Supporting Information

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Solvent-free methodologies for organic brominations using quaternary ammonium tribromides

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General Information

All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F_{254} (0.25mm). NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 with tetra methyl silane as the internal standard for ^1H NMR (400 MHz) and $CDCl_3$ or DMSO-d_6 solvents as internal standard for ^{13}C NMR (100 MHz). IR spectra were recorded in KBr or neat. Melting points were recorded on Buchi B-545 melting point apparatus and are uncorrected.

Spectral Data

4-Bromo- aniline (**1a**): M.p. 56-62^oC. ^1H NMR (400 MHz, $CDCl_3$): δ 3.65 (brs, 2H), 6.55 (d, *J* = 8.4 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H). ^{13}CNMR (100 MHz, $CDCl_3$): δ 105.4, 116.9, 132.2, 142.9. IR (KBr): 3485, 3388, 2931, 2872, 1628, 1500, 1477, 1385, 1300, 1192, 1063, 840, 835, 623, 521 cm^{-1}.

4-Bromo- phenol (**2a**): M.p. 64-68^oC. ^1H NMR (400 MHz, $CDCl_3$): δ 5.03 (brs, 1H), 6.72 (d, *J* = 8.8 Hz, 2H), 7.32 (d, *J* = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 112.9, 117.4, 132.6, 154.8. IR (KBr): 3364, 2932, 2855, 1596, 1491, 1443, 1251, 1237, 835, 612, 508 cm^{-1}.

4-Bromo-2-methyl-phenol (**3a**): M.p. 63.5^oC. ^1H NMR (400 MHz, $CDCl_3$): δ 2.21 (s, 3H), 5.01 (brs, 1H), 6.63 (d, *J* = 8.0 Hz, 1H), 7.14 (dd, J_1 = 8.0 Hz, J_2 = 2.4Hz, 1H), 7.22 (d, *J* = 2.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 16.1, 112.7, 116.7, 126.5, 129.9, 133.7, 153.0.

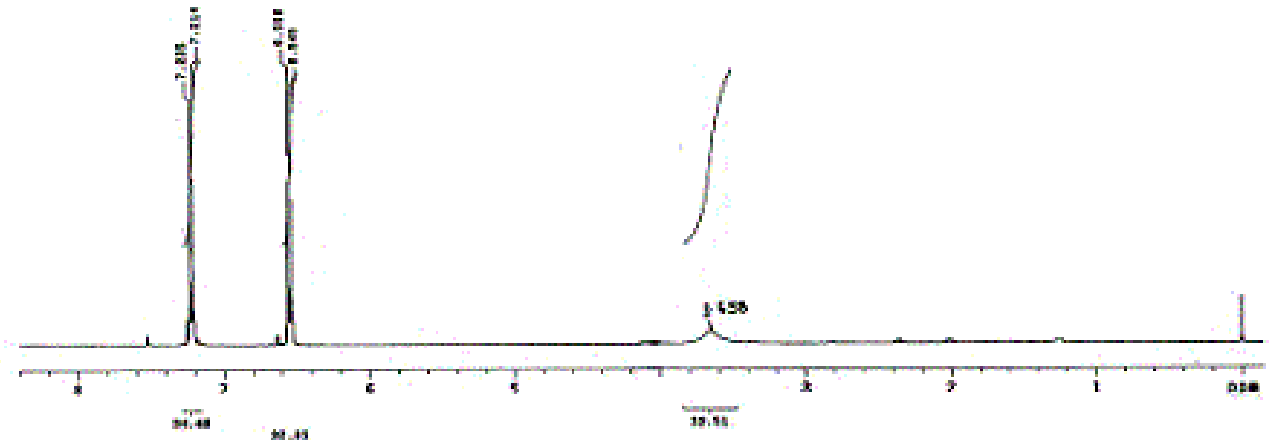
9-Bromoanthracene (**4a**)**:** M.p. 99–101^oC. ^1H NMR (90 MHz, $CDCl_3$): δ 7.46, (t, *J* = 8.2 Hz, 2H), 7.54 (t, *J* = 8.2 Hz, 2H), 7.87 (m, 2H), 8.33 (s, 1H), 8.47 (m, 2H). IR (KBr): 2928, 2855, 1624, 1460, 1380, 1311, 1264, 955, 927, 880, 845, 768, 729, 536 cm^{-1}.

2,4,5-Tribromo-1H-imidazole (**5a**): M.p. 221^oC. ^{13}C NMR (100 MHz, $CDCl_3$): δ 115.6, 139.1. IR (KBr): 3081, 3008, 2921, 2813, 1637, 1537, 1527 1443, 1394, 1300, 1288, 1196 1183, 1004, 980 cm^{-1}. Mass: m/z 304 (M^+).

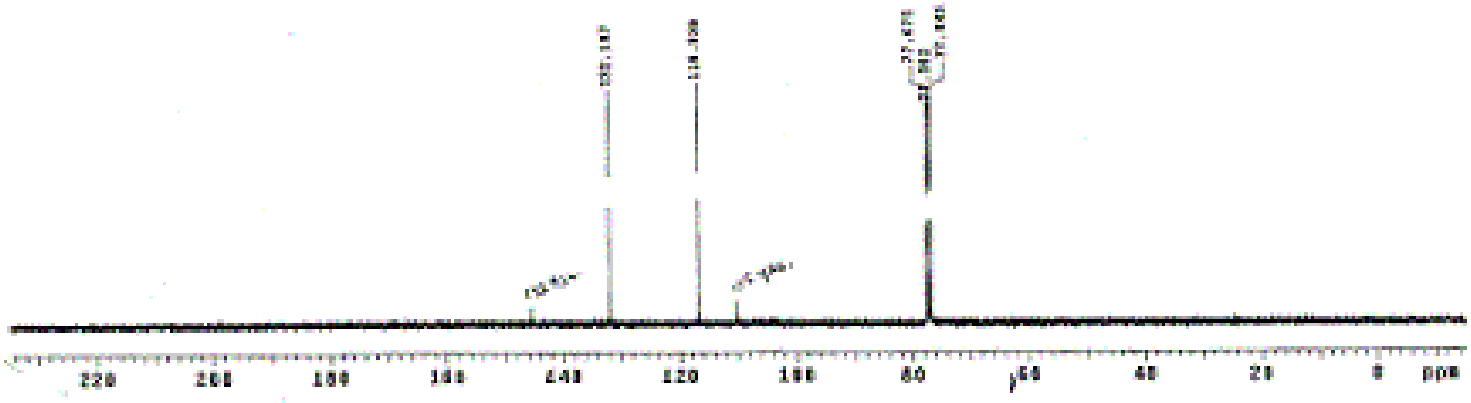
2,3-Dibromo-1,3-diphenyl-propane-1-one (**6a**)**:** M.p. 159-160^oC. ^1H NMR (400 MHz, $CDCl_3$): δ 5.65 (d, *J* = 11.4 Hz, 1H), 5.83 (d, *J* = 11.4 Hz, 1H), 7.39 (m, 3H), 7.53 (m, 4H), 7.66 (m, 1H), 8.10 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 47.2, 50.2, 128.5, 128.7, 129.0, 129.1, 129.2, 129.5, 134.4, 134.6, 138.4, 191.2. IR (KBr): 3068, 3027, 1690, 1593, 1450, 1271, 1235, 984, 805, 779, 723, 692, 579, 564 cm^{-1}.

2-Bromo-1-naphthol (**7a**)**:** ^1H NMR (400 MHz, $CDCl_3$): δ 5.96 (m, 1H), 7.60 (m, 3H), 7.79 (m, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 8.25 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 103.4, 113.5, 122.9, 125.3, 127.1, 127.3, 128.3, 131.2, 132.0, 148.3.

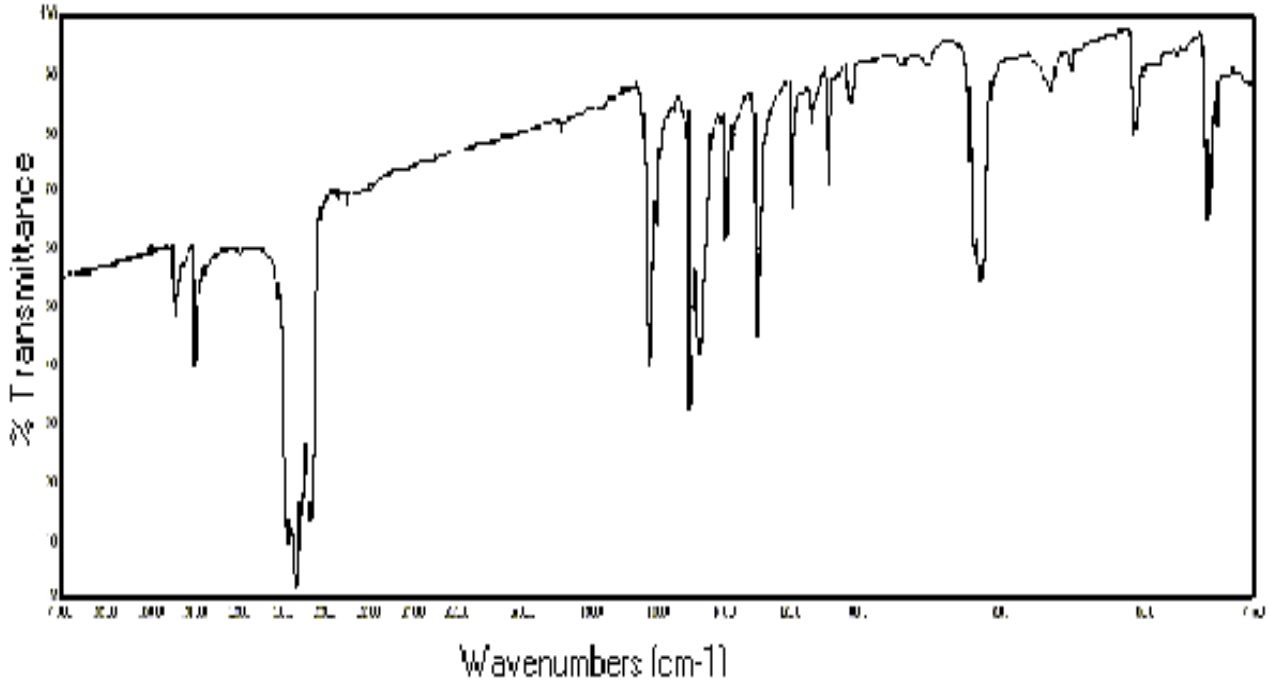
4-Bromo-aniline (1a): ^{1}H NMR($CDCl_3$)



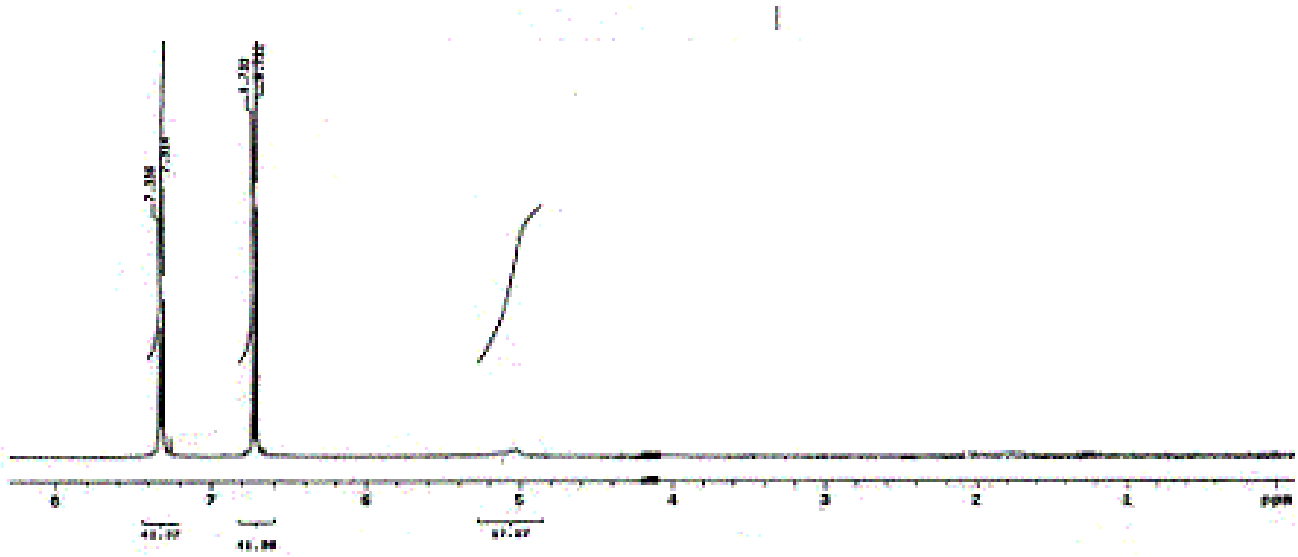
4-Bromo-aniline (1a): ^{13}C NMR($CDCl_3$)



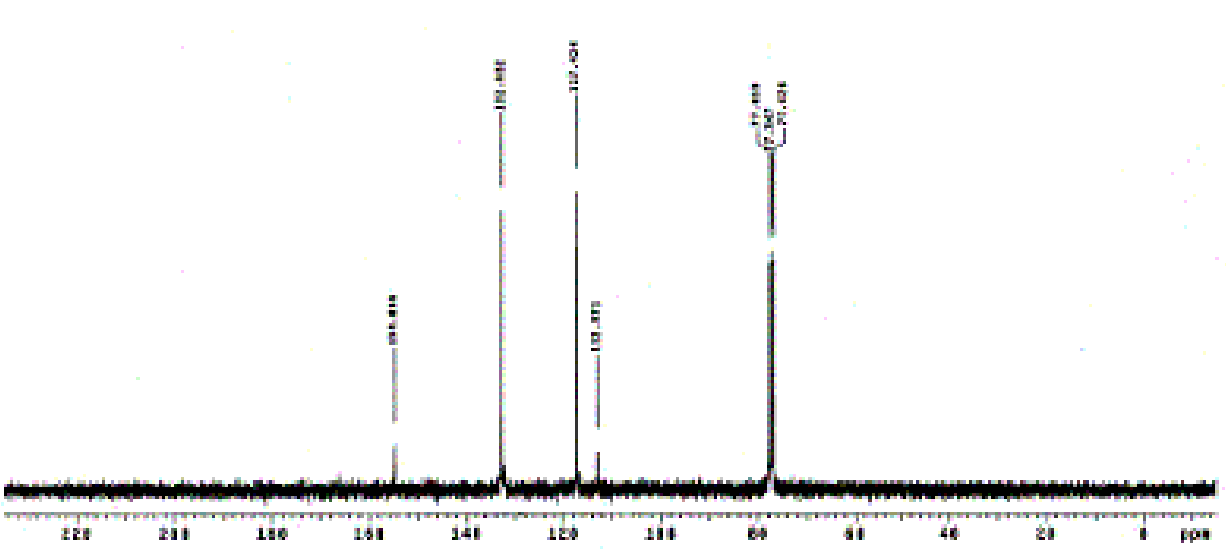
4-Bromoaniline (1a): IR (KBr)



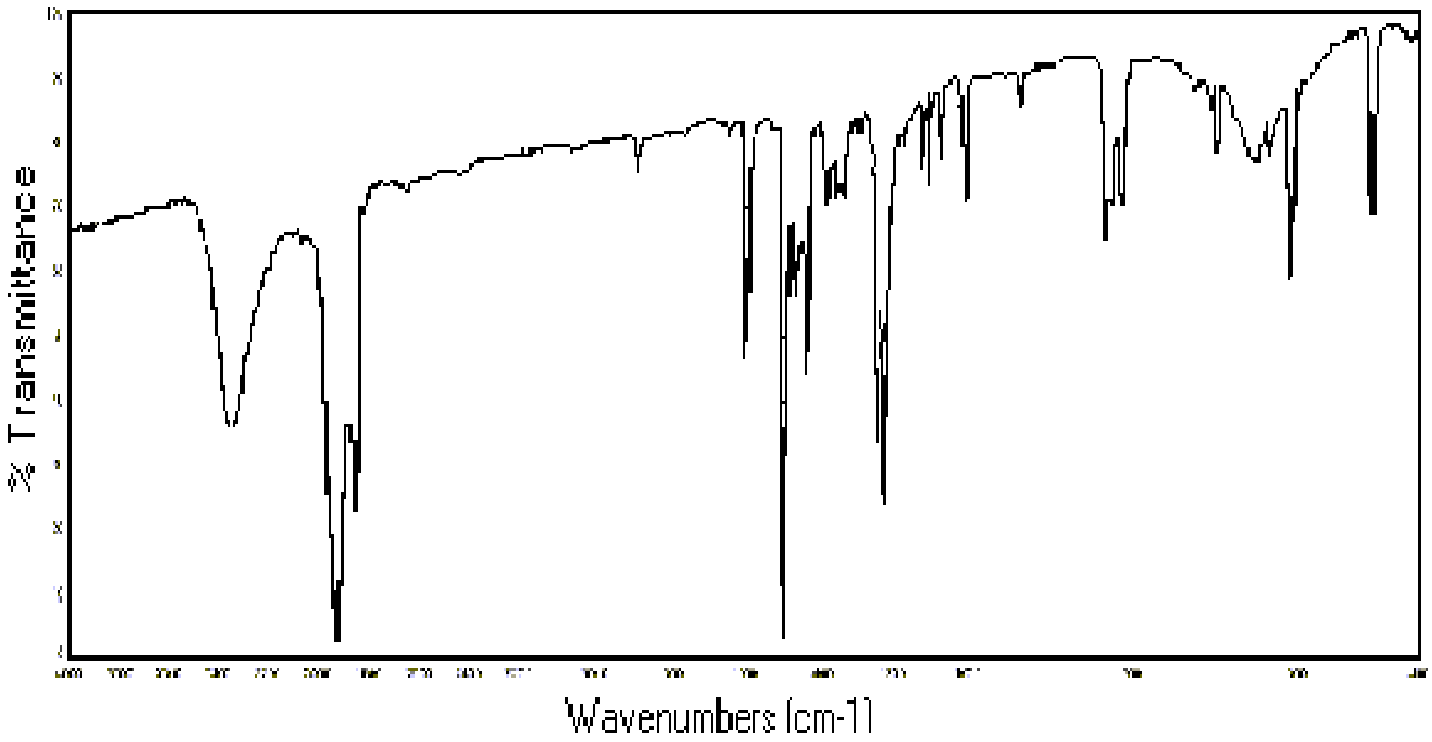
4-Bromo-phenol (2a): ^{1}H NMR($CDCl_3$)



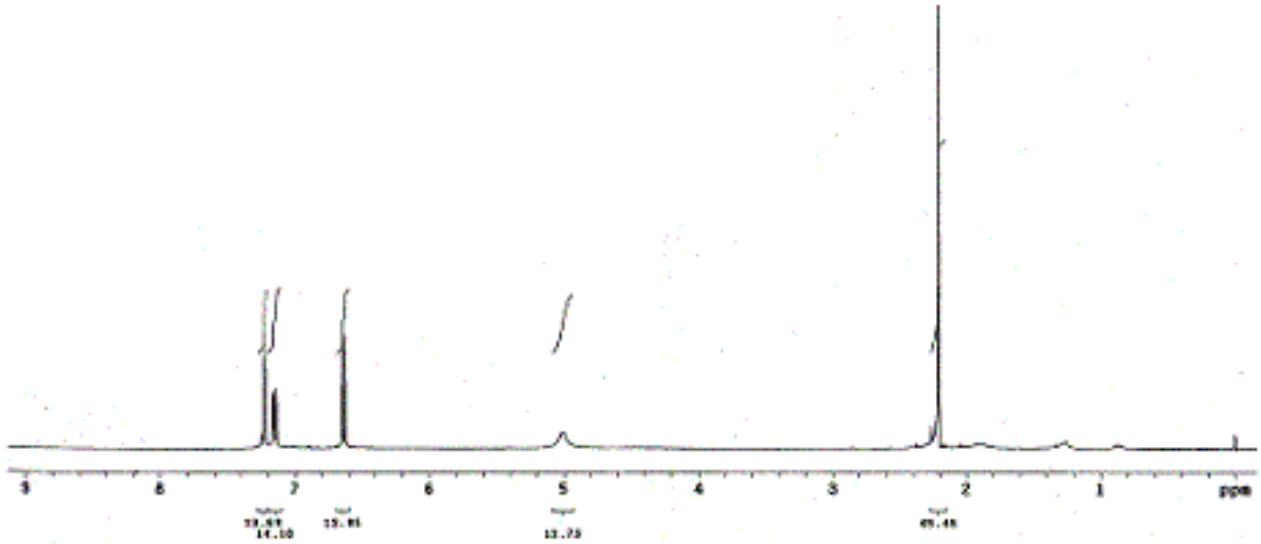
4-Bromo-phenol (2a): ^{13}C NMR($CDCl_3$)



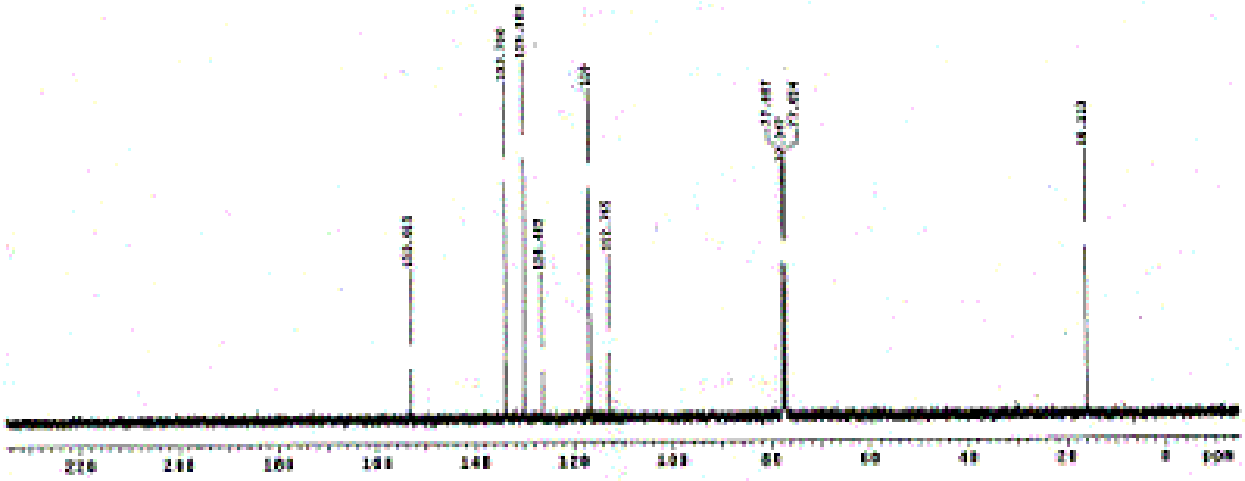
4-Bromophenol (2a): IR (KBr)



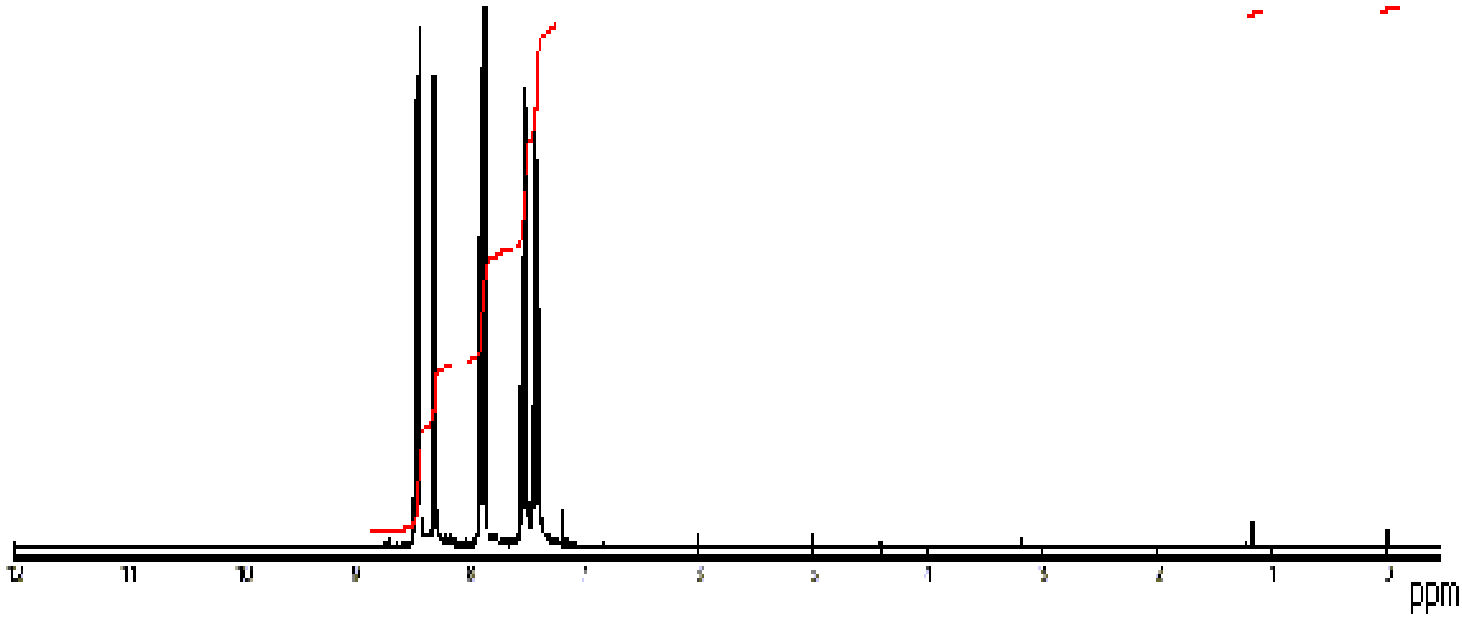
4-Bromo-2-methyl-phenol (3a): ^{1}H NMR ($CDCl_3$)



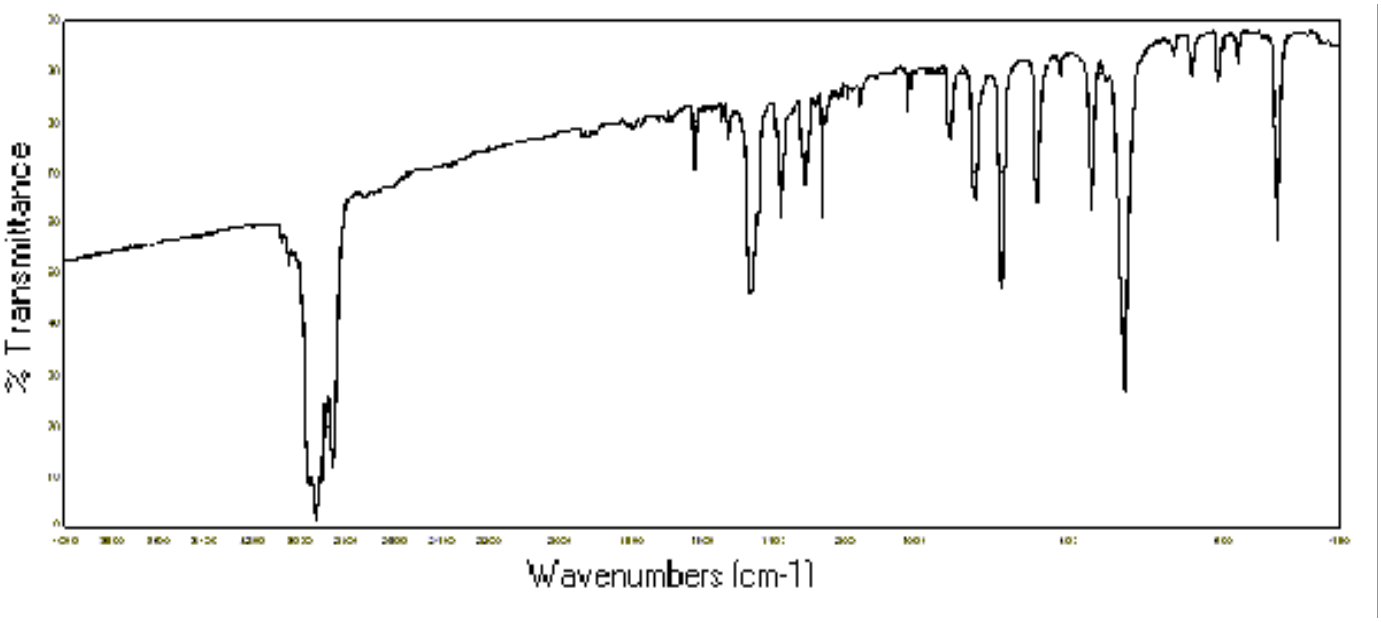
4-Bromo-2-methyl-phenol (3a): ^{13}C NMR ($CDCl_3$)



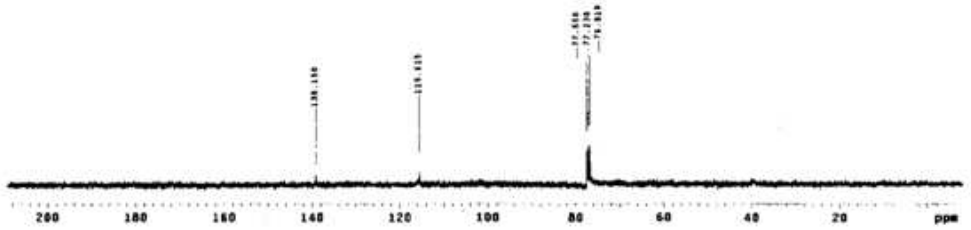
9-Bromoanthracene (4a): ^{1}H NMR ($CDCl_3$)



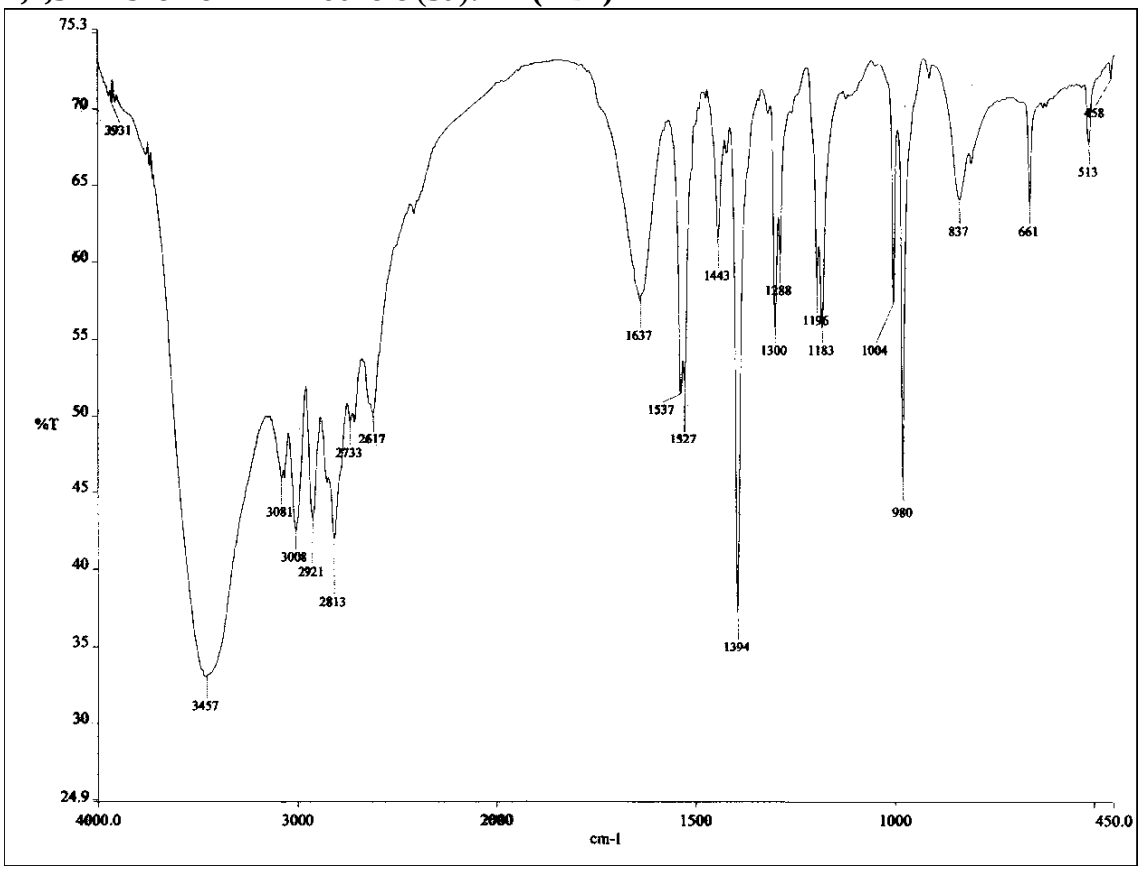
9-Bromoanthracene (4a): IR (KBr)



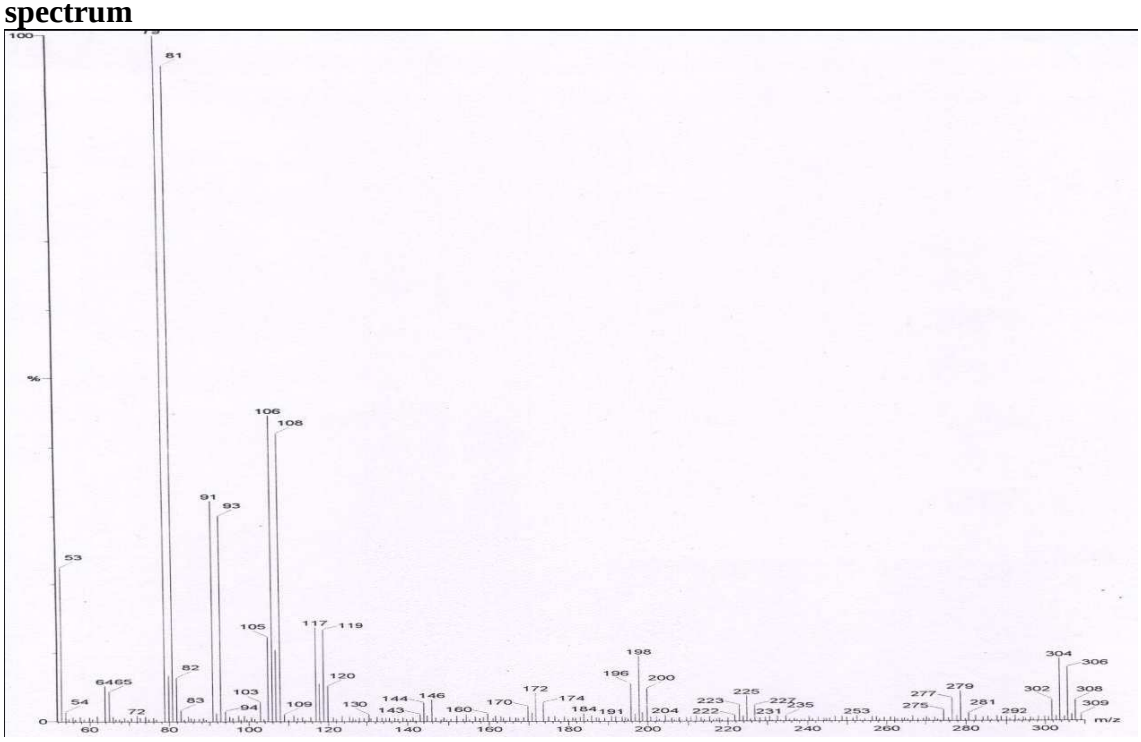
2,4,5-Tribromo-1H-imidazole (5a): ^{13}C NMR ($CDCl_3$)



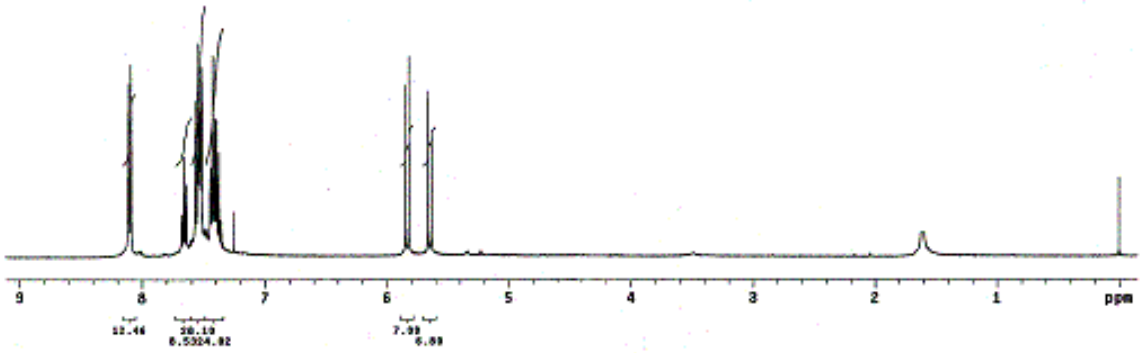
2,4,5-Tribromo-1H-imidazole (5a): IR (KBr)



2,4,5-Tribromo-1H-imidazole (5a): Masss spectrum

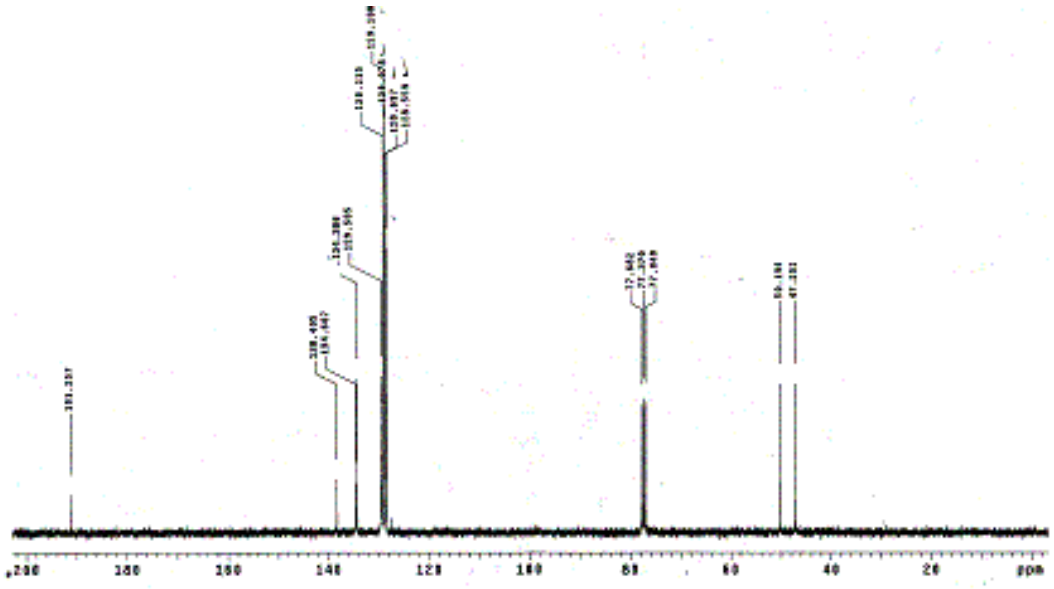


2,3-Dibromo-1,3-diphenyl-propane-1-one (6a): ^{1}H NMR ($CDCl_3$)

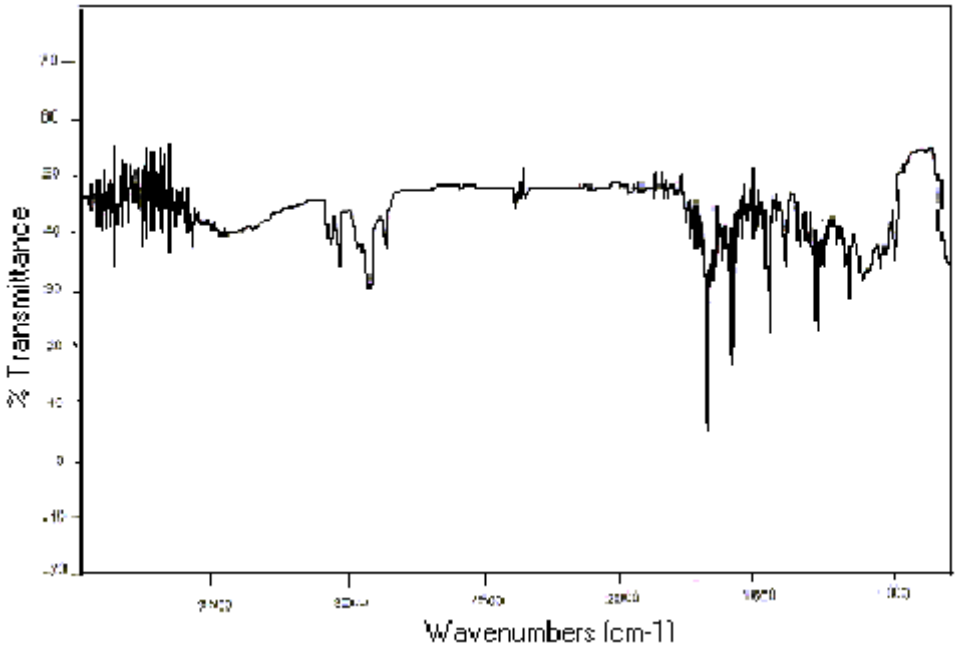


2,3-

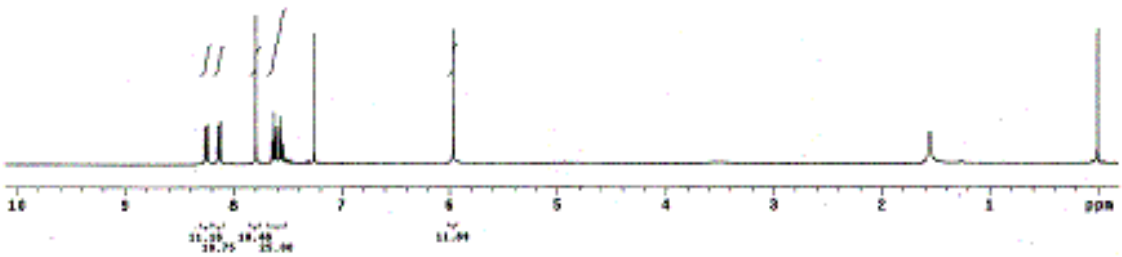
Dibromo-1,3-diphenyl-propane-1-one (6a): ^{13}C NMR($CDCl_3$)



2,3-Dibromo-1,3-diphenyl-propane-1-one (6a): IR (KBr)



2-Bromo-1-naphthol (7a): ^{1}H NMR ($CDCl_3$)



2-Bromo-1-naphthol (7a): ^{13}C NMR ($CDCl_3$)