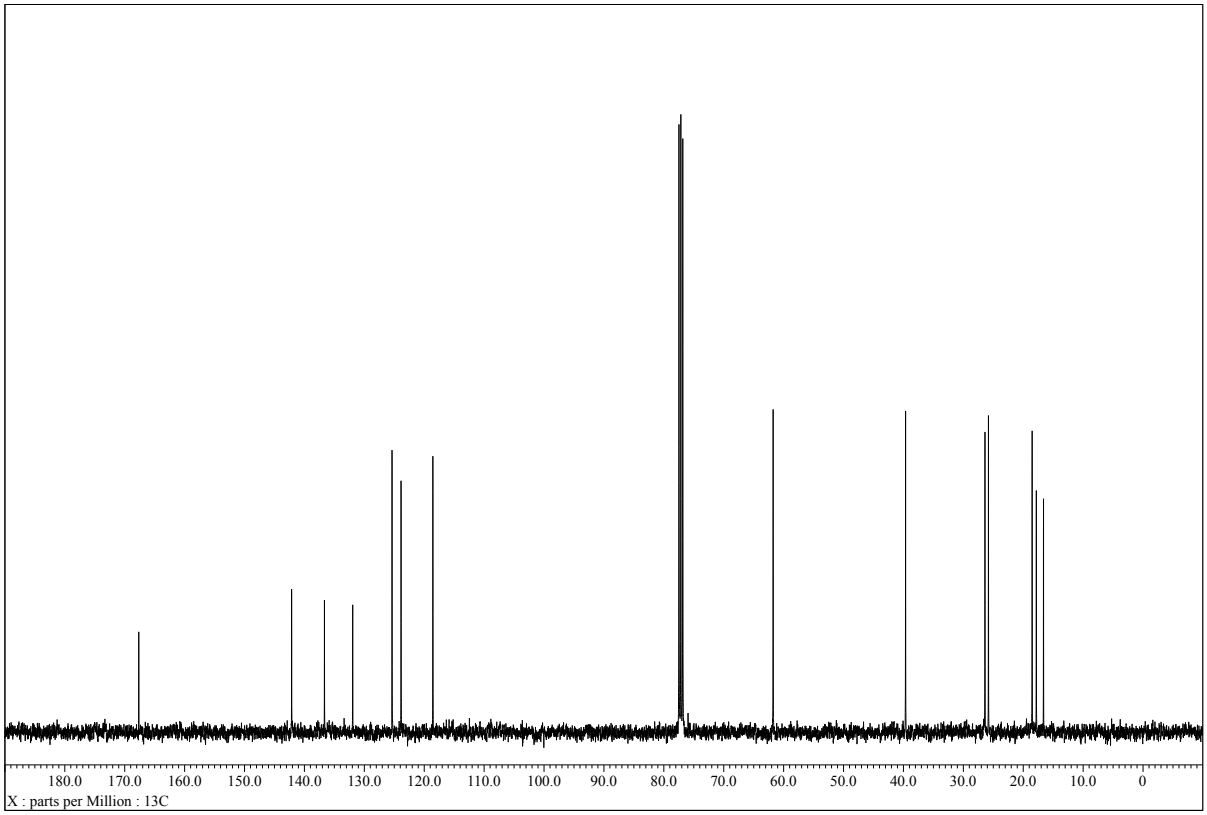
^{1}H and ^{13}C NMR spectra of Dodecyl methacrylate (7c)



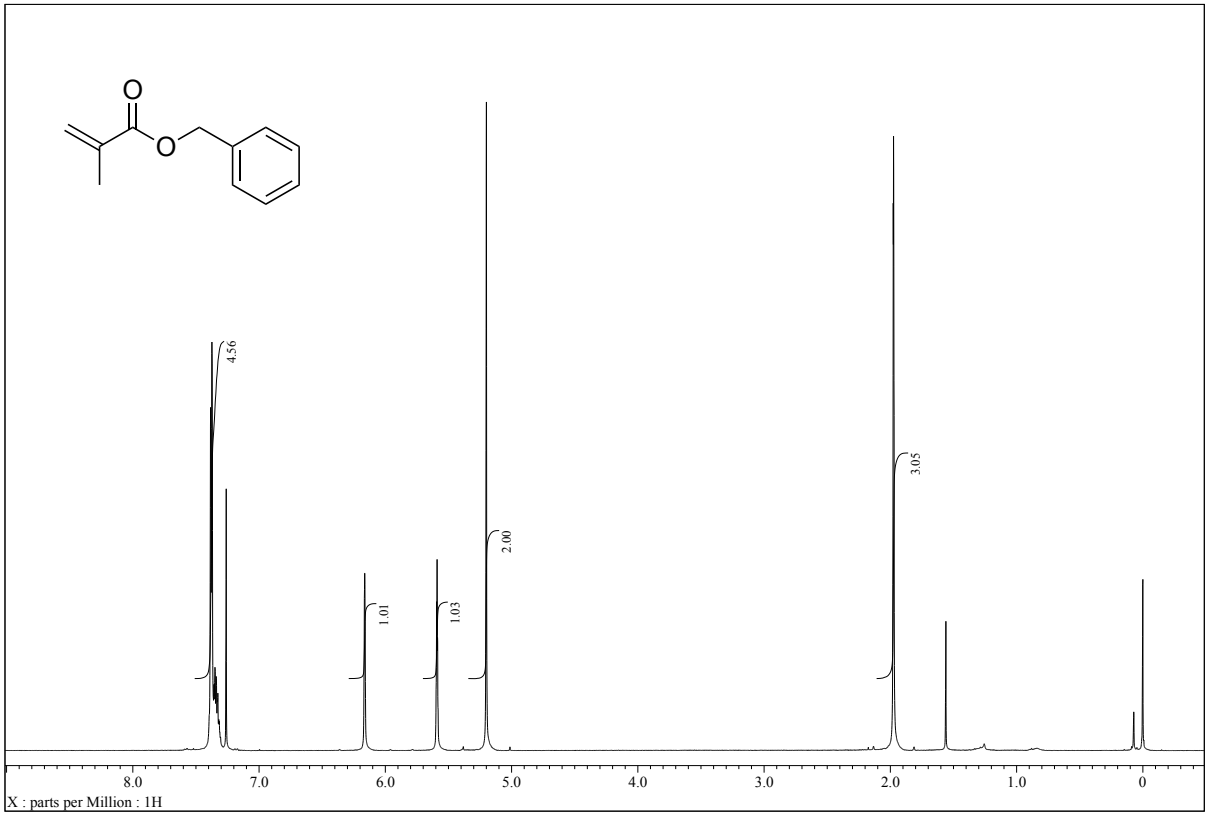


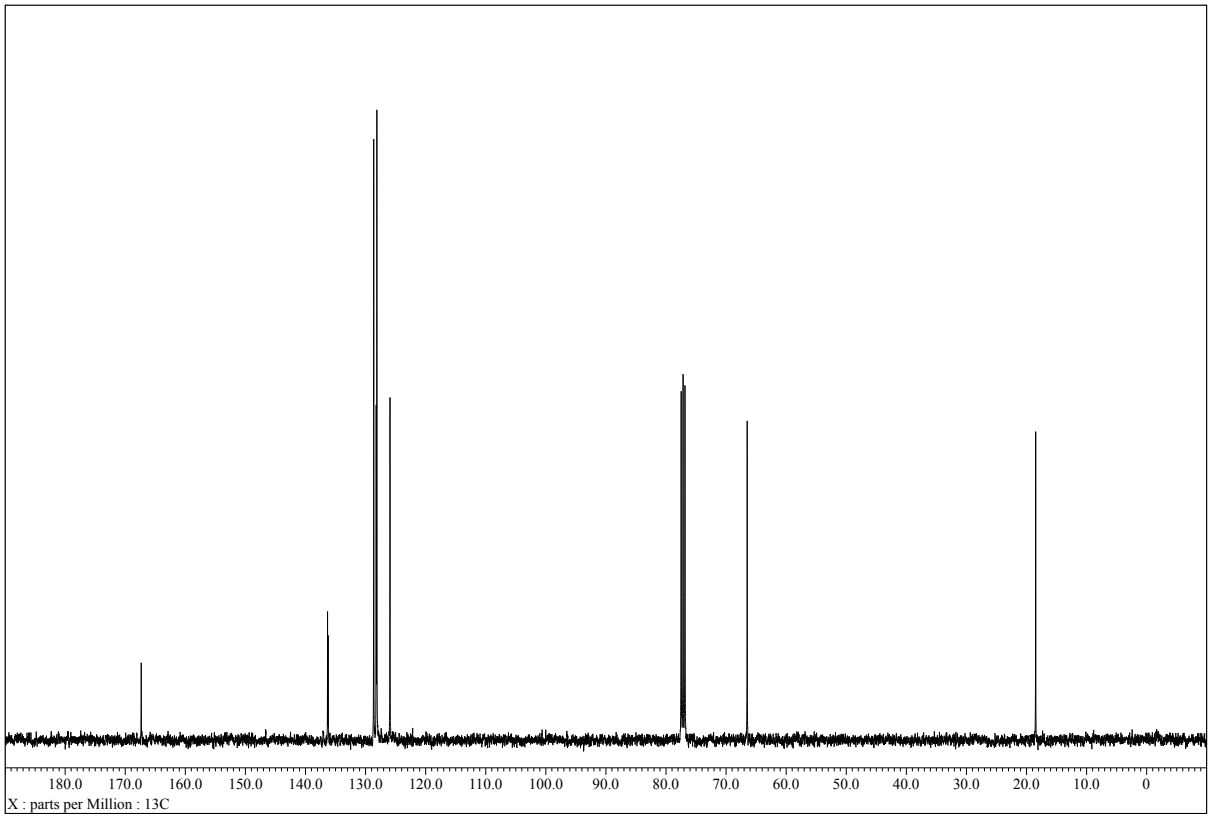
^{1}H and ^{13}C NMR spectra of Geranyl methacrylate (7e)



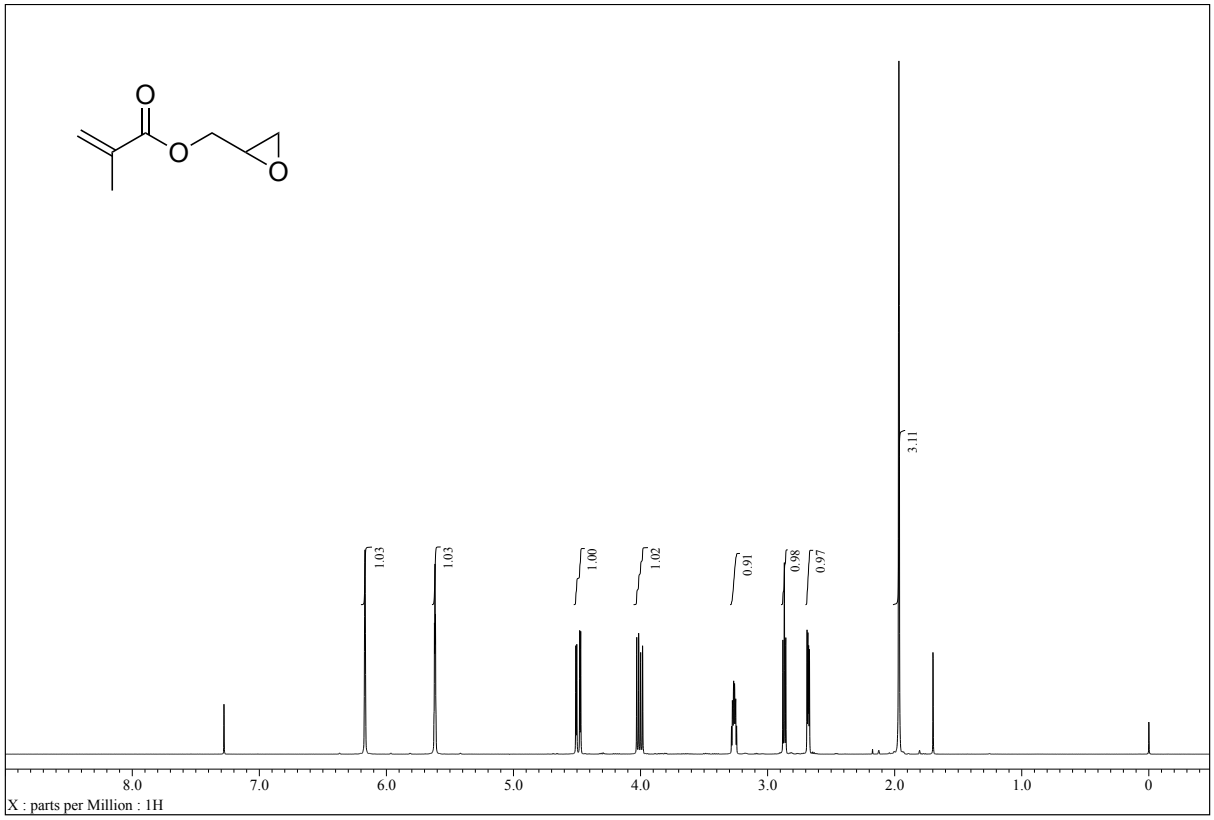


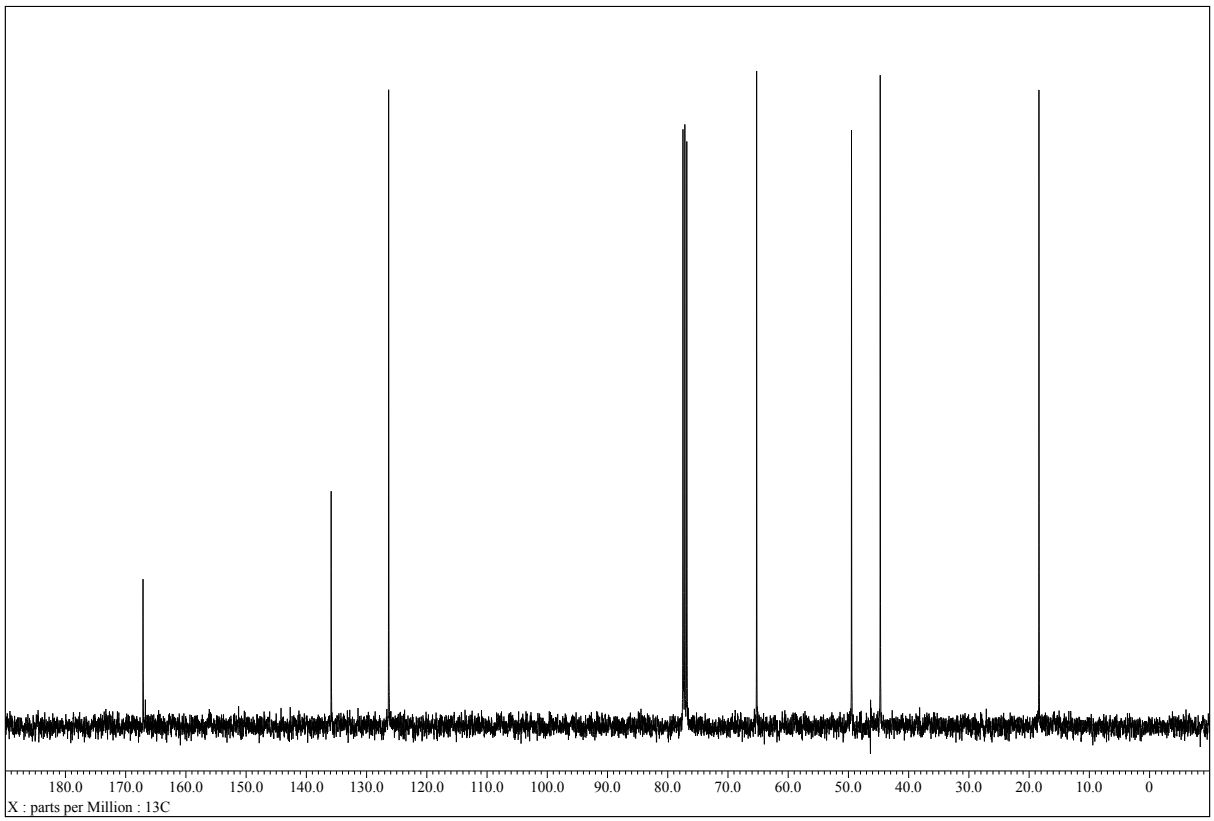
^{1}H and ^{13}C NMR spectra of Benzyl methacrylate (7a):



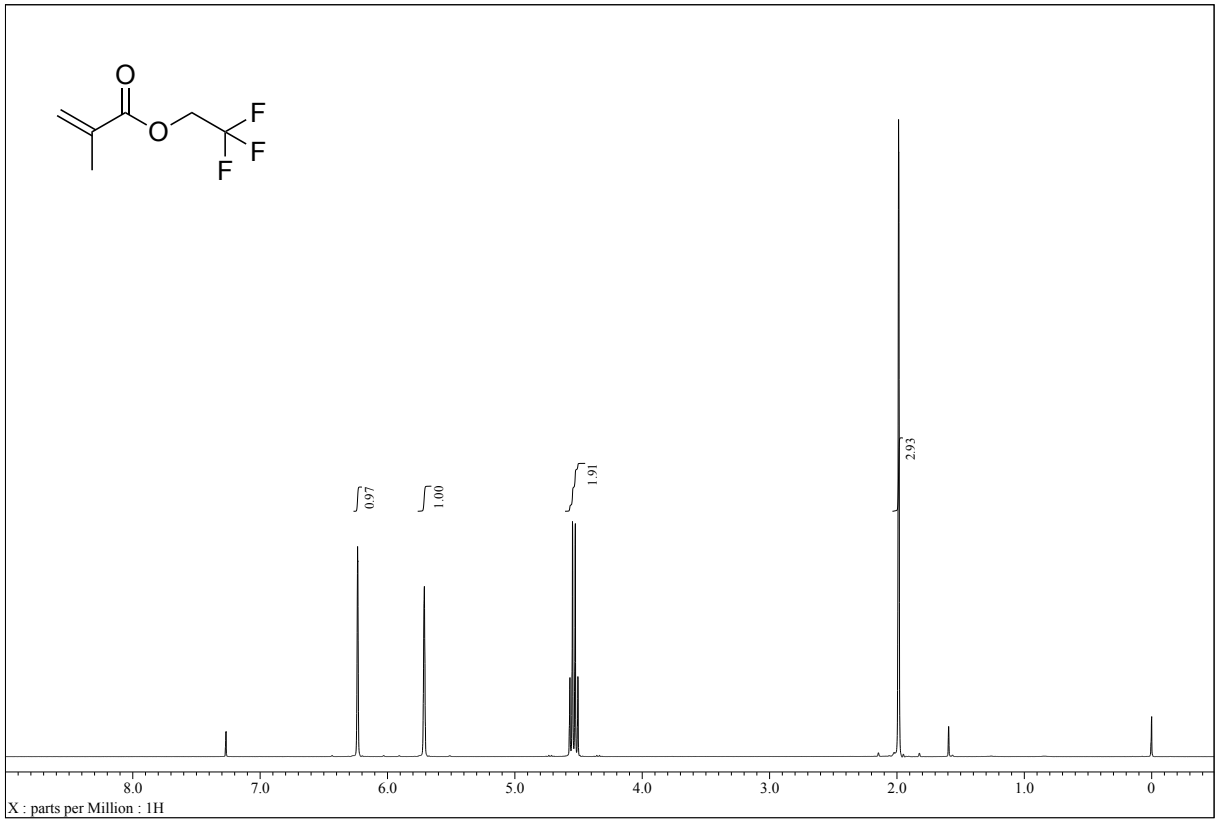


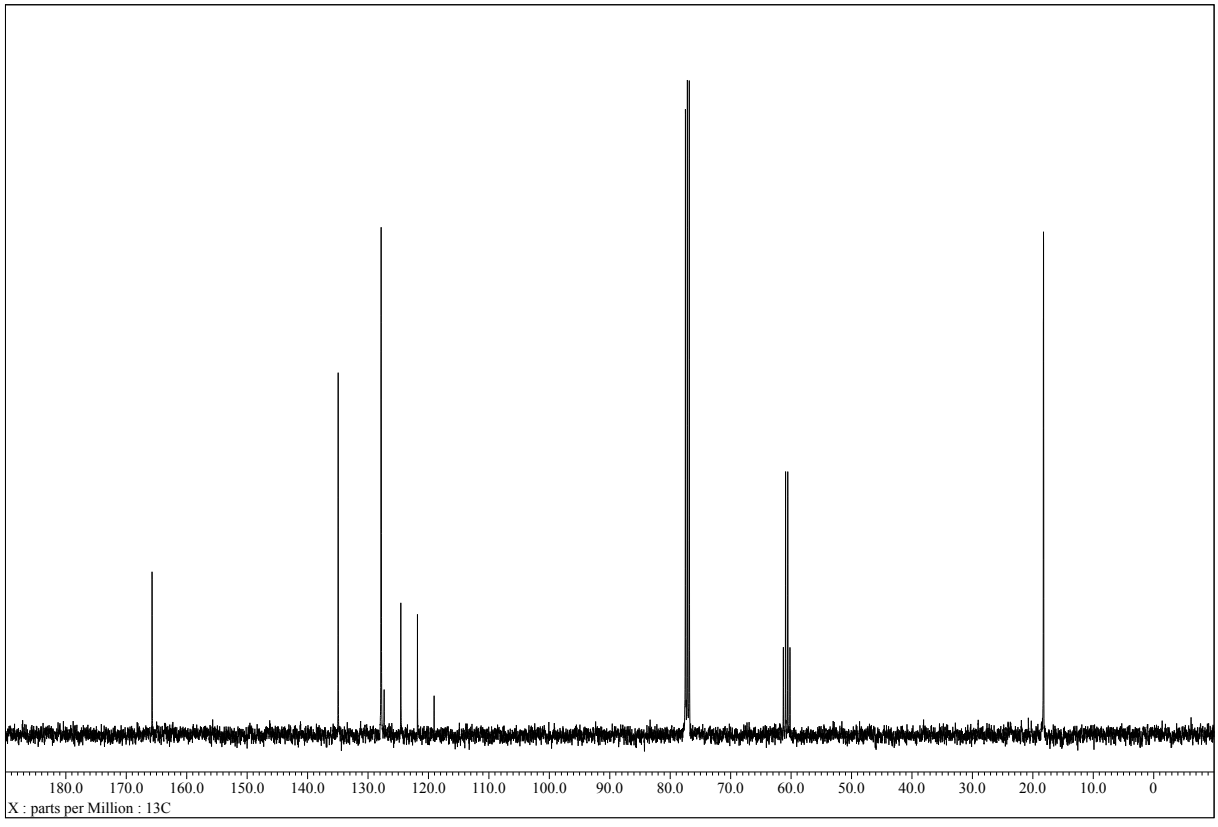
^{1}H and ^{13}C NMR spectra of Oxiran-2-ylmethyl methacrylate (7m):

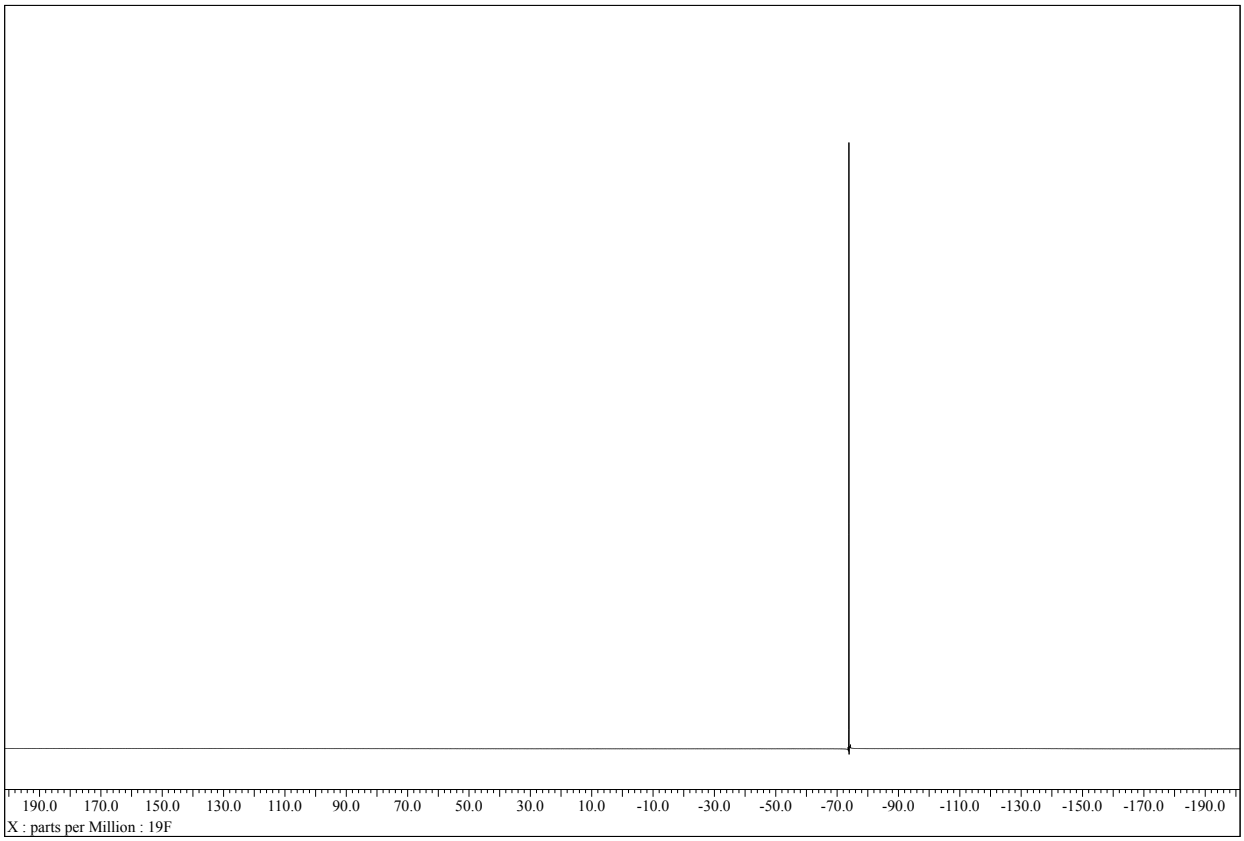




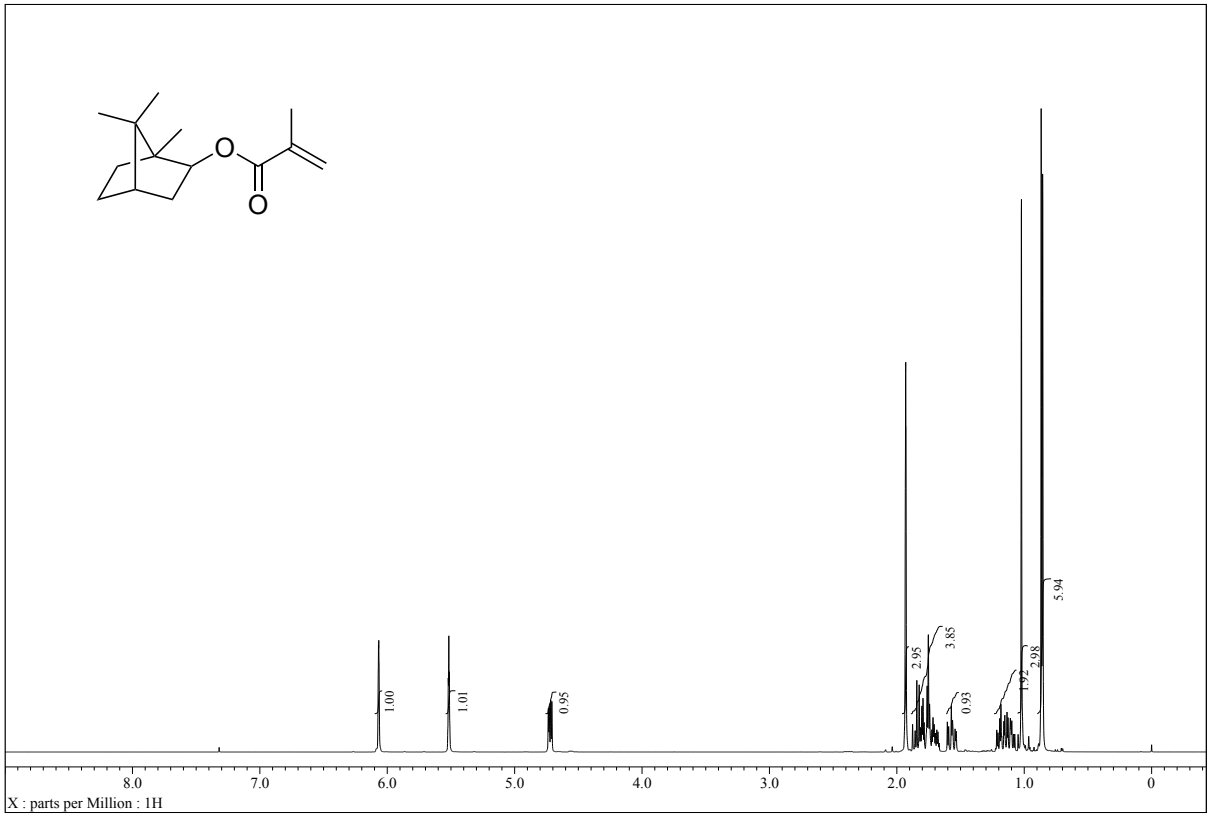
^{1}H,^{13}C and ^{19}F NMR spectra of 2,2,2-Trifluoromethyl methacrylate (7n)

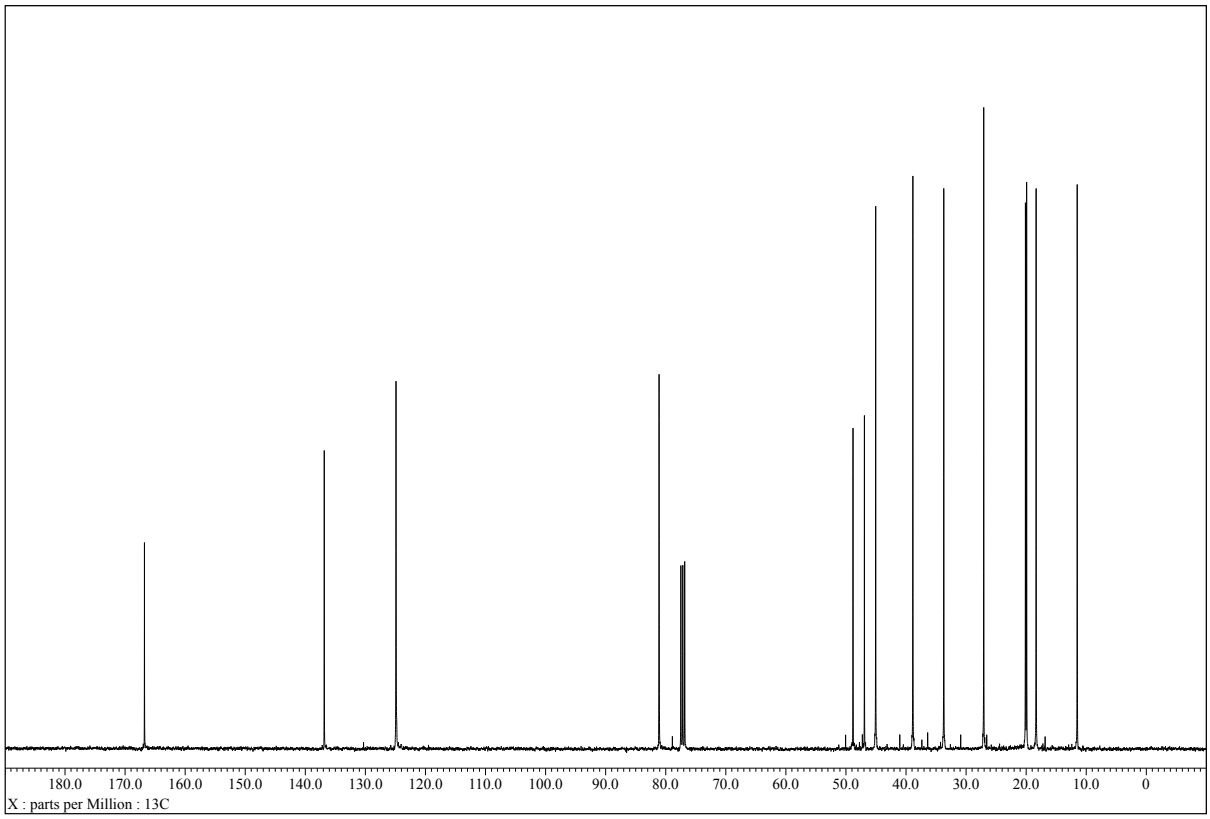




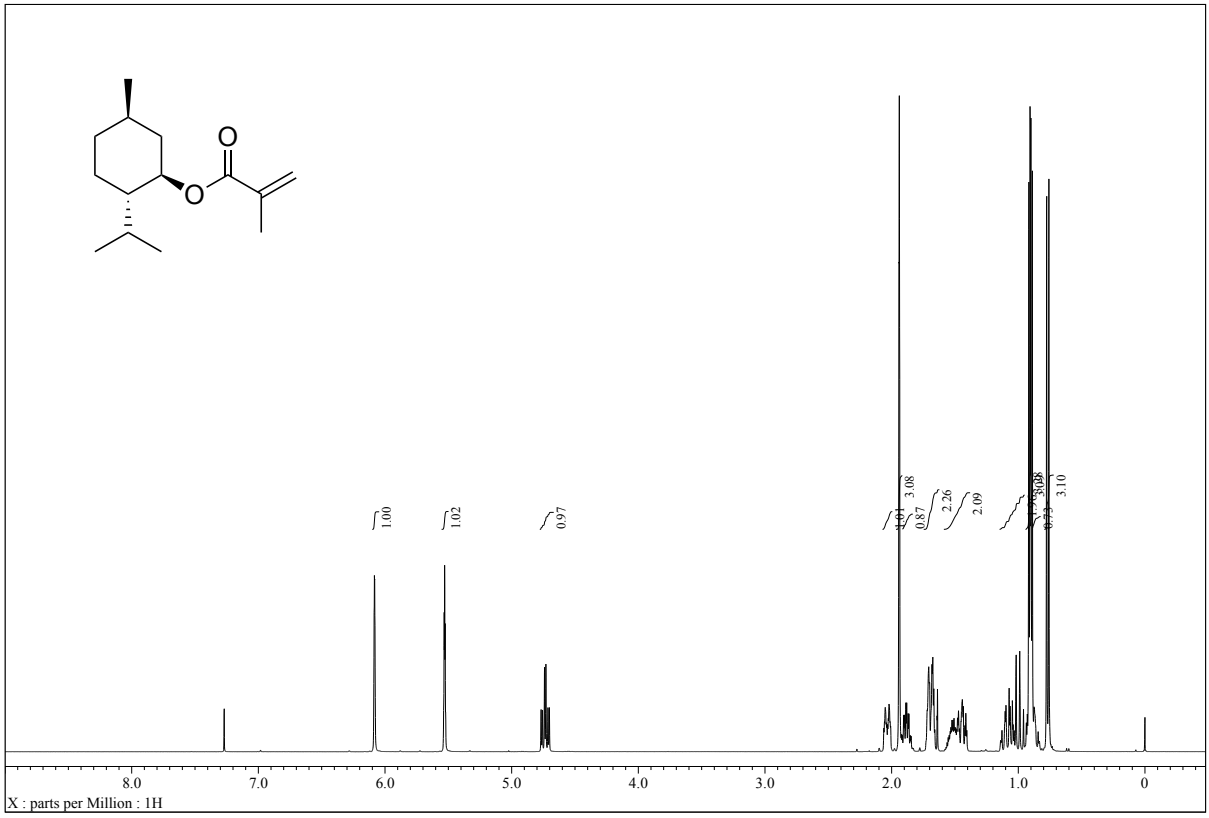

190.0 170.0 150.0 130.0 110.0 90.0 70.0 50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0
X : parts per Million : 19F

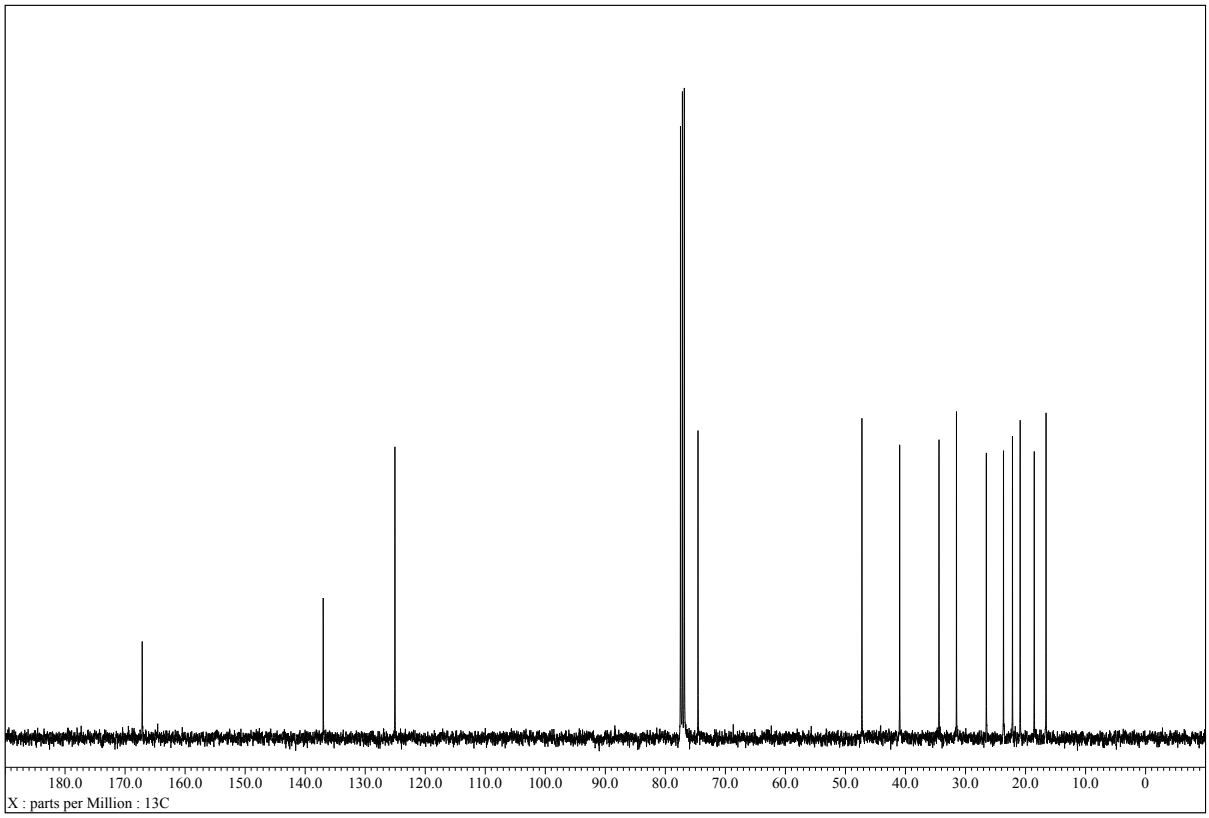
^{1}H and ^{13}C NMR spectra of Isobornyl methacrylate (7b)



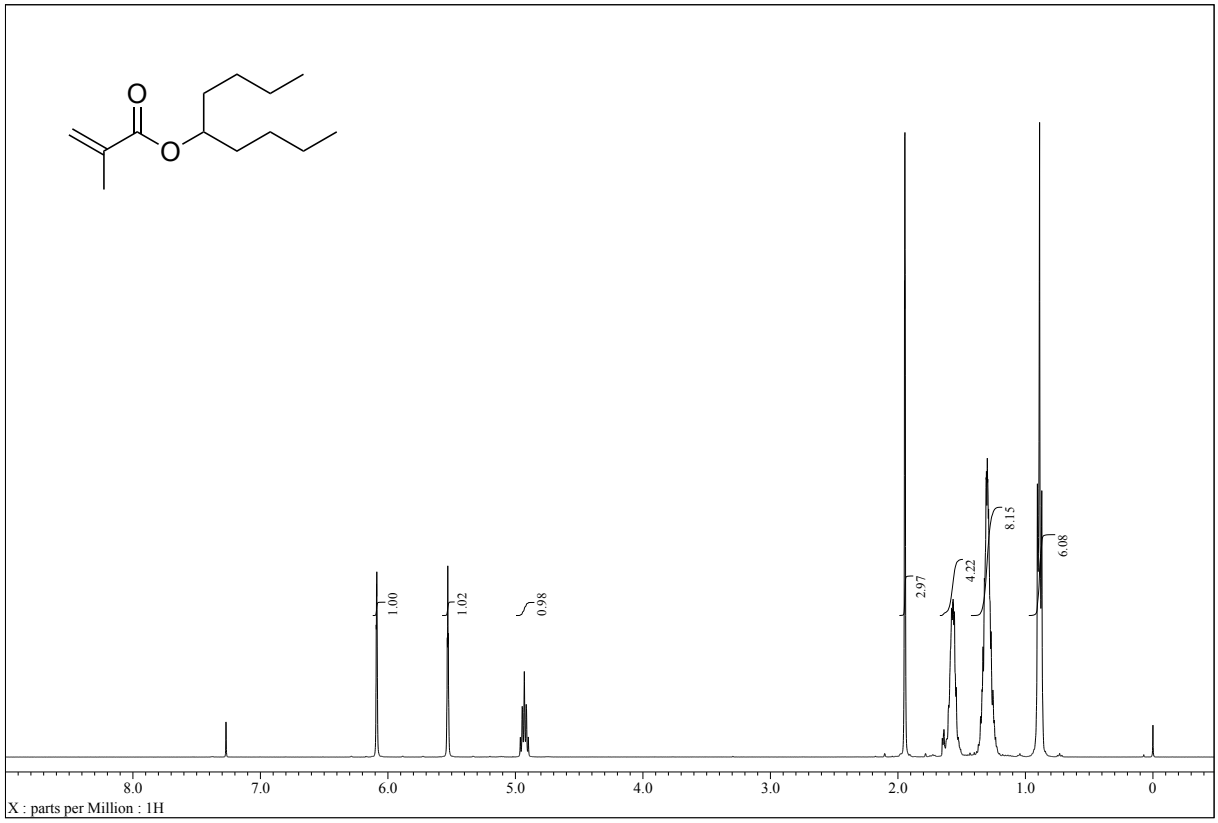


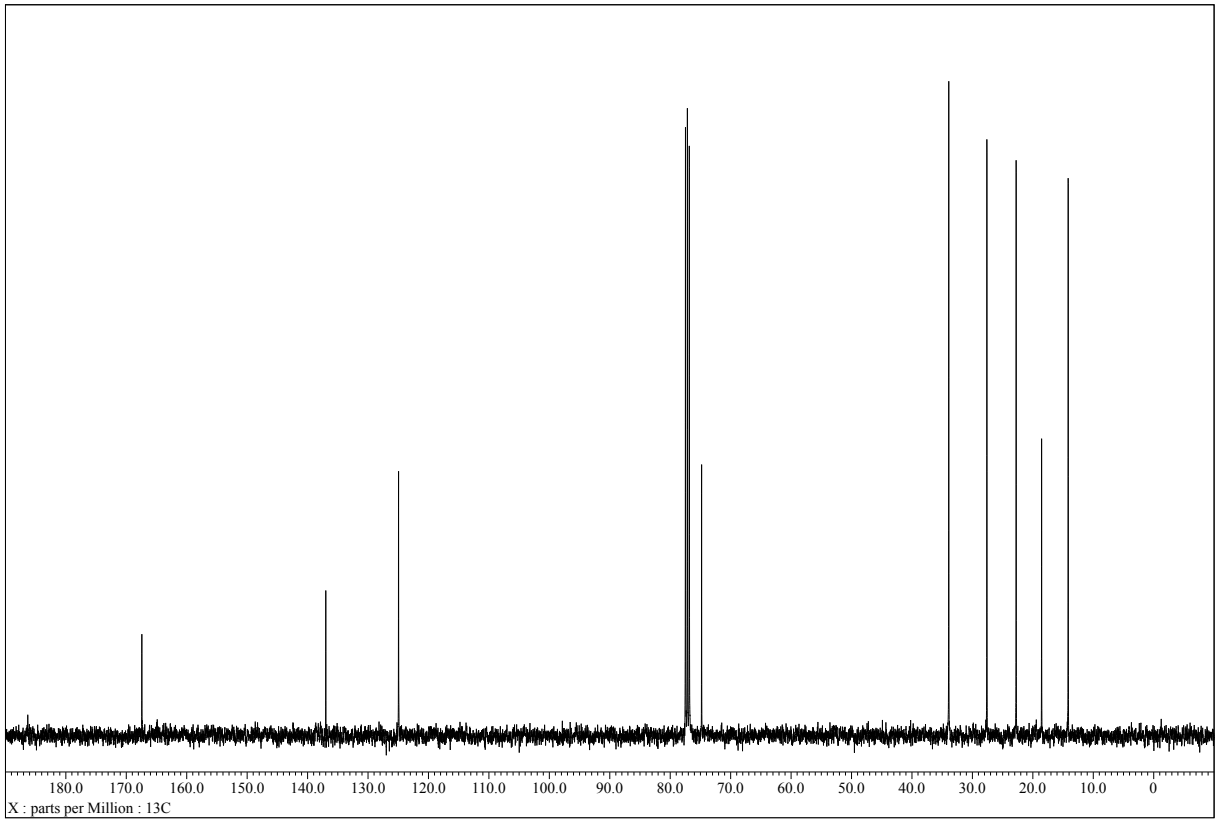
^{1}H and ^{13}C NMR spectra of L-Menthyl methacrylate (7g)



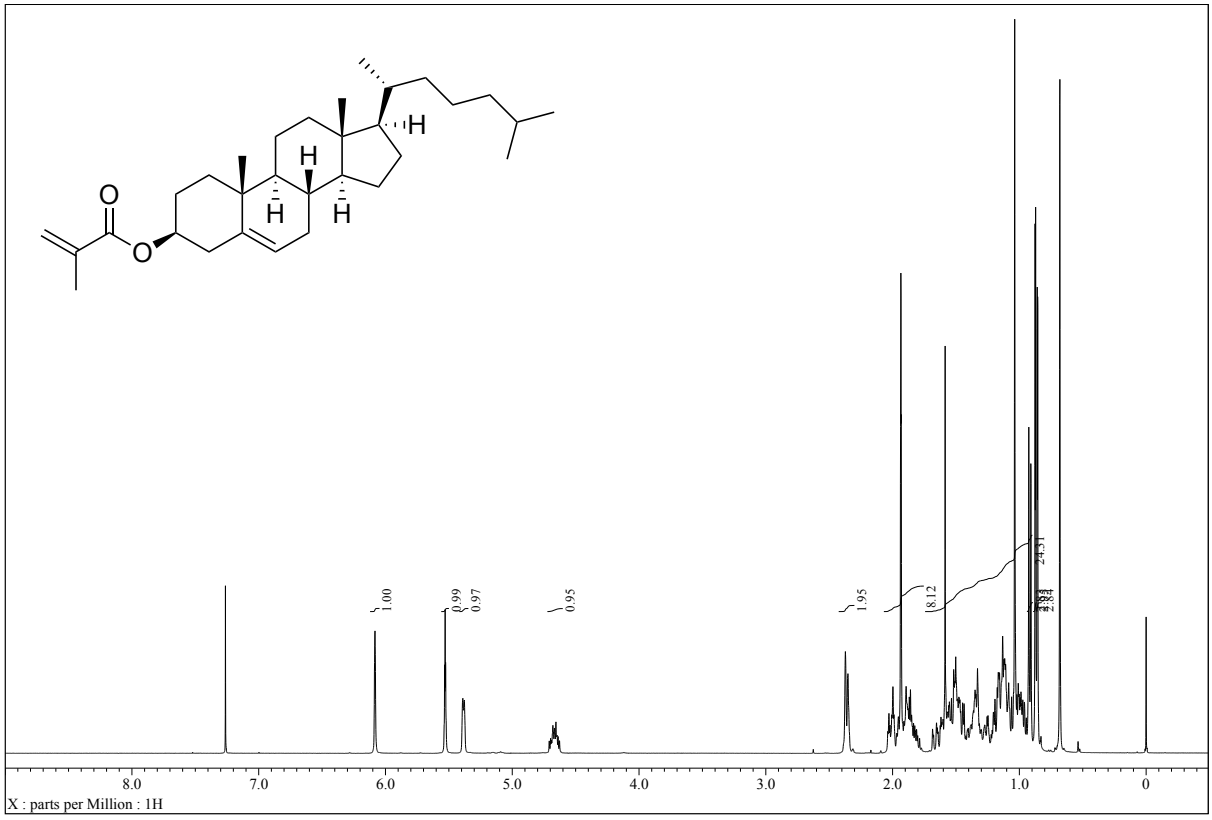


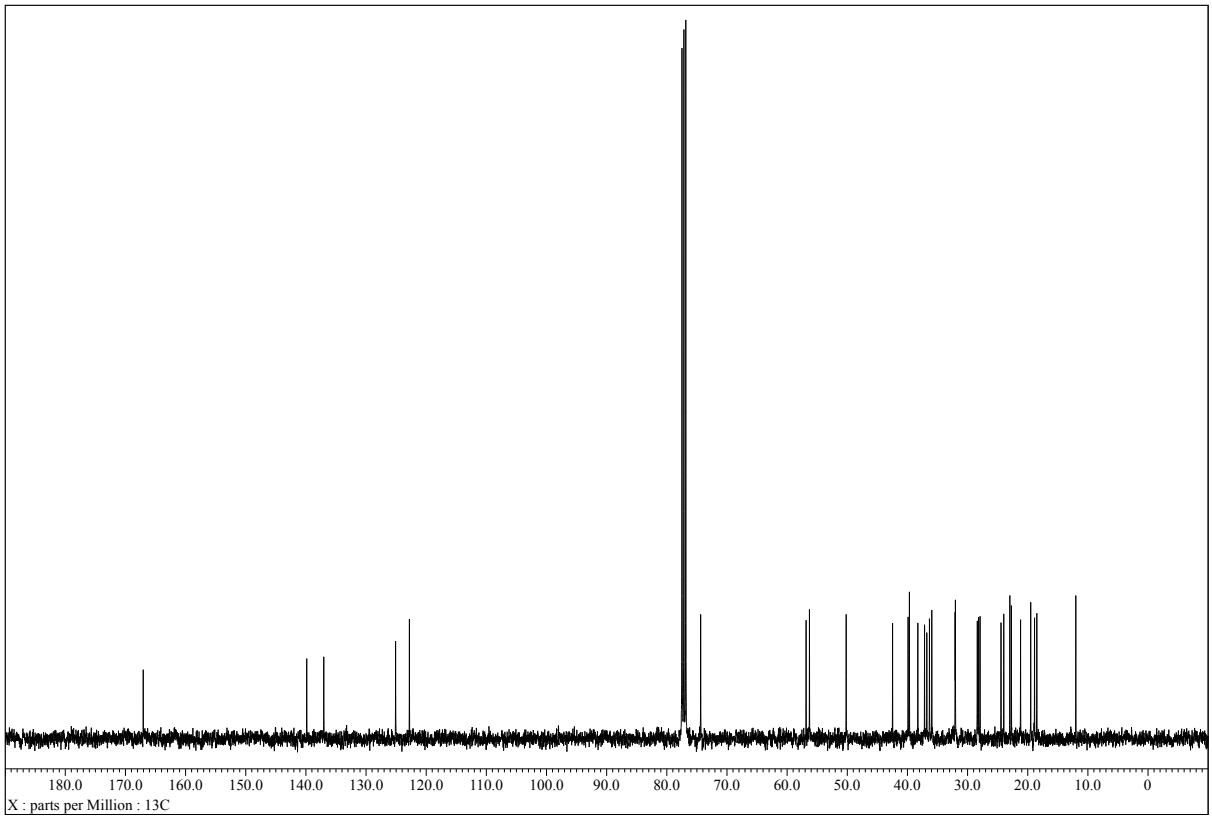
^{1}H and ^{13}C NMR spectra of Nonan-5-yl methacrylate 7h)



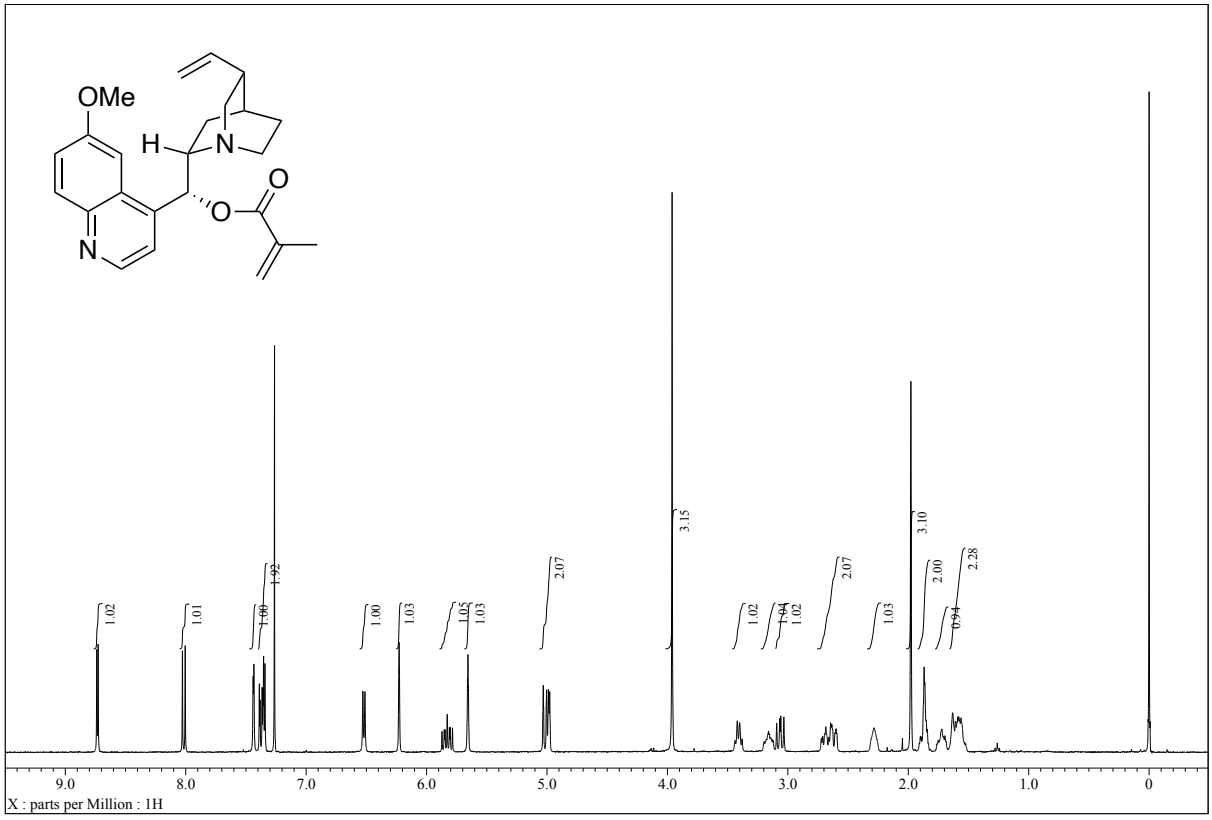


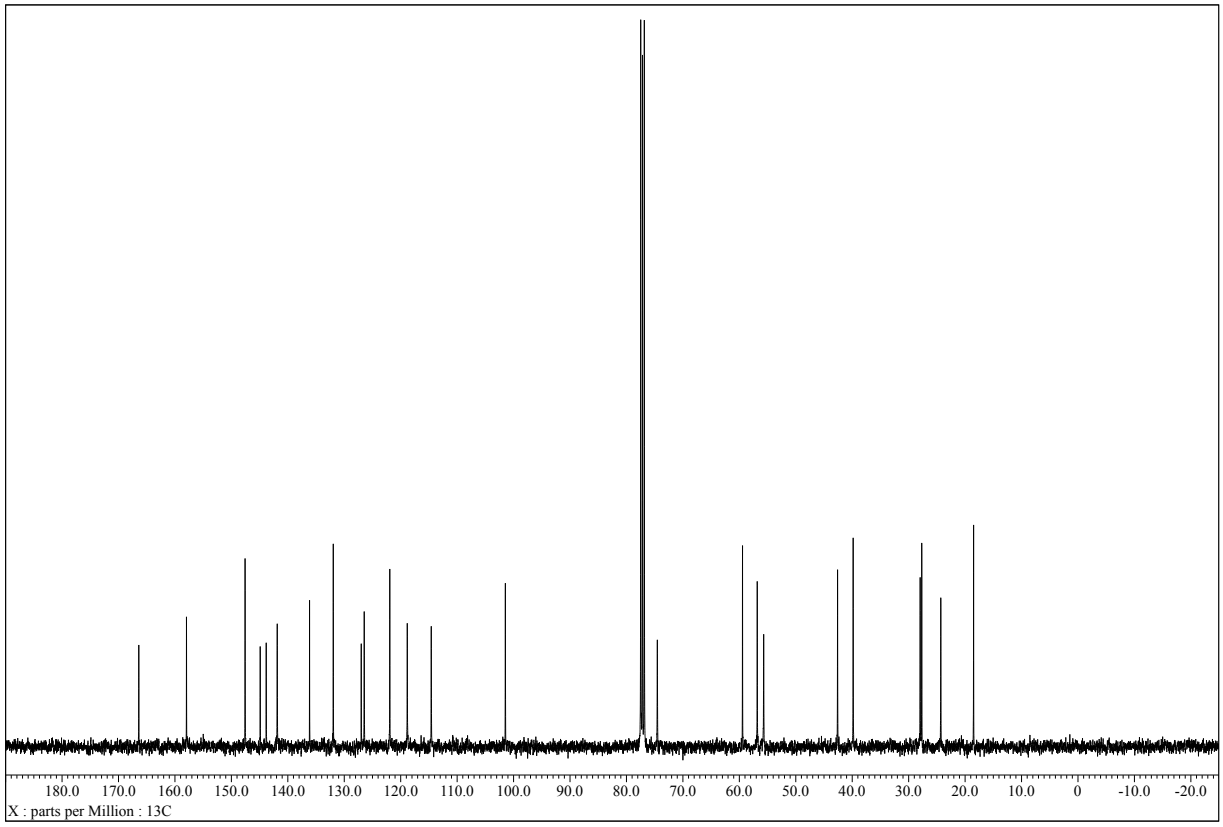
^{1}H and ^{13}C NMR spectra of Cholesteryl methacrylate (7o):



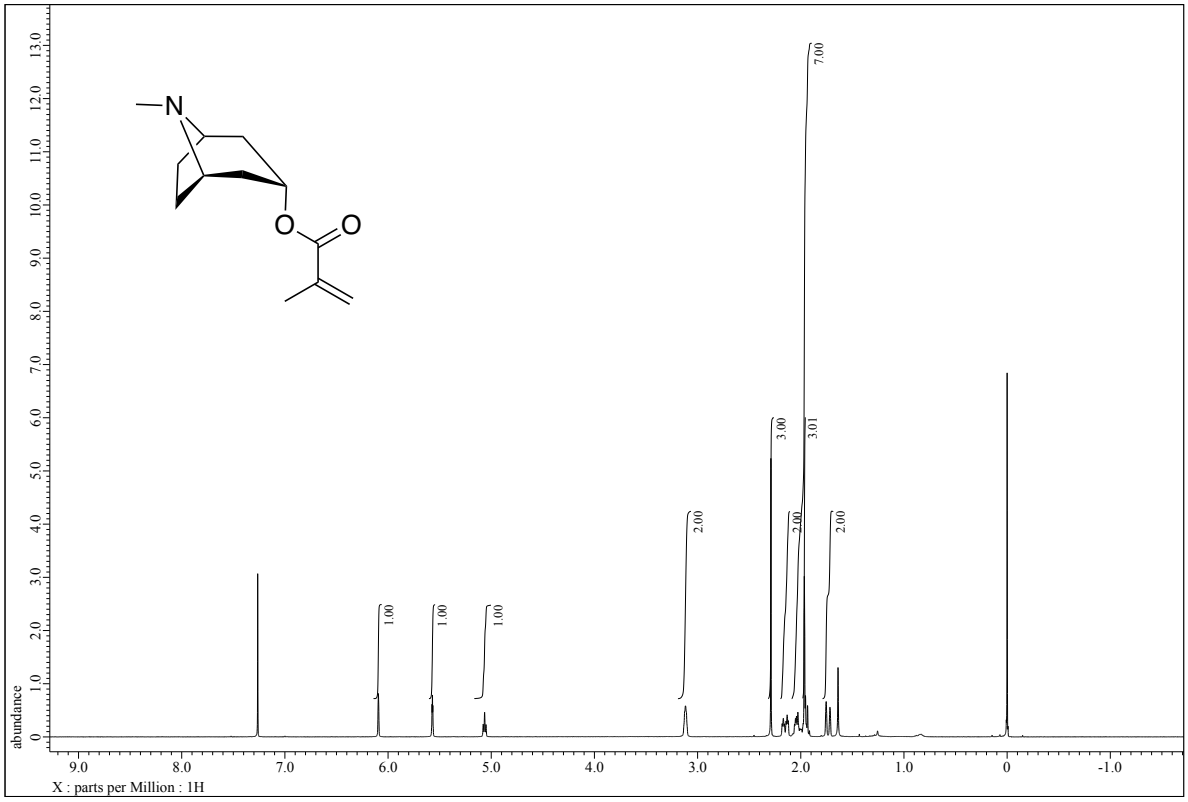


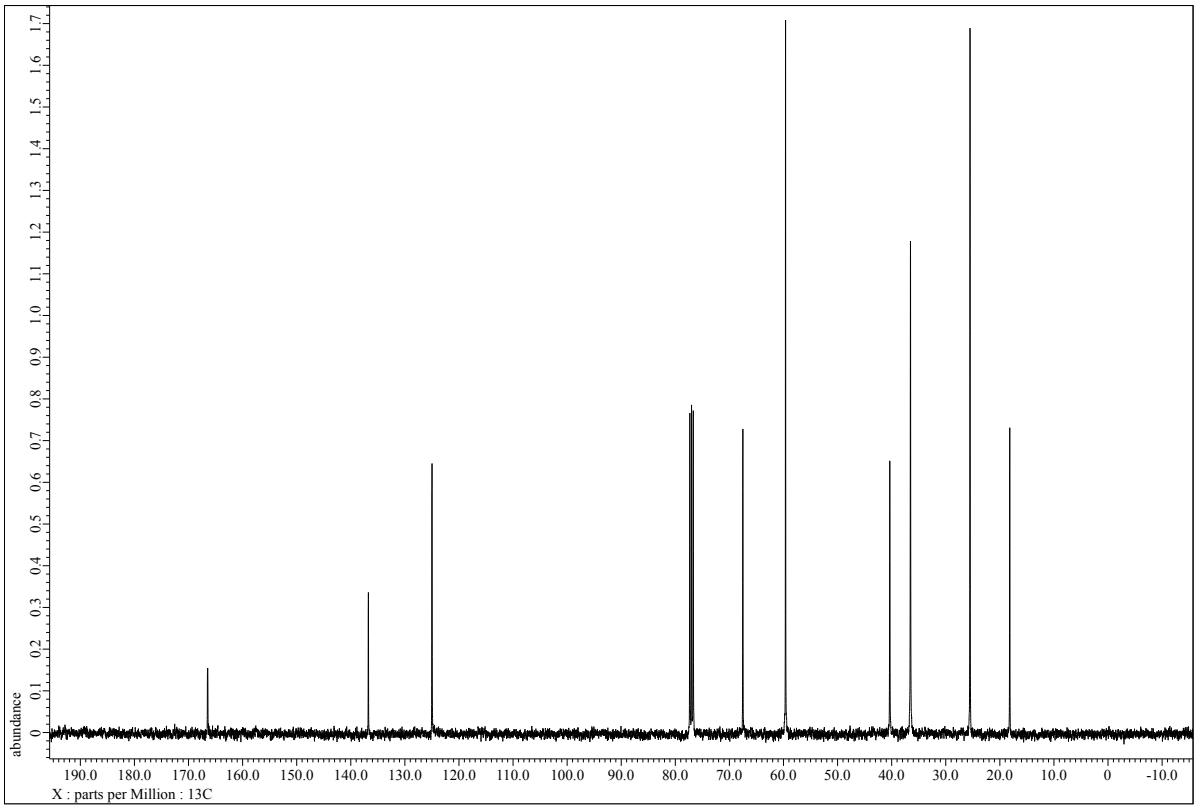
^{1}H and ^{13}C NMR spectra of Quinine methacrylate (7p)



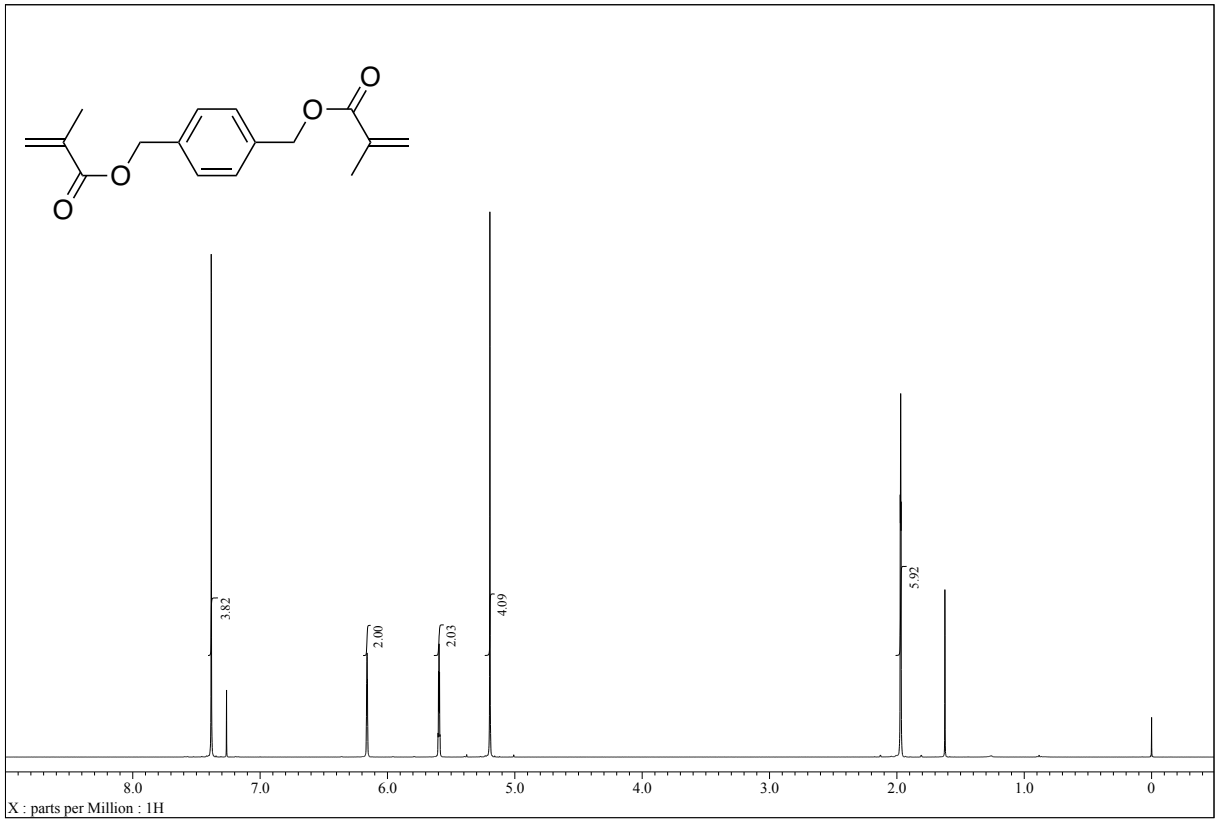


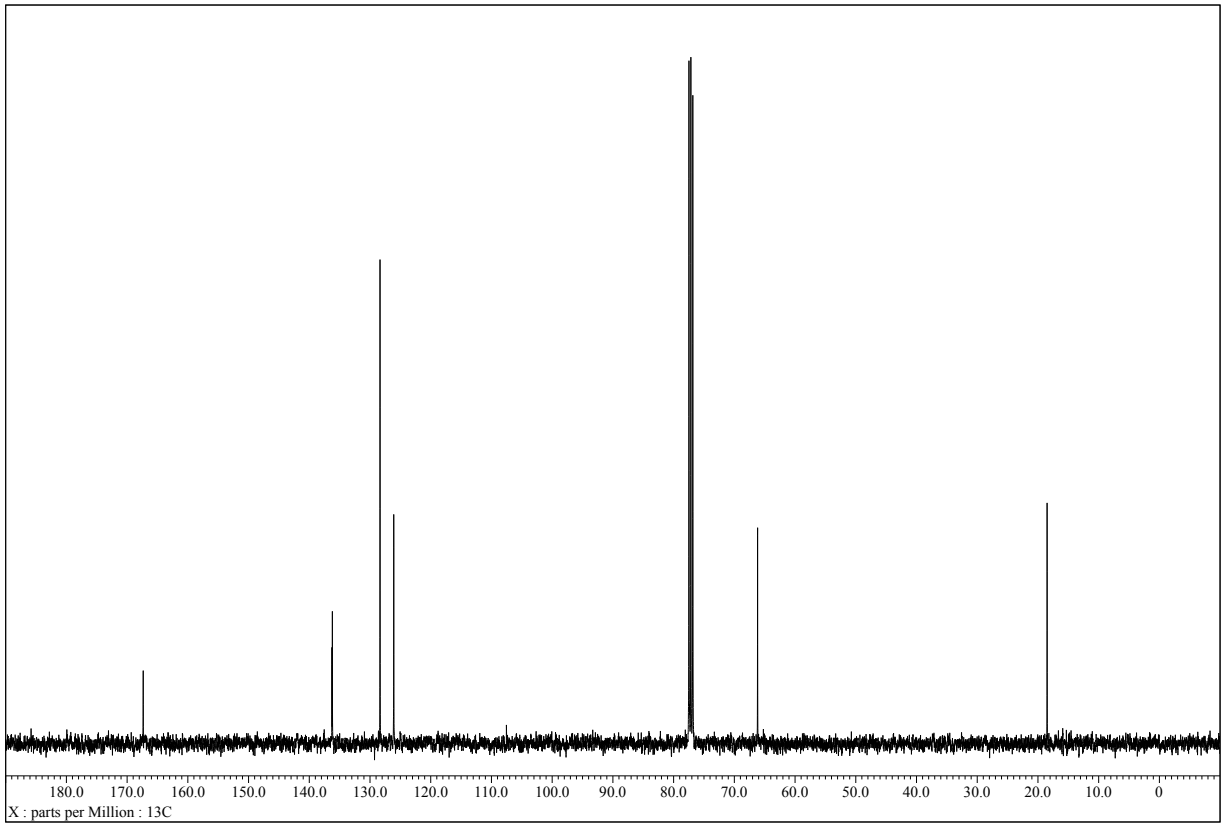
^{1}H and ^{13}C NMR spectra of Tropinyl methacrylate (7q)



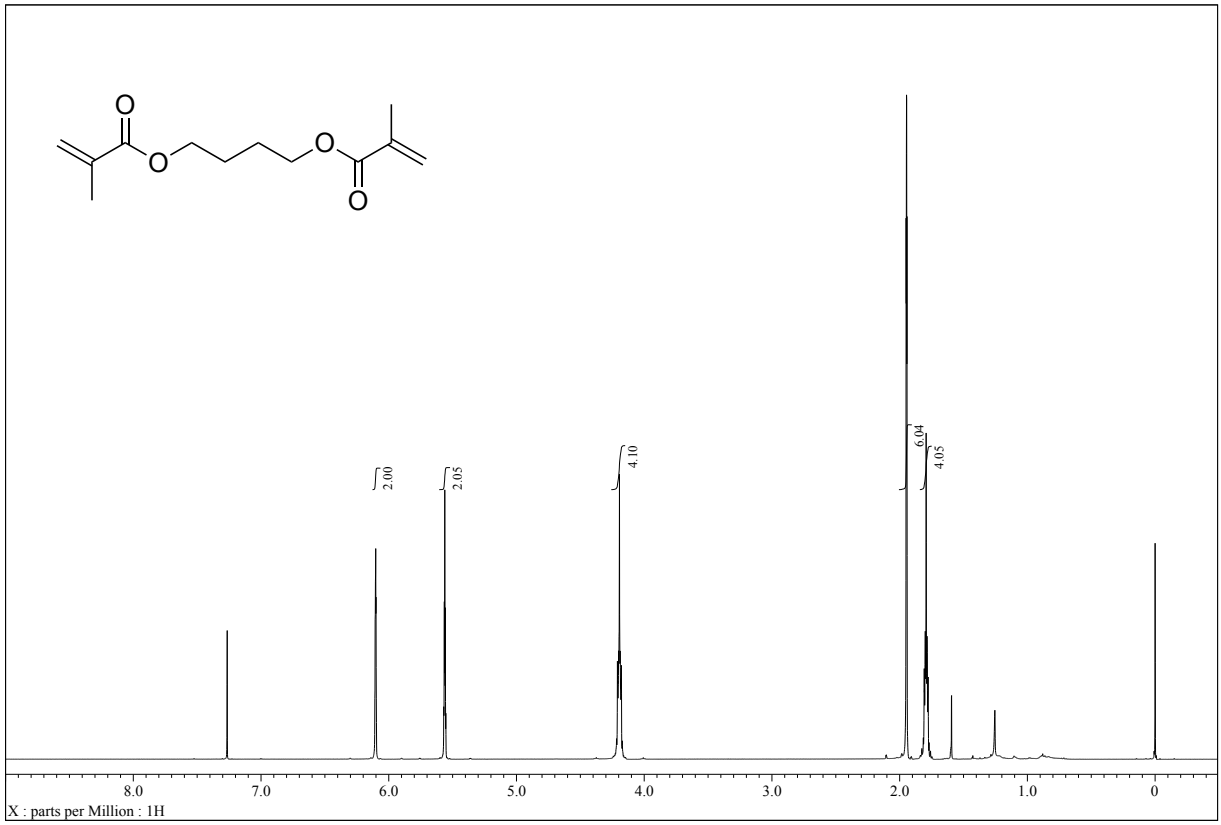


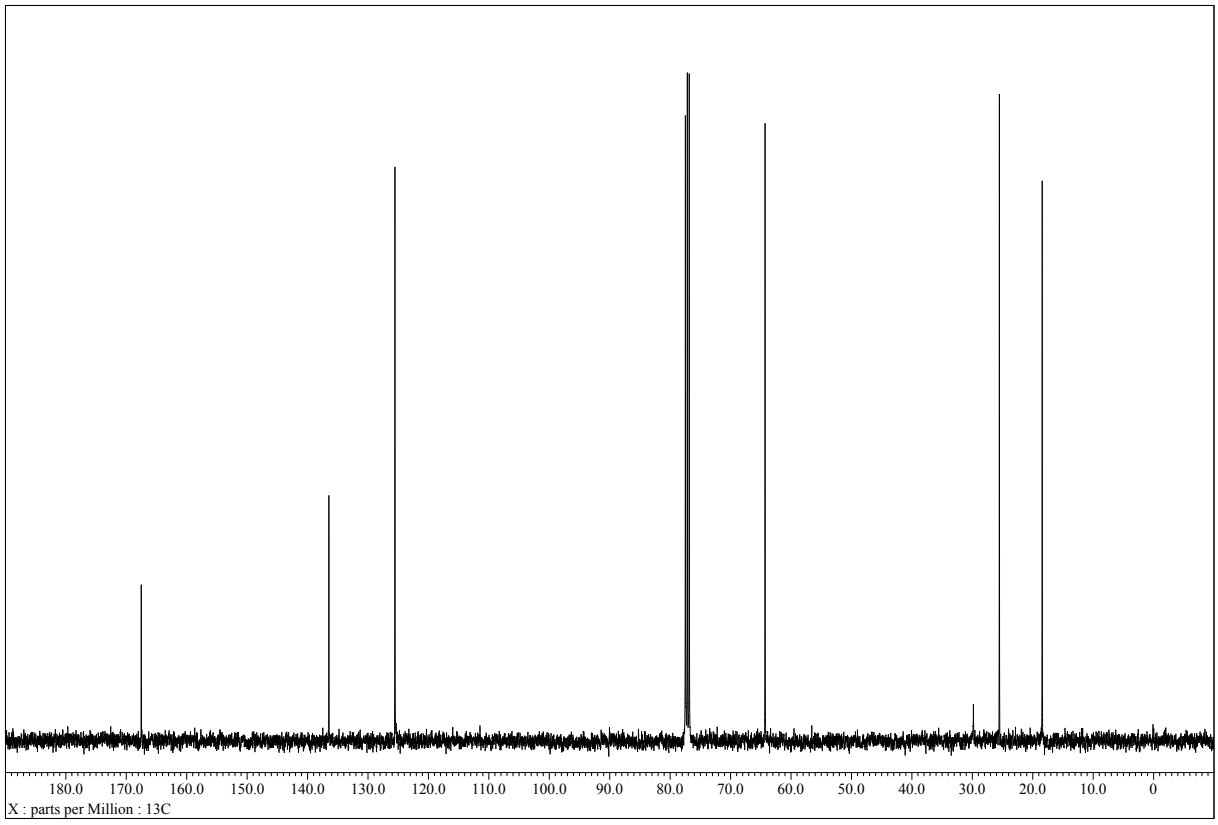
^{1}H and ^{13}C NMR spectra of 1,4-Phenylenebis(methylene) bis(2-methylacrylate) (7r)



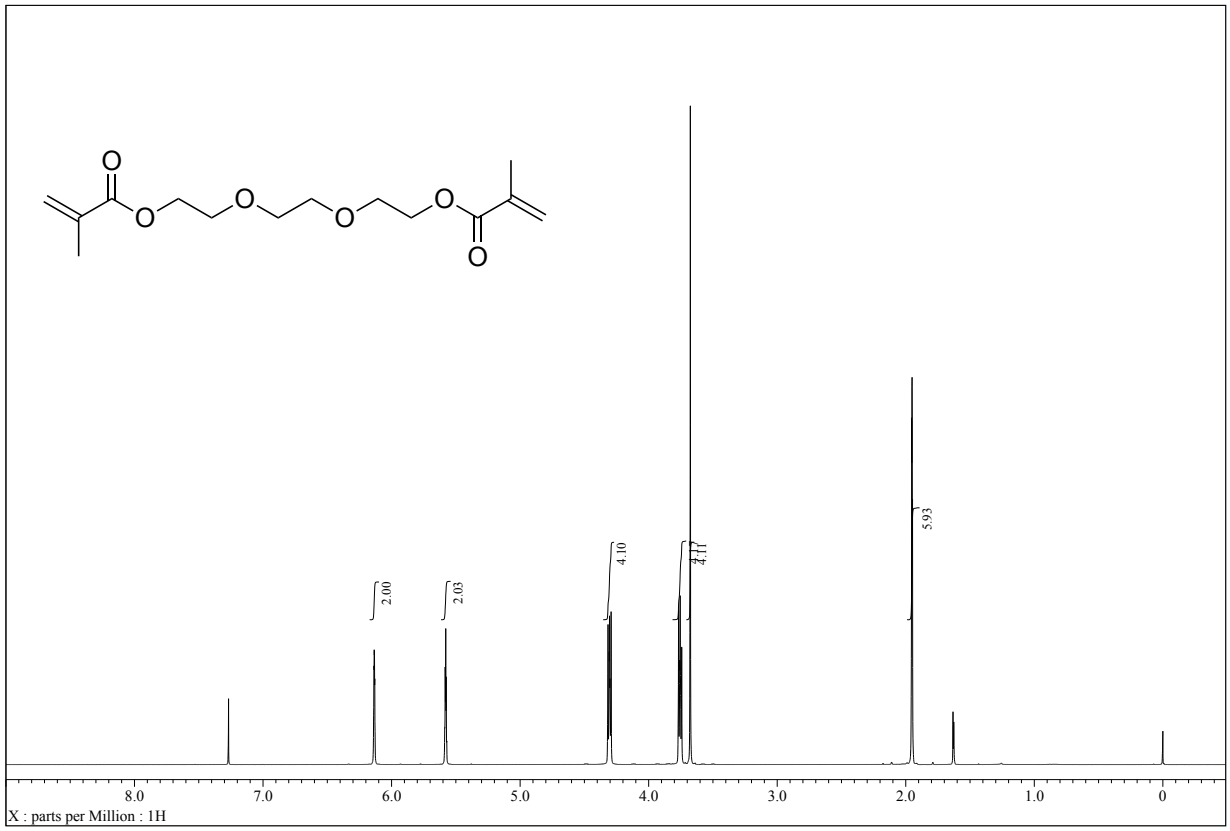


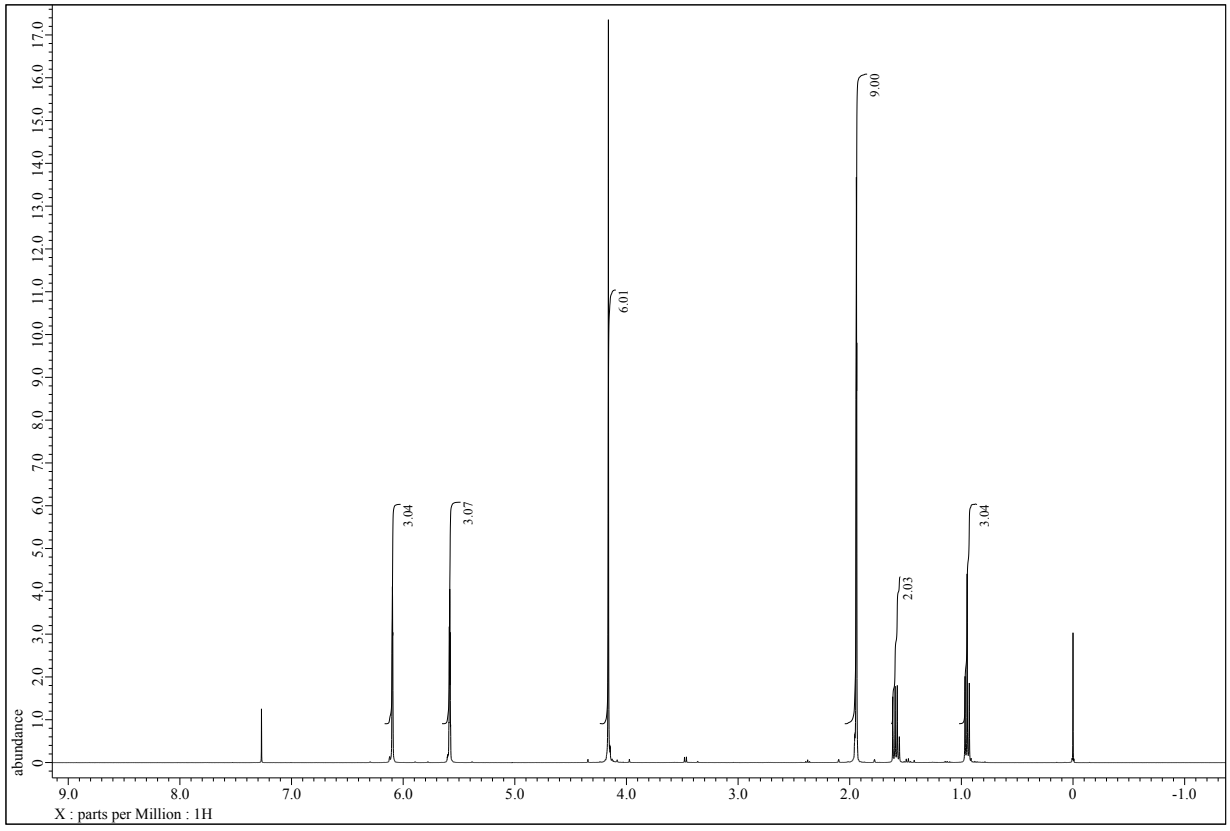
^{1}H and ^{13}C NMR spectra of Butane-1,4-diyl dimethacrylate (7i)





^{1}H and ^{13}C NMR spectra of (Ethane-1,2-diylbis(oxy))bis(ethane-2,1-diyl) dimethacrylate (7k)





^{1}H and ^{13}C NMR spectra of 1,1,1-Trimethylolpropane trimethacrylate (7i)