SUPPORTING INFORMATION

Rapid and total bromination of aromatic compounds using TsNBr_2 without any catalyst

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2, 4, 6-Tribromophenol ^[1]:

IR (KBr, cm^{-1}) ν : 3058, 2989, 2302, 1422, 1265, 896, 748; ^1H NMR (CDCl_3 , 400 MHz) δ : 7.52 (s, 2H), 5.85 (s, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : 148.9, 134.2, 112.7, 110.4.

2-Amino-4, 6-dibromophenol ^[2]:

IR (KBr, cm^{-1}) ν : 3440, 1611, 1526, 1471, 1411, 1315, 1238, 1161, 1072, 884, 835, 812, 763; ^1H NMR (CDCl_3 , 300 MHz) δ : 6.99 (s, 1H), 6.83 (s, 1H), 5.17 (br, 3H); ^{13}C NMR (CDCl_3 , 75 MHz) δ : 145.5, 133.2, 124.7, 116.4, 108.5, 108.4; GCMS (M/Z %): 269 ($\text{M}^+ + 2$, 10), 267 (M^+ , 20), 265 (10), 78 (17), 51 (8), 38 (8), 28 (11), 18 (100).

2, 6-Dibromo-4-fluorophenol ^[3]:

^1H NMR (CDCl_3 , 400 MHz) δ : 7.23 (d, $J = 7.2$ Hz, 2H), 5.74 (s, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : 156.9, 154.4, 146.4, 119.3, 119.0, 109.3.

2, 4, 6-tribromobenzene-1, 3-diol ^[4]:

IR (KBr, cm^{-1}) ν : 3499, 3018, 1216, 771, 669; ^1H NMR (CDCl_3 , 400 MHz) δ : 7.53 (s, 1H), 5.86 (s, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : 149.8, 133.0, 100.4, 98.3.

2, 6-Dibromo-4-nitrophenol^[5]:

IR (KBr, cm^{-1}) v: 3381, 3087, 1573, 1501, 1324, 1228, 1123, 898, 740, 689;
¹HNMR (CDCl_3 , 400 MHz) δ : 8.41 (s, 2H), 6.60 (br, 1H); ¹³CNMR (CDCl_3 , 100 MHz) δ : 155.0, 141.5, 127.9, 115.7; GCMS (M/Z %): 299 ($\text{M}^+ + 2$, 21), 297 (M^+ 44), 295 (23), 267 (38), 251 (6), 223 (13), 185 (17), 170 (32), 141 (18), 90 (53), 62 (100), 53 (55), 30 (40), 18 (56).

1, 3-Dibromo-2-naphthol^[2]:

IR (KBr, cm^{-1}) v: 3283, 1600, 1499, 1432, 1347, 1301, 983, 928, 744, 80;
¹HNMR (CDCl_3 , 400 MHz) δ : 8.05 (d, 1H, J = 8.8 Hz), 7.79 - 7.73 (m, 1H), 7.60 - 7.56 (m, 1H), 7.42 - 7.39 (m, 1H), 7.28 (d, 1H, J = 9.2 Hz), 5.96 (s, 1H), ¹³CNMR (CDCl_3 , 100 MHz) δ : 150.6, 132.3, 129.7, 129.3, 128.2, 127.9, 125.3, 124.2, 117.2, 106.2.

2, 4-Dibromo-6-methoxyphenol^[1]:

IR (KBr, cm^{-1}) v: 3529, 3018, 1601, 1493, 1217, 1038, 770, 670; ¹HNMR (CDCl_3 , 400 MHz) δ : 6.96 (s, 1H), 6.80 (s, 1H), 5.58 (s, 1H), 3.86 (s, 3H); GCMS (M/Z %): 284 ($\text{M}^+ + 2$, 46), 282 (M^+ 100), 267 (93), 267 (93), 239 (56), 157 (13), 131 (18), 79 (45), 50 (73), 29 (13).

2, 4, 6-tribromoanisole^[6]:

¹HNMR (CDCl_3 , 300 MHz) δ 3.81 (s, 3H), 6.68-6.75 (m, 1H), 7.29-7.34 (m, 1H); ¹³CNMR (CDCl_3 , 75 MHz) δ : 154.9, 135.1, 115.4, 112.8, 56.1.

2, 4, 6-Tribromoaniline^[5]:

IR (KBr, cm^{-1}) v: 3401, 3450, 1615, 1376, 704; ¹HNMR (CDCl_3 , 400 MHz) δ 7.50 (s, 2H), 4.56 (s, 2H) GCMS (M/Z %) 329 (M, 100), 250 (35), 170 (40), 65 (8).

2, 6-Dibromo-4-nitroaniline^[5]:

IR (KBr, cm^{-1}) v: 3477, 3385, 2928, 2350, 1577, 1453, 1260, 664; ¹HNMR (DMSO, 300 MHz) δ 8.25 (s, 2H), 6.80 (s, 2H) ¹³CNMR (DMSO, 75 MHz) δ : 149.3, 136.46, 128.1, 105.4; GCMS (M/Z %) 294 (M^+ , 5), 136 (3), 89 (45), 73 (48).

2, 6-Dibromo-4-methylaniline^[7]:

IR (KBr, cm^{-1}) v: 3421, 3470, 1618, 1285, 705 ¹HNMR (CDCl_3 , 400 MHz) δ 2.2 (s, 3H), 4.3 (s, 2H), 7.2 (s, 2H) GCMS (M/Z %) 267 ($\text{M}^+ + 4$, 47), 265 ($\text{M}^+ + 2$, 95), 263 (M^+ , 54), 184 (90), 105 (45), 89 (5), 65 (12).

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2014-03-07B.001.001.1R.3

20100622-13-phpr.001.001.1f.esp

2, 4, 6-tribromobenzene-1, 3-diol

Mass analysis
ISH3 340 (1.699)

, 30-DEC-2008 + 12:32:04

Scan El+
3.55e6

2-Amino-4,6-dibromophenol

2, 6-Dibromo-4-nitrophenol

Mass analysis
ISH7 590 (2.950)

, 22-DEC-2008 + 13:46:04
Scan EI+
3.29e6

2, 6-Dibromo-4-nitrophenol

2, 4-Dibromo-6-methoxyphenol

1, 3-Dibromo-2-naphthol

88.088.001.1r.esp

PC-150 • 28-Nov-2006 + 11:33:47
1 Scan E1+
3 3668

28-Nov-2006 + 11:33:47
1 Scan E1+
TIC
4.9761

2, 6-Dibromo-4-methylaniline

PC 159

IP-4NO₂/NH₂

8.251

6.800

3.430

2, 6-Dibromo-4-nitroaniline

[P-4NO2/NH2

NAME 2014-08-06b
EXPNO 1
PROCNO 1
Date 20140806
Time 14.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1200
DS 2
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 -0.50 dB
PL1W 34.66611099 W
SFO1 75.4778101 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 2.50 dB
PL12 19.20 dB
PL13 23.00 dB
PL2W 8.07971478 W
PL12W 0.17274120 W
PL13W 0.07201053 W
SFO2 300.1412006 MHz
SI 32768
SF 75.4702919 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

IP-2OH/NH2

— 7.271
— 6.991
— 6.826

— 5.173

2-Amino-4, 6-dibromophenol

NAME 2014-08-12-a
EXPNO 1
PROCNO 1
Date_ 20140812
Time 14.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.188846 Hz
AQ 2.6477044 sec
RG 114
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.50 usec
PL1 2.50 dB
PL1W 8.05146408 W
SFO1 300.1418535 MHz
SI 16384
SF 300.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

IP-2OH/NH2

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PROCNO    1
Date_     20140812
Time      15.58
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TD        32768
SOLVENT   CDCl3
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DS        2
SWH        18028.846 Hz
FIDRES     0.550197 Hz
AQ         0.9088159 sec
RG         203
DW         27.733 usec
DE         6.50 usec
TE        300.0 K
D1         2.0000000 sec
DELTA     0.0300000 sec
TD0       1

===== CHANNEL f1 =====
NUC1       13C
P1         9.80 usec
PL1        -0.50 dB
PL1W       34.66611099 W
SFO1       75.4778101 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      100.00 usec
PL2        2.50 dB
PL12       19.20 dB
PL13       23.00 dB
PL2W       8.07971478 W
PL12W      0.17274120 W
PL13W      0.07201053 W
SFO2       300.1412006 MHz
SI         32768
SF         75.4702752 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
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