The Aldrich Library of FT-IR Spectra

EDITION I

Charles J. Pouchert

VOLUME 2

THE ALDRICH LIBRARY

of

FT-IR SPECTRA

Edition I

Volume 2

CHARLES J. POUCHERT

Volume II

AROMATIC KETONES

A

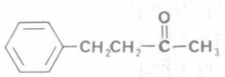
B1600-3 *CAS [2550-26-7]*
Benzylacetone, 98%

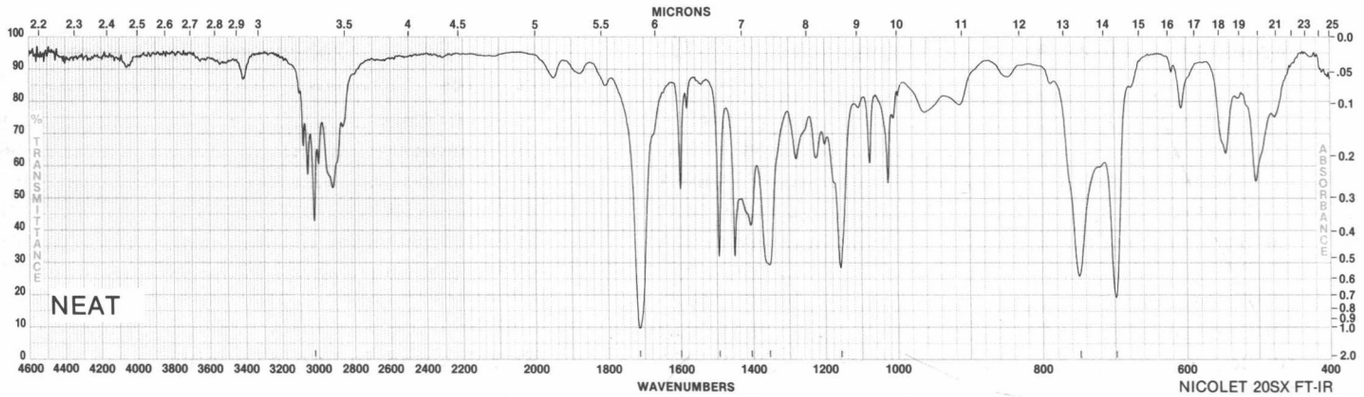
FW 148.21
bp 235°C
d 0.989

Fp 209°F
n_D^{20} 1.5122

IR III, 848B
NMR II, 2,3A

3027.3 1496.9 1162.0
1717.3 1408.8 750.4
1602.7 1357.8 699.7





B

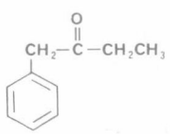
13722-7 *CAS [1007-32-5]*
1-Phenyl-2-butanone, 98%

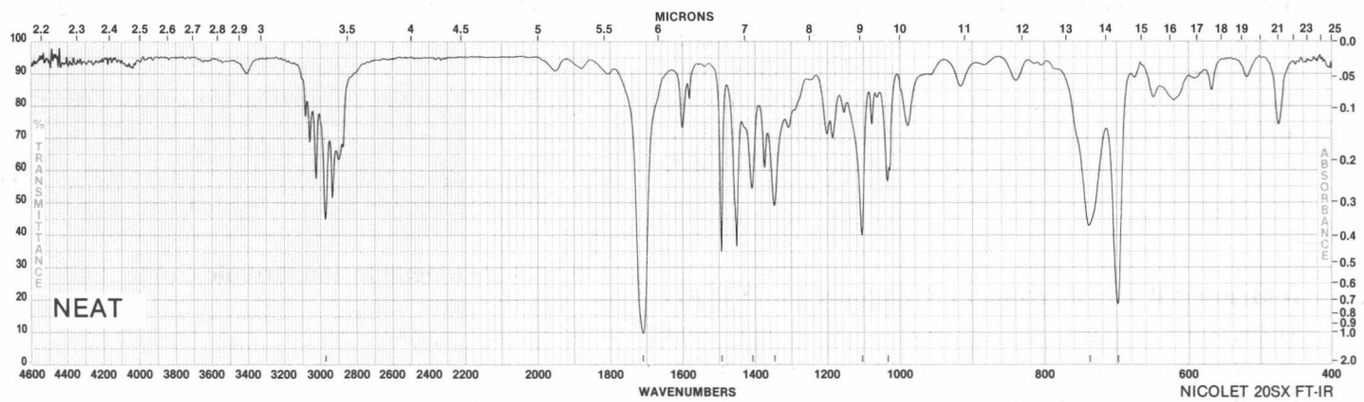
FW 148.21
bp 112°C/15mm
d 0.998

Fp 195°F
n_D^{20} 1.5122

IR III, 848C
NMR II, 2,2D

2977.5 1411.4 1037.8
1713.0 1350.1 739.1
1495.8 1108.8 699.2





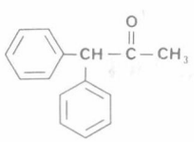
C

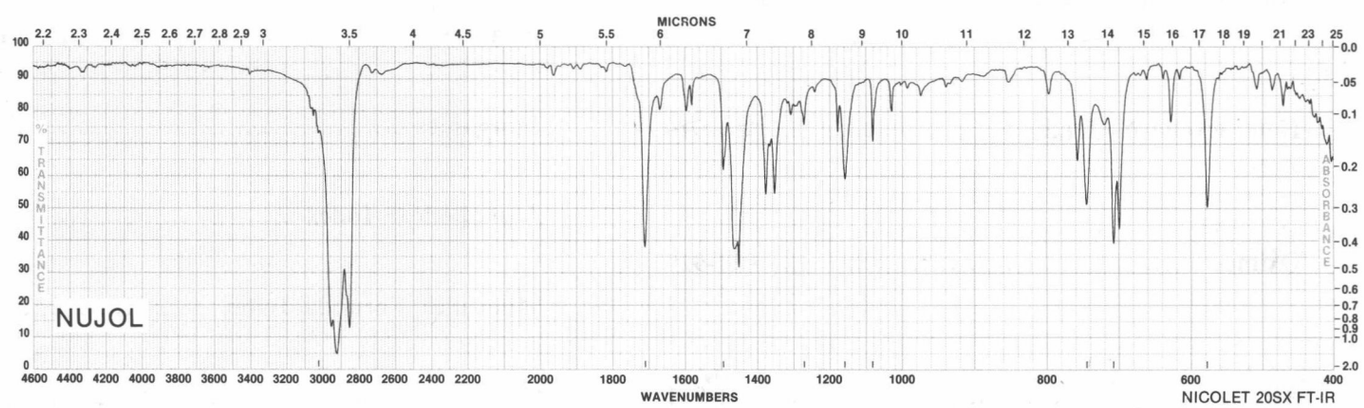
D20440-4 *CAS [781-35-1]*
1,1-Diphenylacetone, 98%

FW 210.28
mp 59-63°C

IR III, 848D
NMR II, 2,3C

3025.3 1271.4 745.0
1710.6 1158.6 707.5
1494.6 1081.7 577.7





D

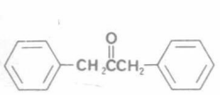
D20460-9 *CAS [102-04-5]*
1,3-Diphenylacetone, 99%

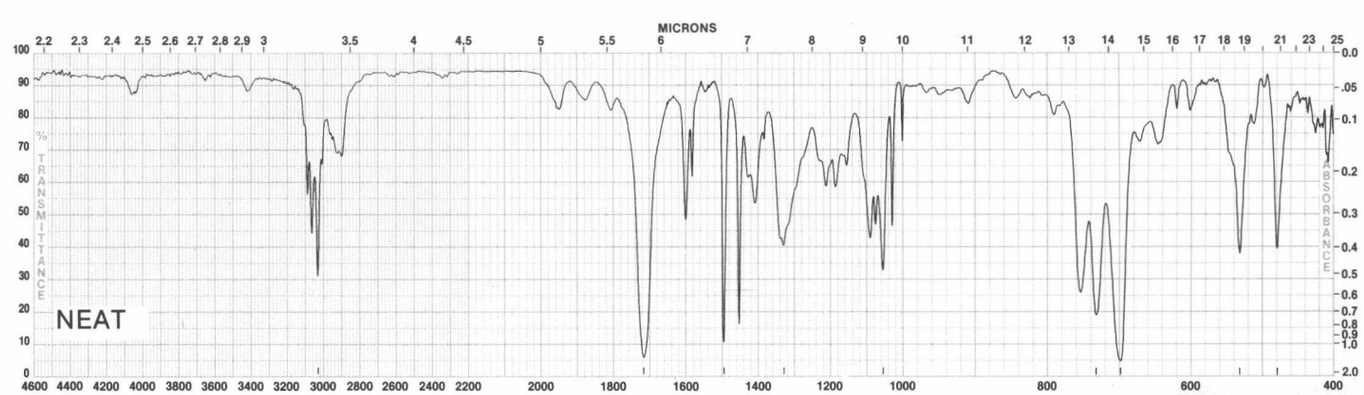
FW 210.28
mp 32-34°C
bp 330°C

Fp >235°F

IR III, 848E
NMR II, 2,3D

3029.0 1495.7 732.1
1715.6 1331.8 698.3
1601.8 1056.0 532.0





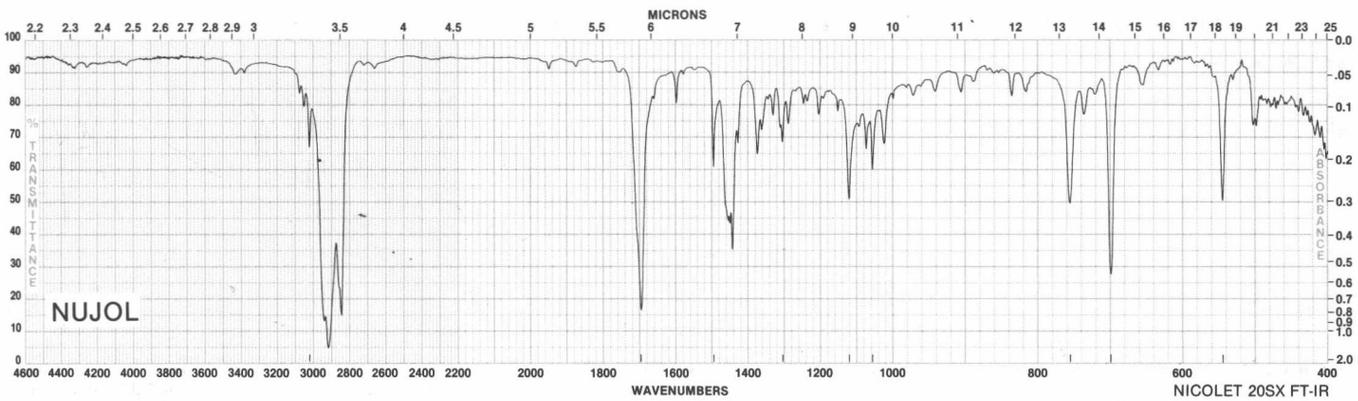
P2227-3 *CAS [1444-65-1]*
2-Phenylcyclohexanone, 98%

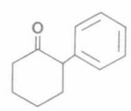
FW 174.24
mp 53-56°C
Fp >235°F

IR III, 848F
NMR II, 2,5B

3030.3 1308.3 757.4
1700.5 1125.1 700.6
1499.0 1060.1 546.2

A





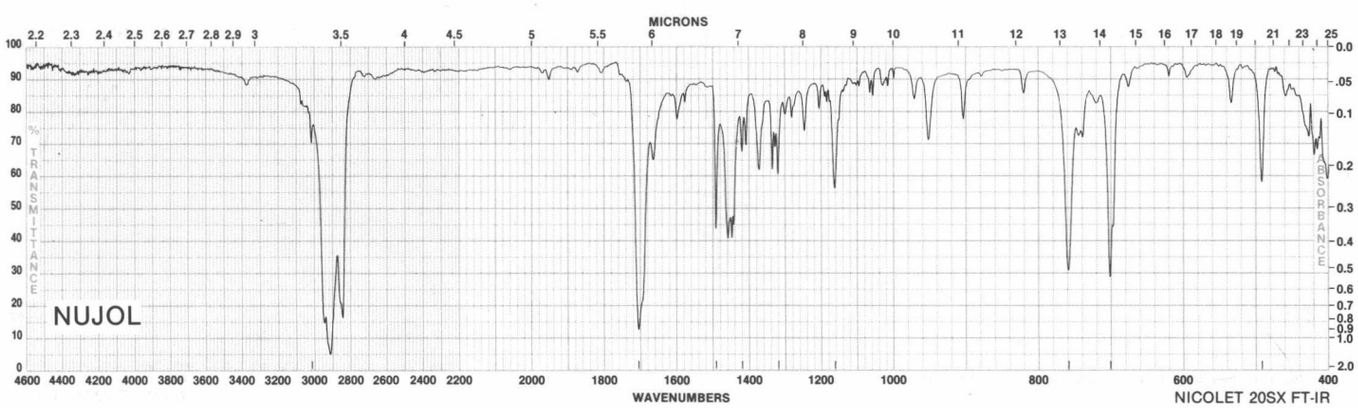
19623-1 *CAS [4894-75-1]*
4-Phenylcyclohexanone, 98 + %

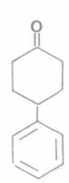
FW 174.24
mp 78-80°C

IR III, 848G
NMR II, 2,5C

3025.9 1423.7 760.8
1709.8 1323.6 703.0
1496.2 1167.0 492.9

B





16432-1 *CAS [15547-89-4]*
2-(3-Methoxyphenyl)cyclohexanone, 97%

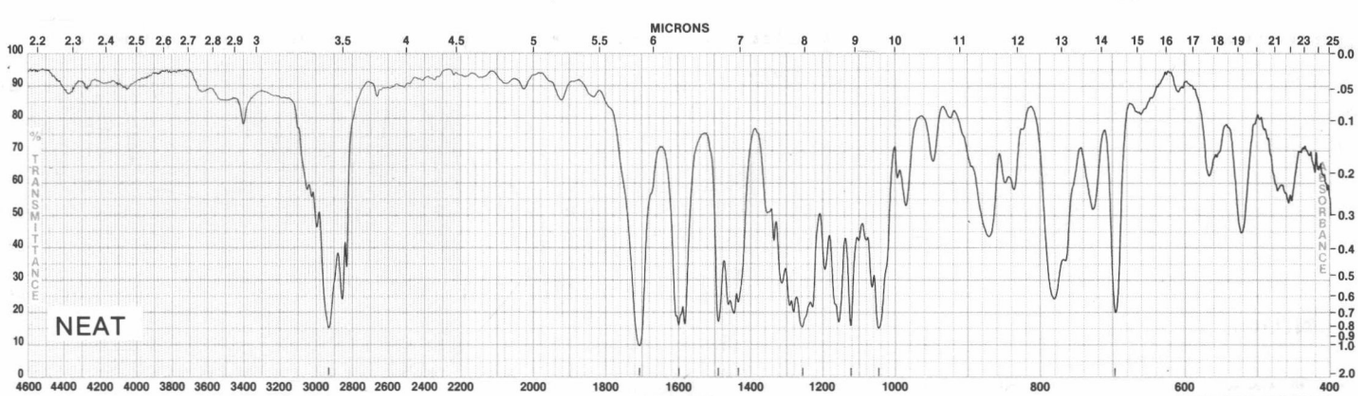
FW 204.27
d 1.100
Fp >235°F

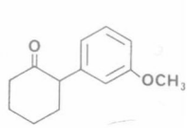
n_D^{20} 1.5470

IR III, 848H

2936.9 1492.9 1124.9
1710.0 1437.1 1048.2
1602.1 1259.1 697.5

C





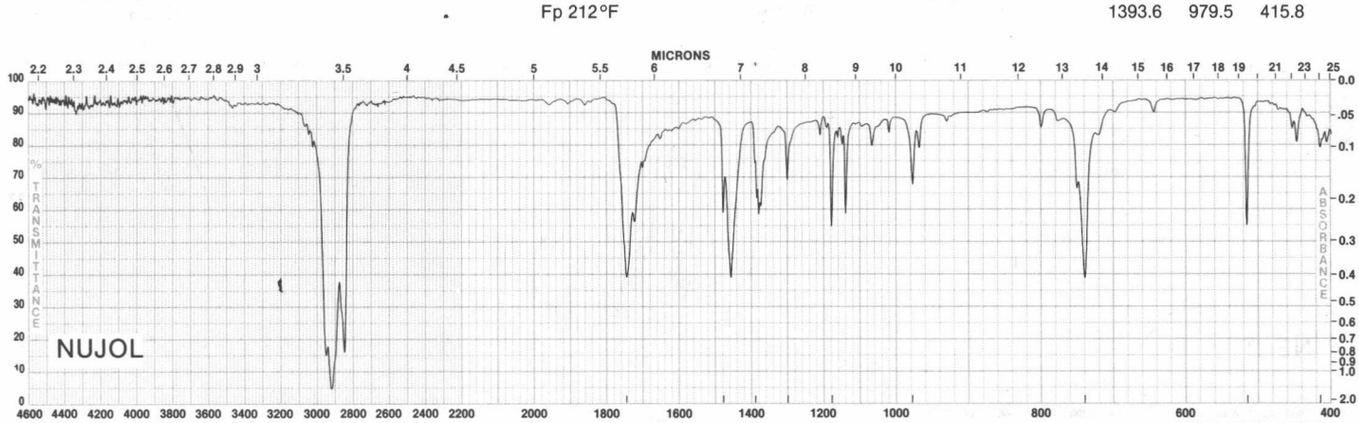
14669-2 *CAS [615-13-4]*
2-Indanone, 98%

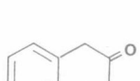
FW 132.16
mp 54-56°C
Fp 212°F

IR III, 849B
NMR II, 2,4A

1748.6 1304.1 742.0
1481.8 1182.4 517.3
1393.6 979.5 415.8

D





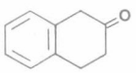
AROMATIC KETONES

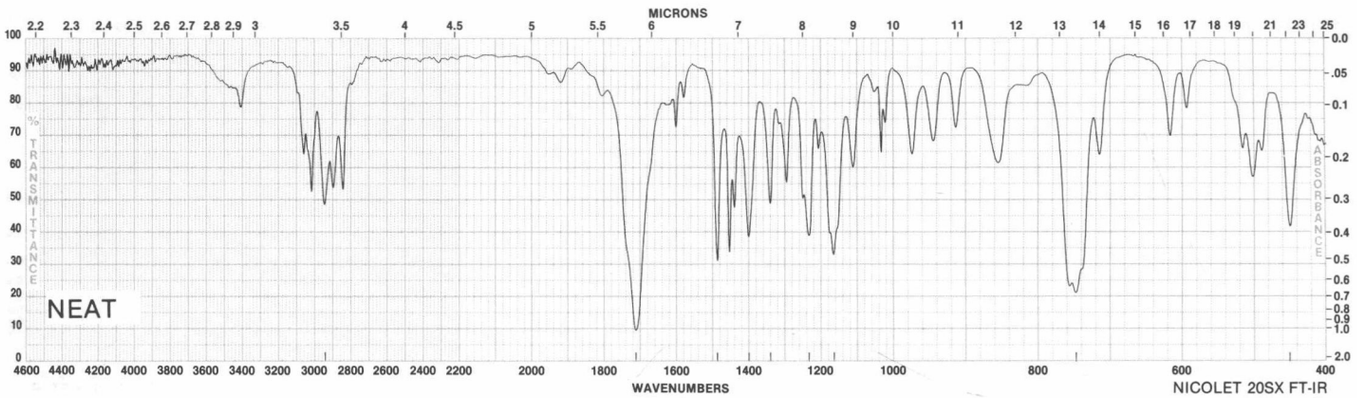
A

T1920-8 *CAS [530-93-8]*
β-Tetralone, 99%

FW 146.19 | d 1.106 | IR III, 849C
mp 18°C | Fp >235°F | NMR II, 2,4B
bp 131°C/11mm | n_D^{20} 1.5598

2949.8 1404.0 1169.4
1716.3 1343.5 750.0
1491.0 1237.5 452.5



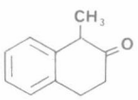


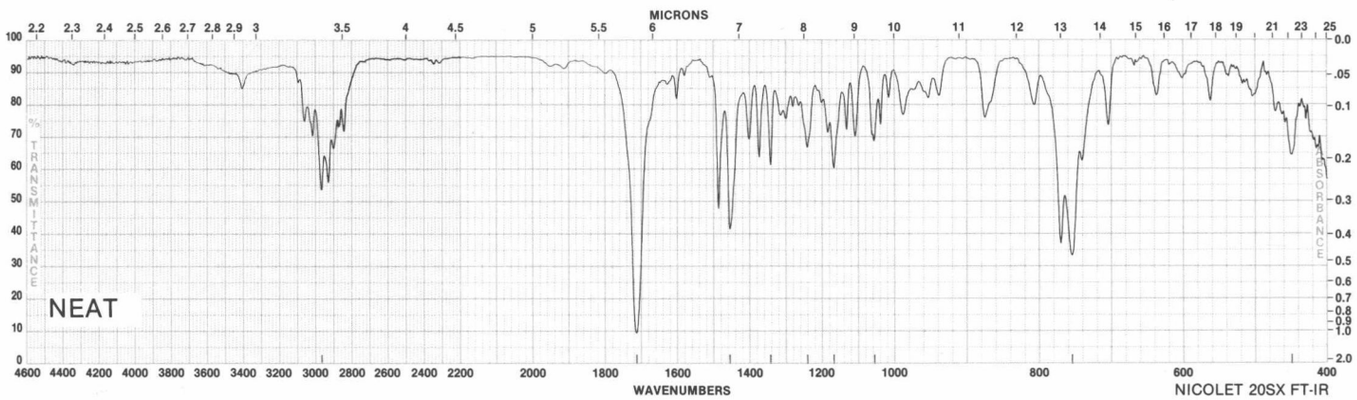
B

M8290-6 *CAS [4024-14-0]*
1-Methyl-2-tetralone, tech., 90%

FW 160.22 | Fp >235°F | IR III, 849D
bp 261°C | n_D^{20} 1.5530 | NMR II, 2,5A
d 1.020

2975.0 1344.6 1058.3
1716.0 1243.4 755.0
1457.8 1169.9 449.9



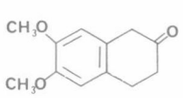


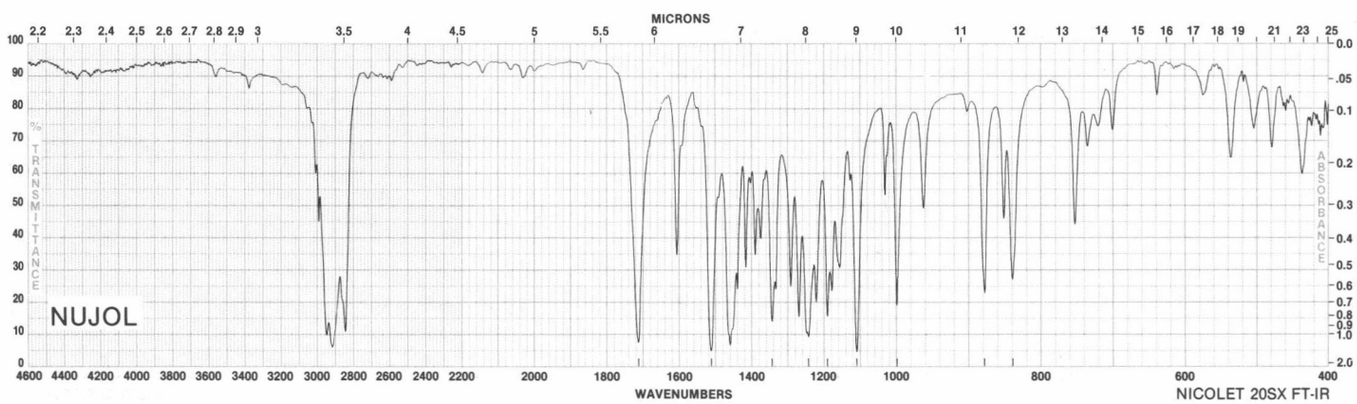
C

22926-1 *CAS [2472-13-1]*
6,7-Dimethoxy-2-tetralone, 99%

FW 206.24 | NMR II, 2,4D
mp 87-89°C

1716.0 1246.5 1002.4
1515.1 1194.0 880.0
1347.0 1113.3 841.4



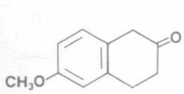


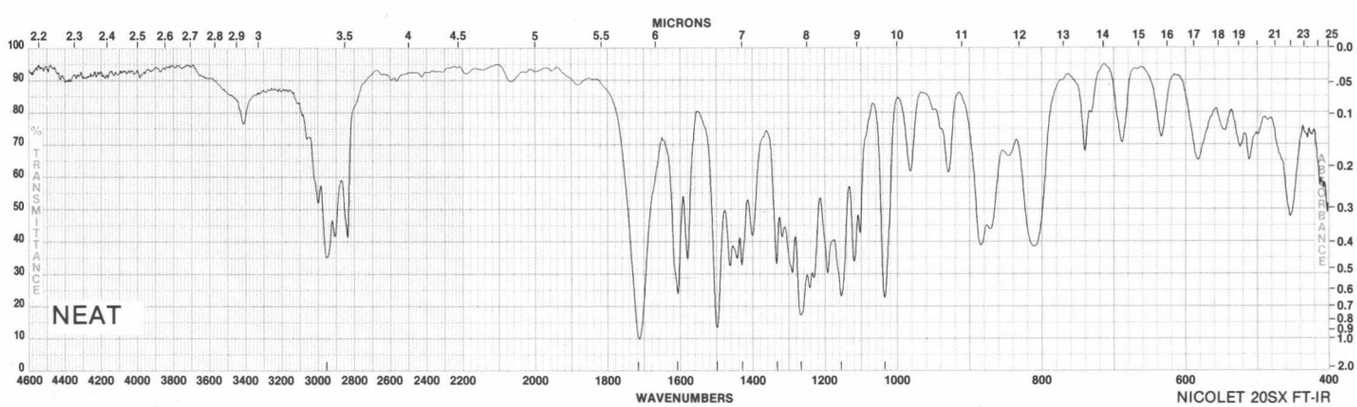
D

18406-3 *CAS [2472-22-2]*
6-Methoxy-2-tetralone, 95%

FW 176.22 | IR III, 849F
Fp >235°F
n_D^{20} 1.5645

2952.9 1501.2 1269.8
1716.5 1432.3 1157.9
1610.0 1336.3 1037.4



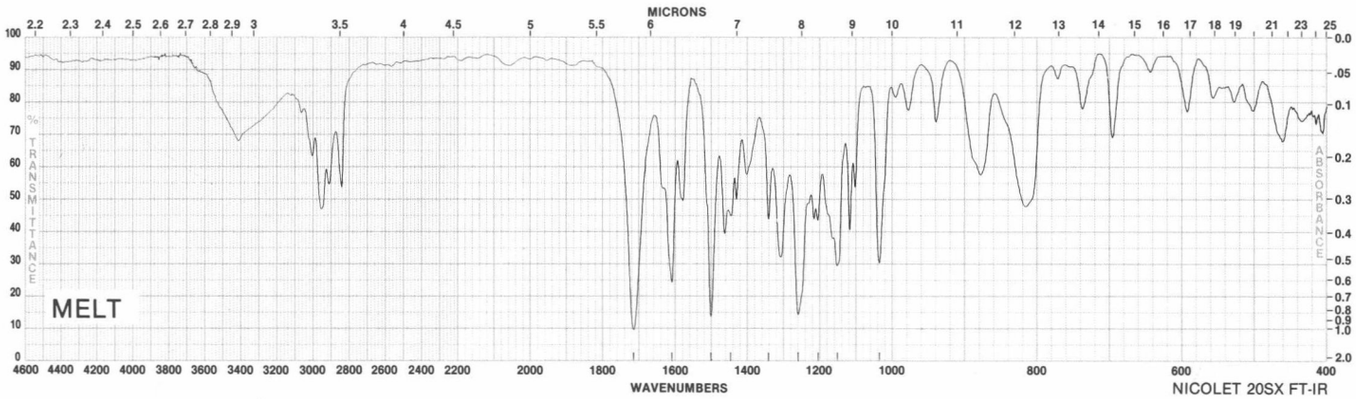


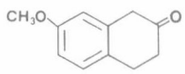
16418-6 *CAS [4133-34-0]*
7-Methoxy-2-tetralone, 97%

FW 176.22 Fp >235°F IR III, 849G
bp 126°C/1.5mm n_D^{20} 1.5595
d 1.130

1716.4 1447.6 1207.2
1610.9 1343.6 1154.3
1503.1 1261.7 1037.7

A



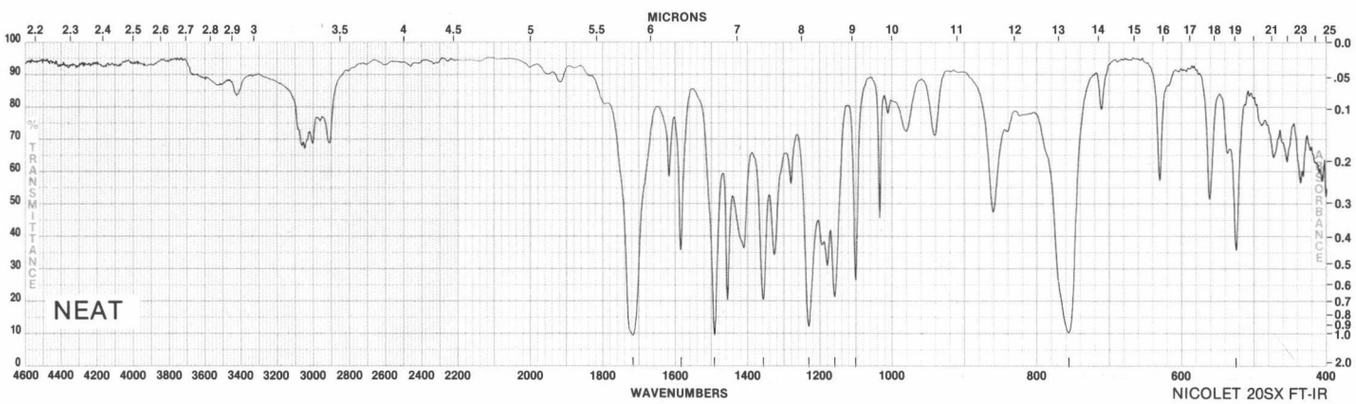


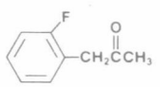
20874-4 *CAS [2836-82-0]*
(2-Fluorophenyl)acetone, 99%

FW 152.17 Fp 185°F IR III, 849H
bp 47°C/0.05mm n_D^{20} 1.4989 NMR II, 2,1B
d 1.077

1719.1 1359.2 1102.5
1586.4 1233.0 757.2
1493.6 1161.3 525.5

B



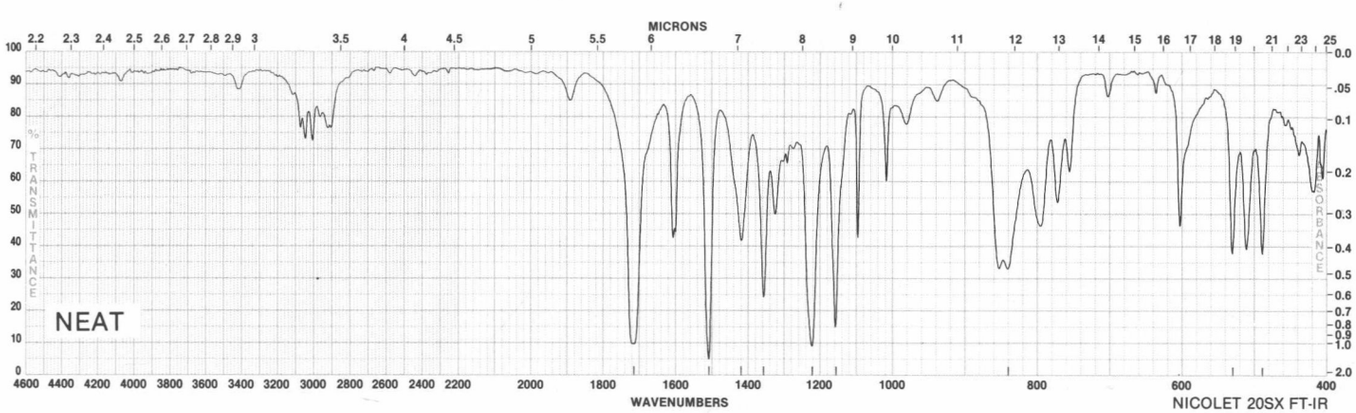


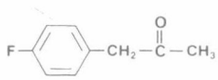
20945-7 *CAS [459-03-0]*
(4-Fluorophenyl)acetone, 98%

FW 152.17 Fp 197°F IR III, 850A
bp 107°C/18mm n_D^{20} 1.4958 NMR II, 2,1C
d 1.139

1714.0 1358.1 840.0
1601.7 1223.0 530.1
1508.9 1157.5 488.9

C



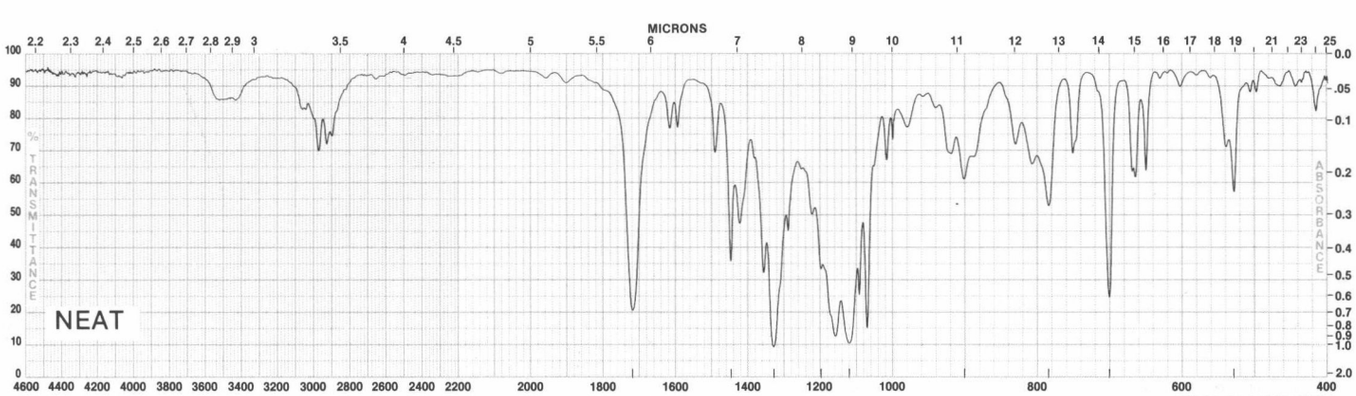


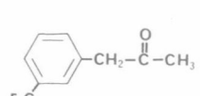
19379-8 *CAS [21906-39-8]*
3-(Trifluoromethyl)phenylacetone, 97%

FW 202.18 Fp 192°F IR III, 850B
bp 90°C/0.5mm n_D^{20} 1.4570 NMR II, 2,1D
d 1.204

1722.5 1202.4 786.5
1451.4 1124.4 702.8
1333.3 903.2 530.5

D





AROMATIC KETONES

A

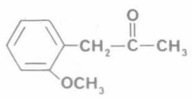
21398-5 *CAS [521-62-1]*
2-Methoxyphenylacetone, 98%

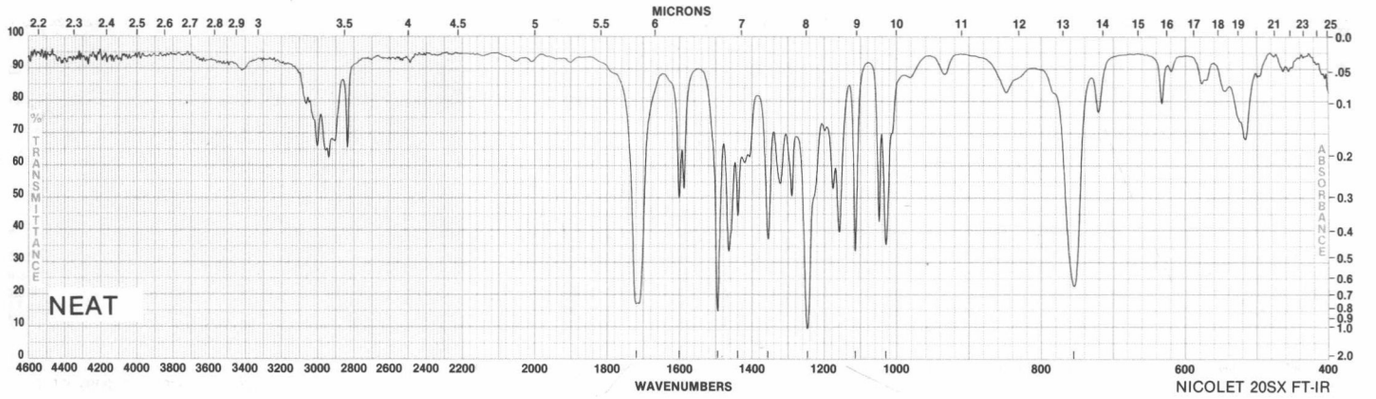
FW 164.20
bp 130°C/10mm
d 1.054

Fp >235°F
nᴅ 1.5250

IR III, 850C

1721.1 1439.7 1115.3
1601.9 1355.9 1030.7
1496.0 1247.2 754.9





B

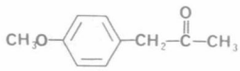
19917-6 *CAS [122-84-9]*
4-Methoxyphenylacetone, 97 + %

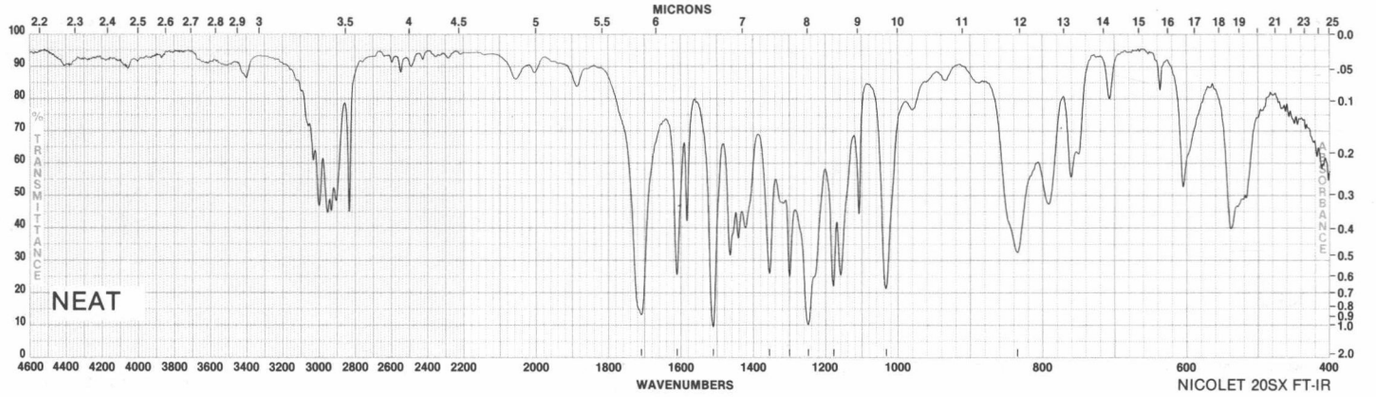
FW 164.20
bp 145°C/25mm
d 1.067

Fp 215°F
nᴅ 1.5250

IR III, 850D
NMR II, 2,2B

1710.5 1356.2 1179.0
1611.9 1301.0 1034.2
1511.7 1248.8 834.6





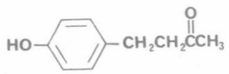
C

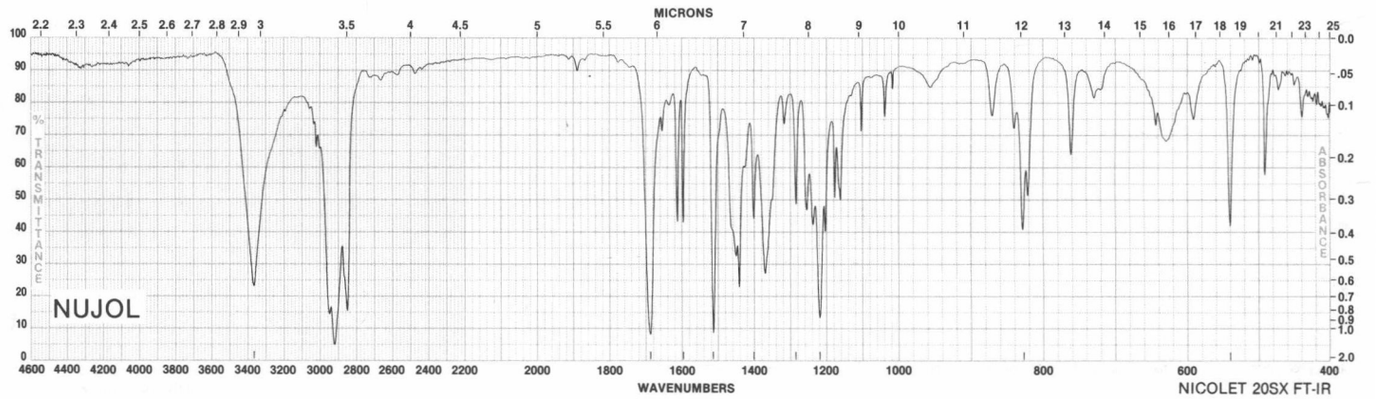
17851-9 *CAS [5471-51-2]*
4-(4-Hydroxyphenyl)-2-butanone, 99%

FW 164.20
mp 82-83°C

IR III, 850F
NMR II, 2,3B

3370.9 1516.0 1221.4
1690.0 1404.0 829.2
1598.6 1287.5 541.2





D

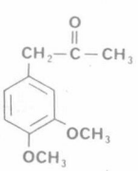
14121-6 *CAS [776-99-8]*
3,4-Dimethoxyphenylacetone, 97%

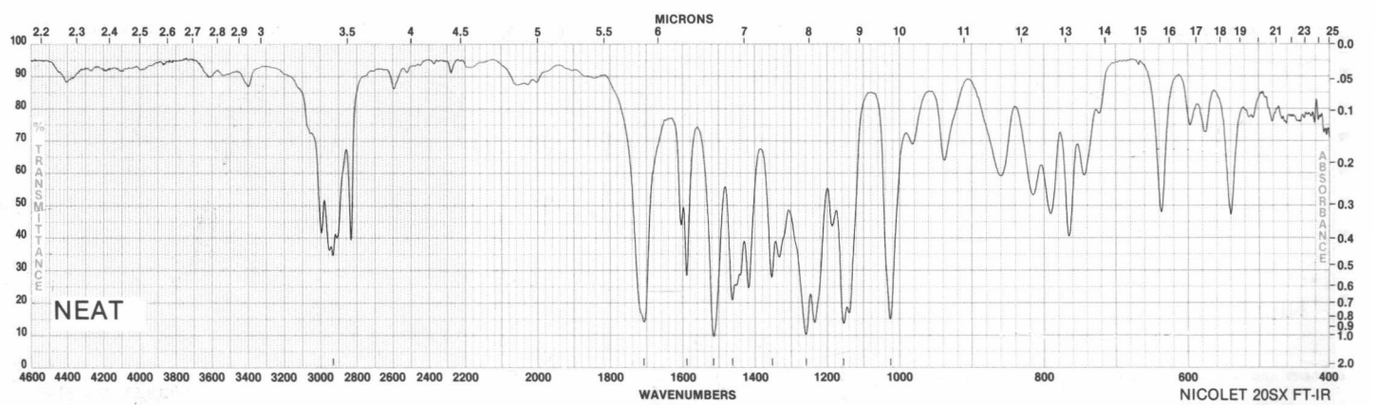
FW 194.23
d 1.115
Fp >235°F

nᴅ 1.5358

IR III, 850G
NMR II, 2,2C

2937.3 1516.9 1262.1
1709.5 1465.2 1157.7
1591.4 1356.4 1028.4





15202-1 *CAS [621-87-4]*
Phenoxy-2-propanone, 99%

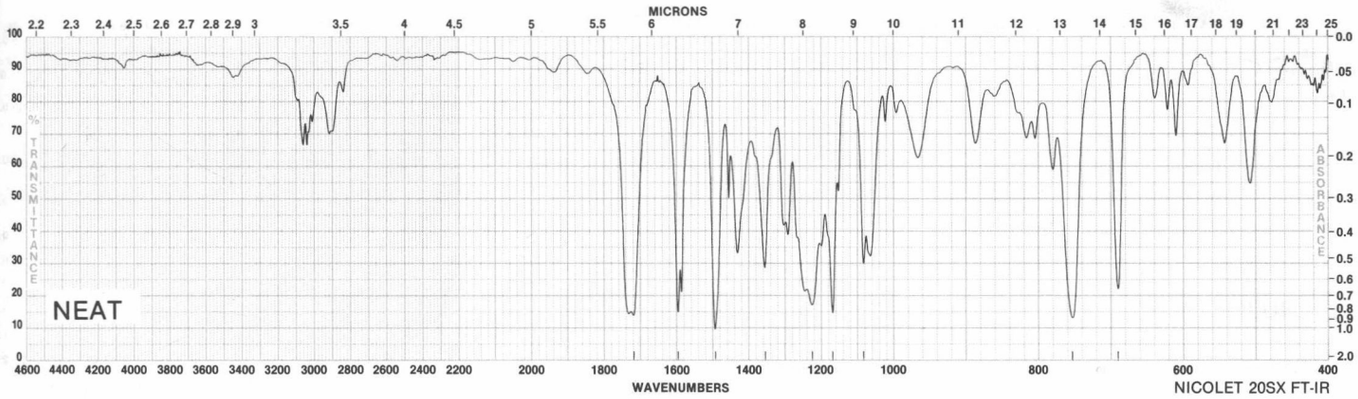
FW 150.18
bp 229-230°C
d 1.097

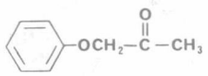
Fp 185°F
n_D^{20} 1.5210

IR III, 851B
NMR II, 2,5D

1722.3 1358.0 1085.5
1599.0 1228.4 754.9
1496.1 1171.7 691.7

A





18517-5 *CAS [775-16-6]*
1-Benzyl-3-pyrrolidinone, 98%

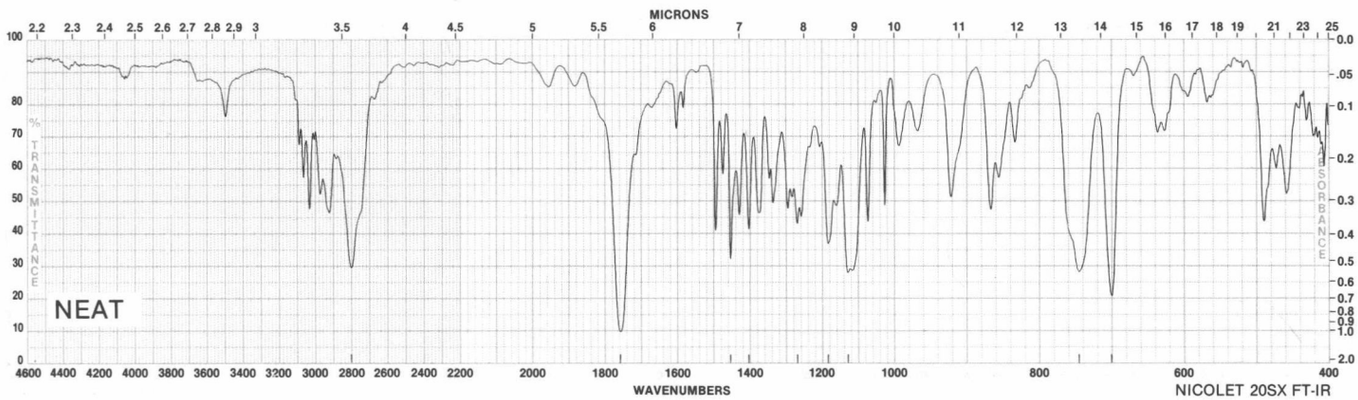
FW 175.23
bp 77°C/0.01mm
d 1.091

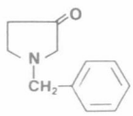
Fp >235°F
n_D^{20} 1.5378

IR III, 851E
NMR II, 2,6A

2798.2 1403.6 1130.1
1756.7 1269.7 744.6
1453.9 1184.5 699.9

B





B2980-6 *CAS [3612-20-2]*
1-Benzyl-4-piperidone, 99 + %

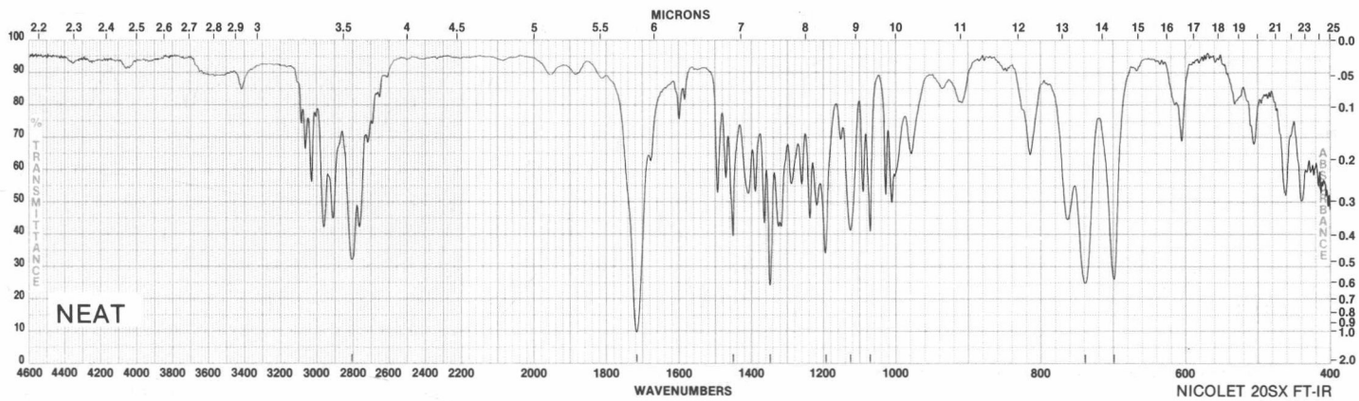
FW 189.26
bp 134°C/7mm
d 1.021

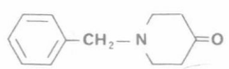
Fp >235°F
n_D^{20} 1.5399

IR III, 851F
NMR II, 2,6B

2807.3 1349.6 1071.8
1718.4 1195.4 738.7
1453.4 1126.7 699.3

C





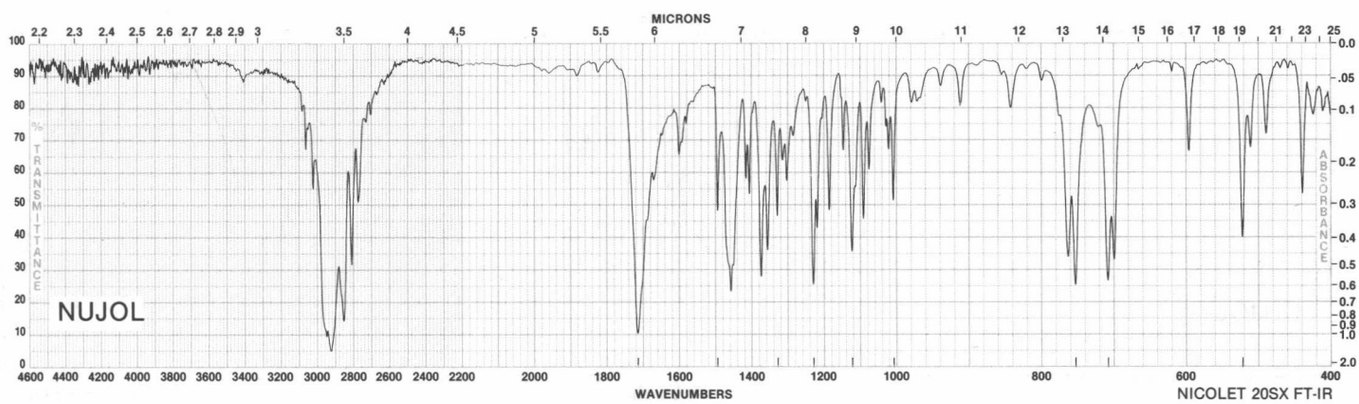
13138-5 *CAS [39742-60-4]*
1-Phenethyl-4-piperidone, 97%

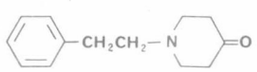
FW 203.29
mp 57-60°C

IR III, 851G
NMR II, 2,6C

1716.1 1230.6 753.0
1495.5 1123.7 708.4
1330.4 1009.4 522.4

D





AROMATIC KETONES

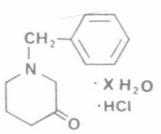
A

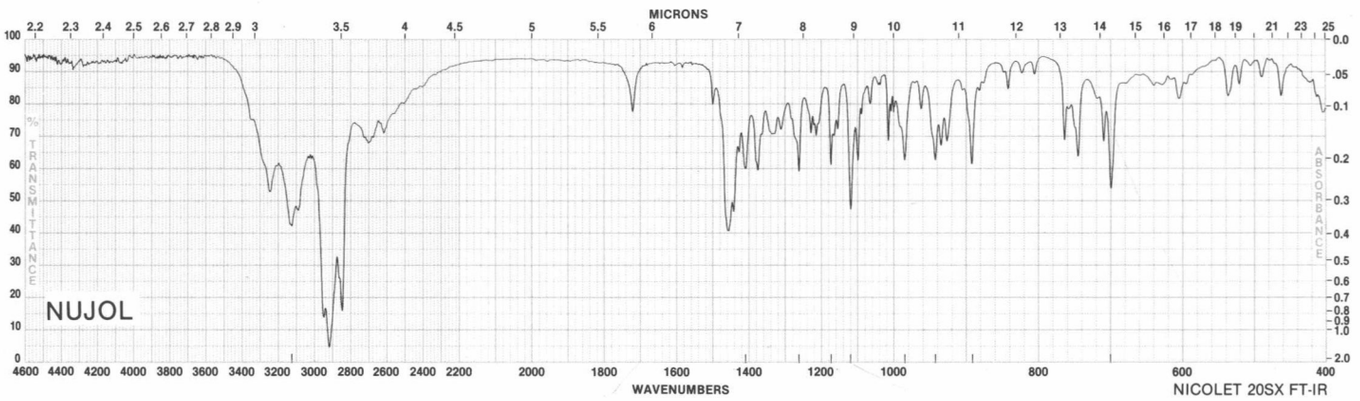
15311-7 *CAS [50606-58-1]*
1-Benzyl-3-piperidone hydrochloride hydrate

FW 225.72

IR III, 852A
NMR II, 2,6D

3130.4 1176.2 943.8
1411.8 1121.7 893.4
1264.1 986.1 701.6





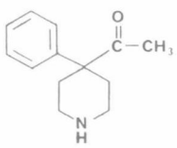
B

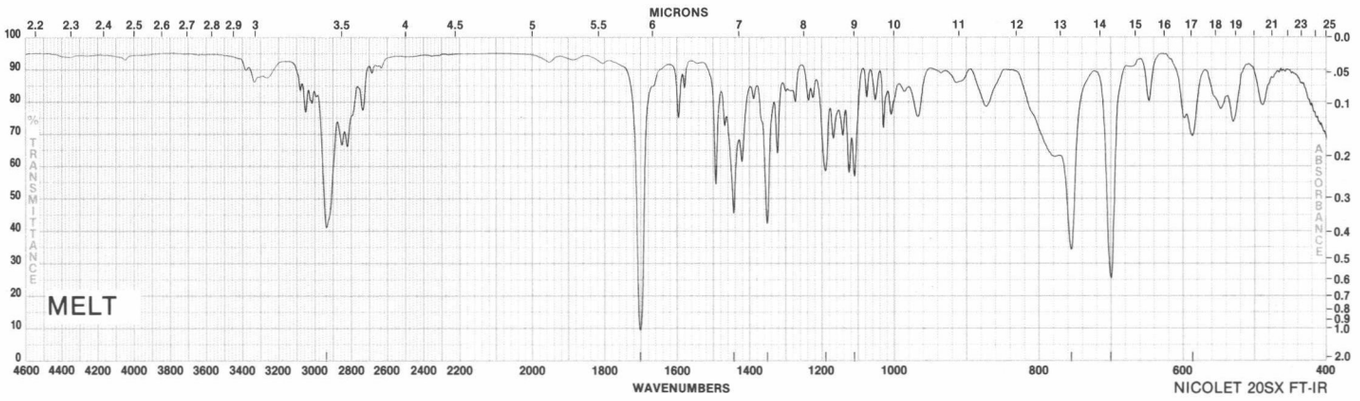
A2040-5 *CAS [34798-80-6]*
4-Acetyl-4-phenylpiperidine

FW 203.29
mp 44-46°C
Fp >235°F

IR III, 852B

2944.6 1353.0 756.2
1703.6 1192.2 700.8
1445.6 1111.6 588.0





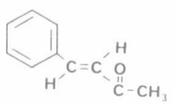
C

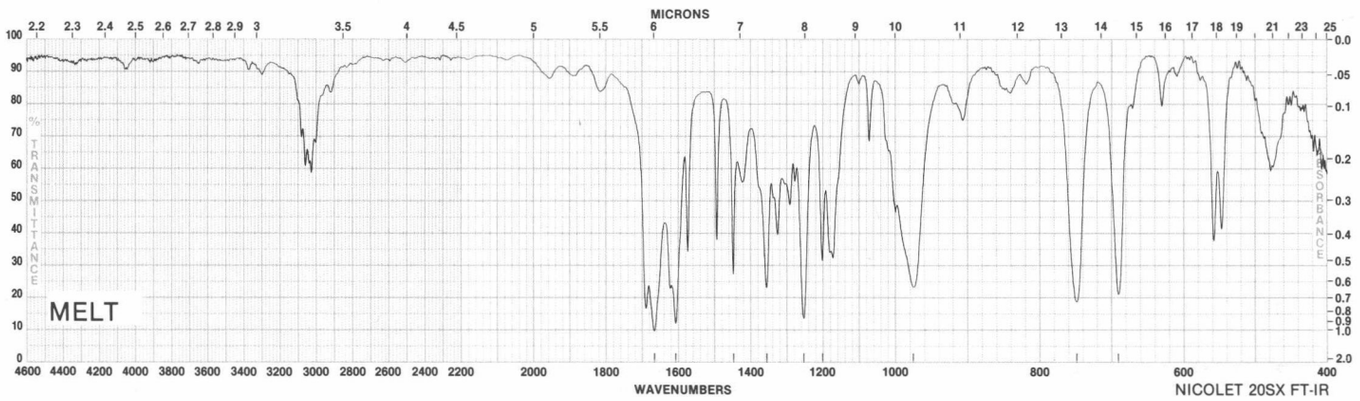
14788-5 *CAS [122-57-6]*
***trans*-4-Phenyl-3-buten-2-one,** 99%

FW 146.19
mp 35-39°C
bp 260-262°C
Fp 150°F

IR III, 852D
NMR II, 2,53D
Merck 10,1144

1669.3 1358.4 975.7
1610.1 1255.7 748.8
1450.0 1203.9 690.6





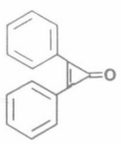
D

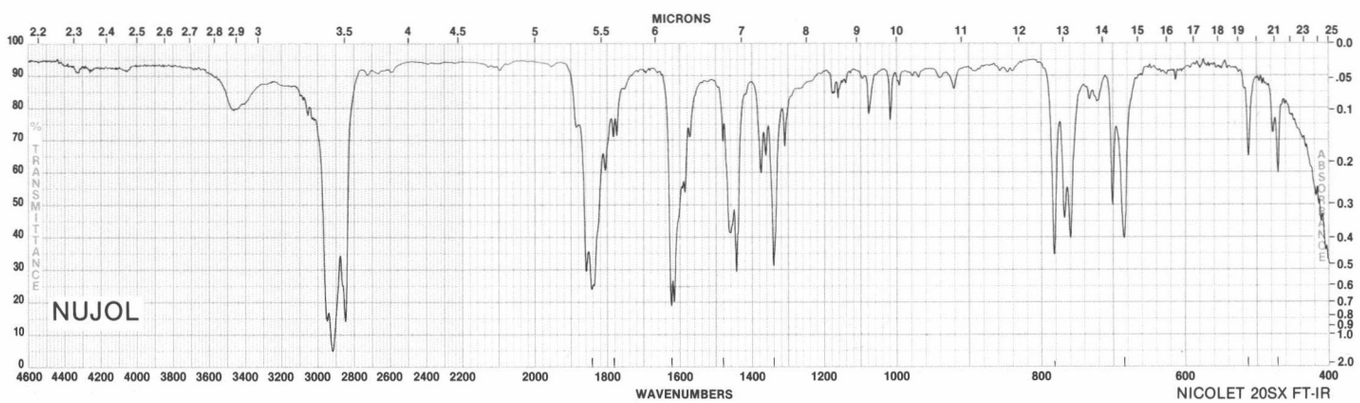
17737-7 *CAS [886-38-4]*
Diphenylcyclopropenone, 98%

FW 206.24
mp 119-121°C

IR III, 853B
NMR II, 2,11A

1846.0 1482.7 685.2
1785.1 1343.0 512.5
1626.4 782.4 471.6





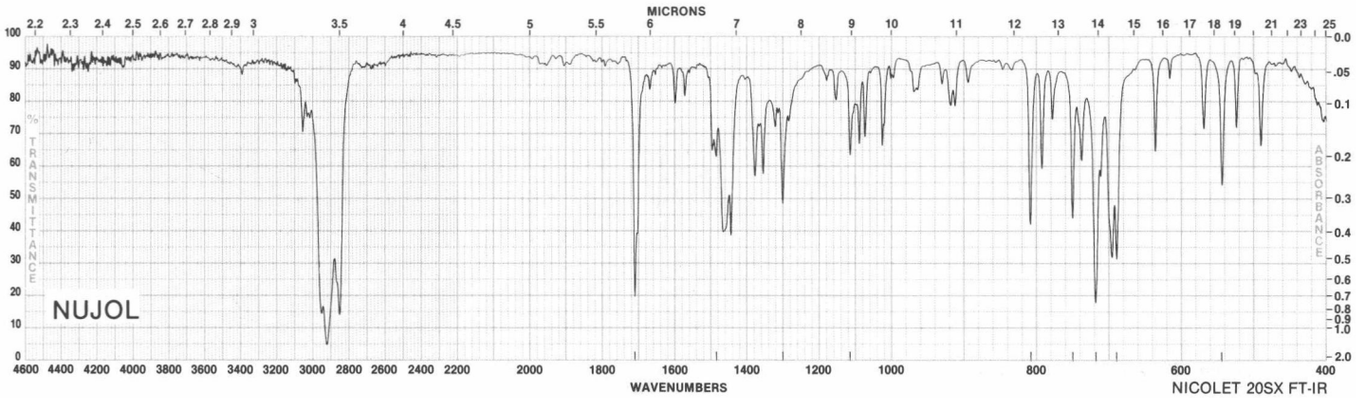
T2580-1 *CAS [479-33-4]*
Tetraphenylcyclopentadienone, 98%

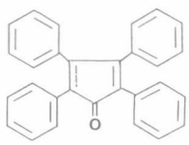
FW 384.48
mp 217-220°C

IR III, 853C
NMR II, 2,58B

1710.5 1116.2 718.8
1485.0 809.3 689.8
1300.7 750.5 544.8

A





A1070-1 *CAS [98-86-2]*
Acetophenone, 99%

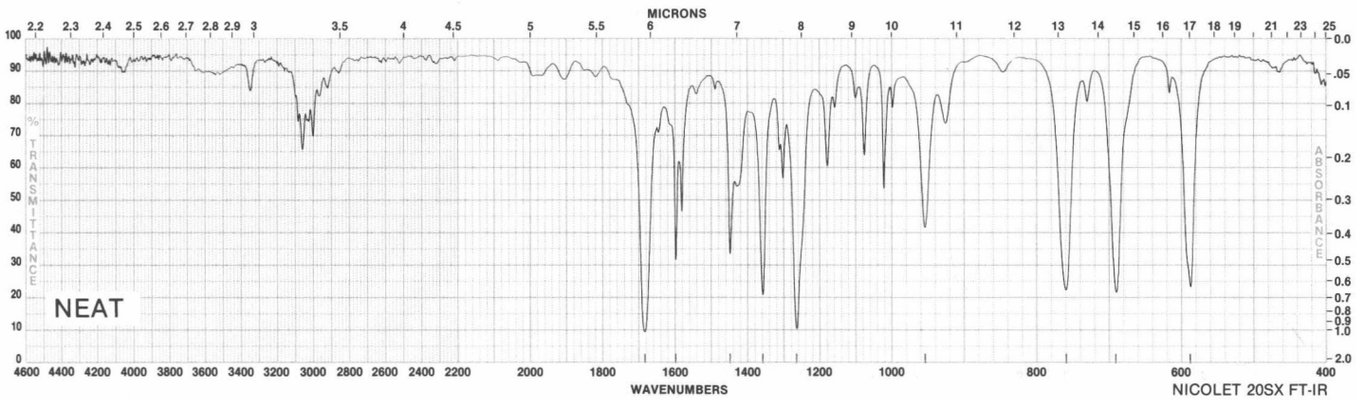
FW 120.15
mp 19-20°C
bp 202°C

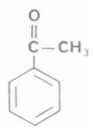
d 1.030
Fp 180°F
n_D^{20} 1.5325

IR III, 853E
NMR II, 2,7D
Merck 10,65

1685.2 1359.4 760.3
1599.0 1266.3 690.5
1449.3 955.4 588.3

B





P5160-5 *CAS [93-55-0]*
Propiophenone, 99%

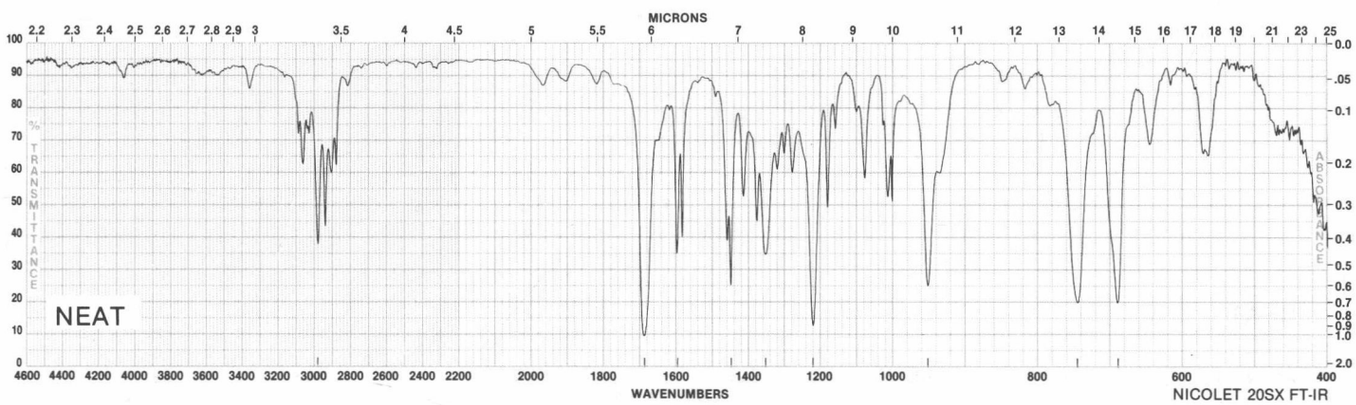
FW 134.18
mp 18°C
bp 218°C

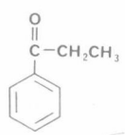
d 1.009
Fp 190°F
n_D^{20} 1.5258

IR III, 853F
NMR II, 2,8A
Merck 10,7731

2978.5 1449.0 951.9
1688.0 1353.2 745.5
1597.3 1220.5 690.3

C





12433-8 *CAS [495-40-9]*
Butyrophenone, 99%

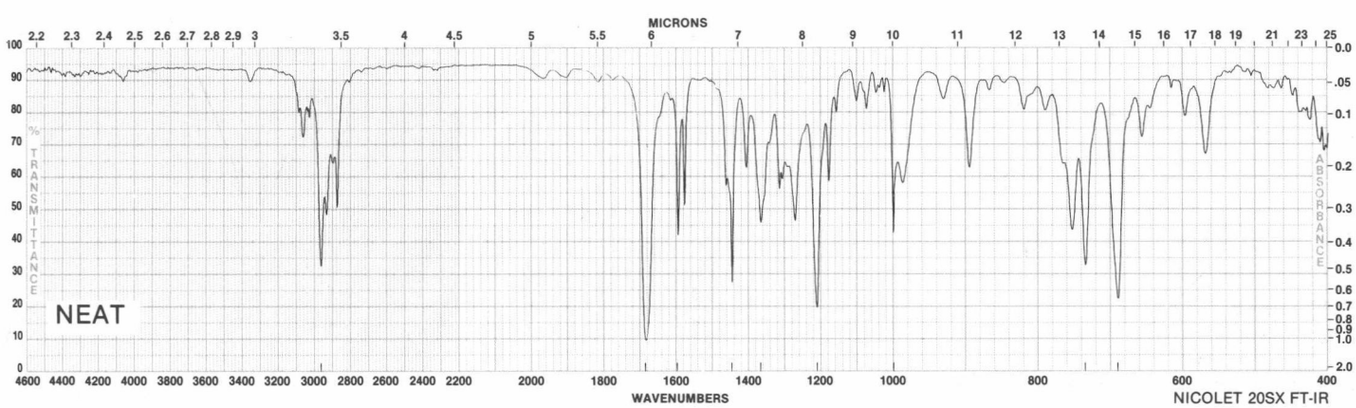
FW 148.21
mp 11-13°C
bp 220-222°C

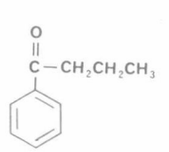
d 1.021
Fp 192°F
n_D^{20} 1.5195

IR III, 853G
NMR II, 2,8B

2962.9 1448.3 1002.2
1687.2 1368.7 735.5
1597.8 1213.4 690.6

D





AROMATIC KETONES

A

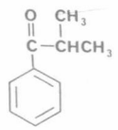
13036-2 *CAS [611-70-1]*
Isobutyrophenone, 97%

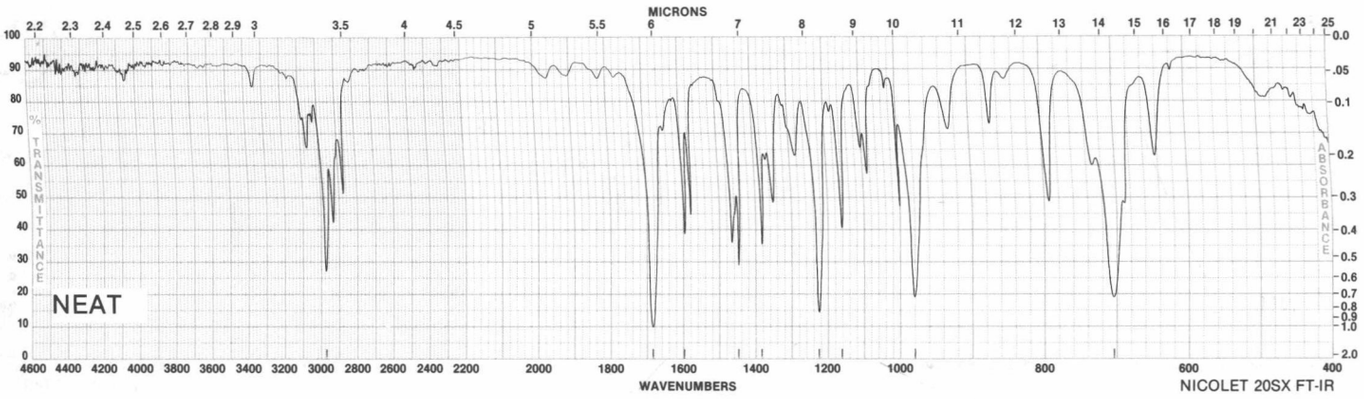
FW 148.21
bp 217°C
d 0.988

Fp 184°F
n_D^{20} 1.5172

IR III, 853H
NMR II, 2,9D

2972.7 1447.3 1161.6
1684.0 1383.1 979.6
1596.6 1224.6 703.3





B

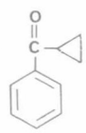
12551-2 *CAS [3481-02-5]*
Cyclopropyl phenyl ketone, 97%

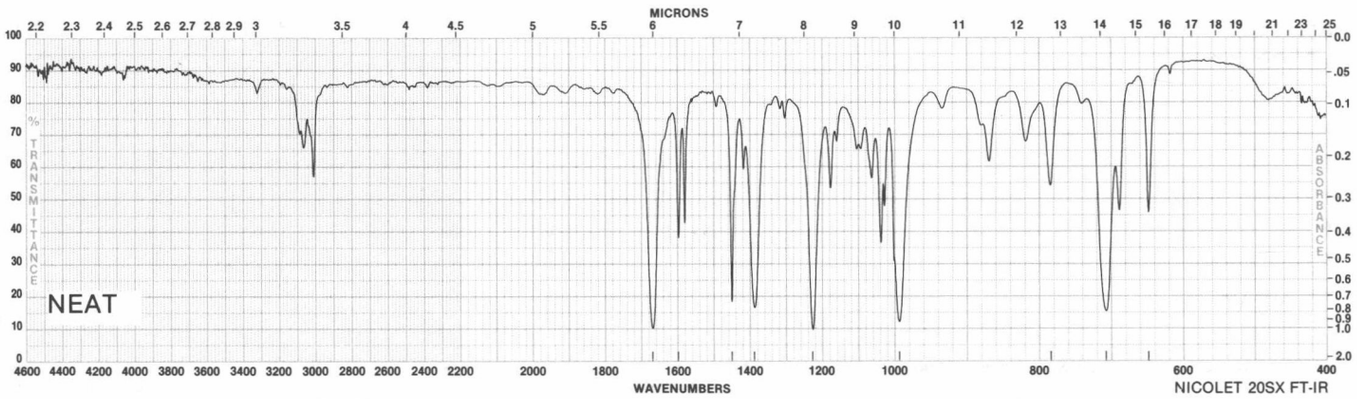
FW 146.19
mp 7-9°C
bp 123°C/15mm

d 1.058
Fp 195°F
n_D^{20} 1.5534

IR III, 854A
NMR II, 2,10A

1668.4 1386.6 783.3
1596.6 1225.8 705.5
1449.4 992.6 646.6





C

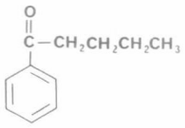
V65-9 *CAS [1009-14-9]*
Valerophenone, 99%

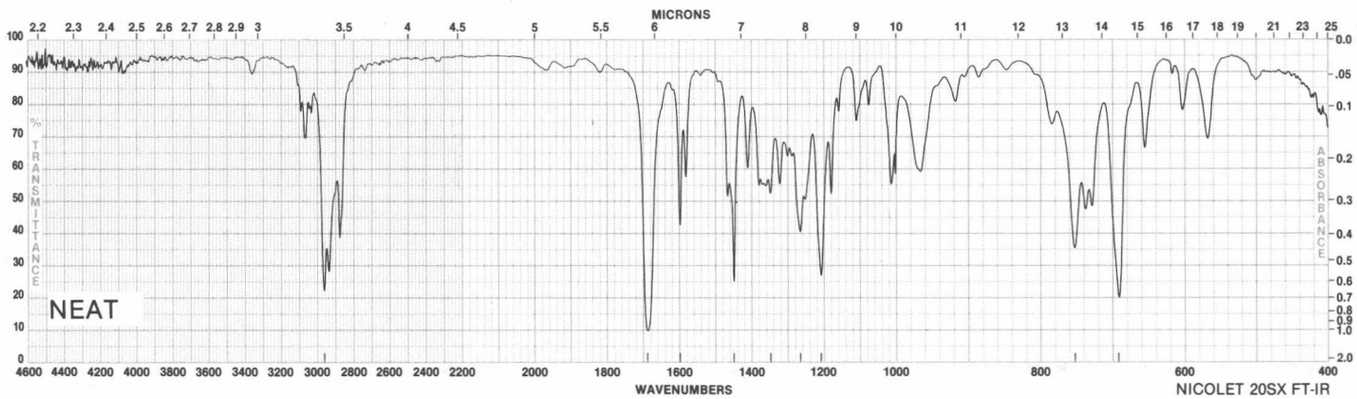
FW 162.23
bp 107°C/5mm
d 0.988

Fp 217°F
n_D^{20} 1.5143

IR III, 854B
NMR II, 2,8C

2958.4 1448.5 1208.0
1686.9 1347.4 752.2
1597.1 1265.4 690.5





D

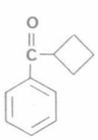
10836-7 *CAS [5407-98-7]*
Cyclobutyl phenyl ketone, 98%

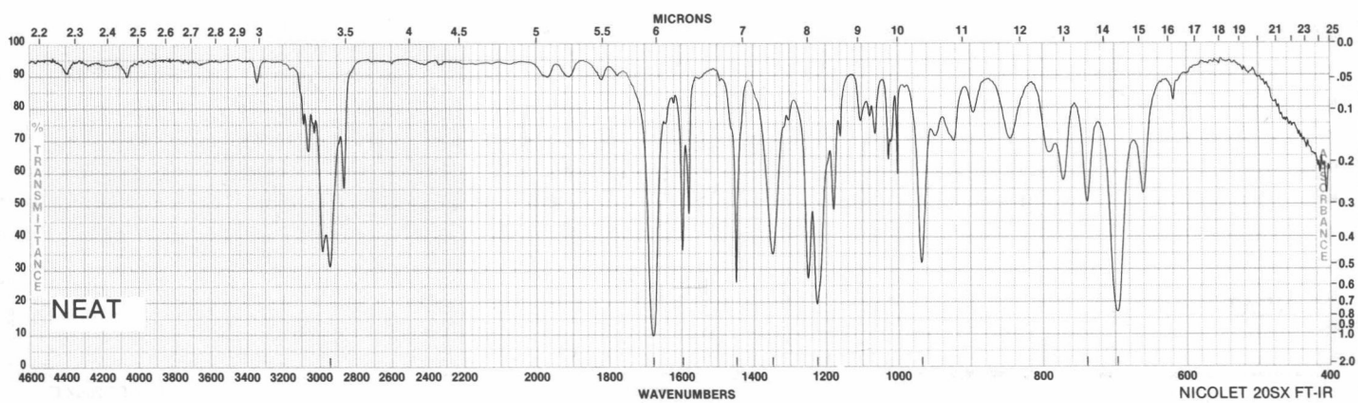
FW 160.22
bp 118°C/7mm
d 1.050

Fp >235°F
n_D^{20} 1.5470

IR III, 854C
NMR II, 2,11B

2943.5 1448.3 967.1
1678.4 1347.9 738.1
1597.2 1224.3 695.9





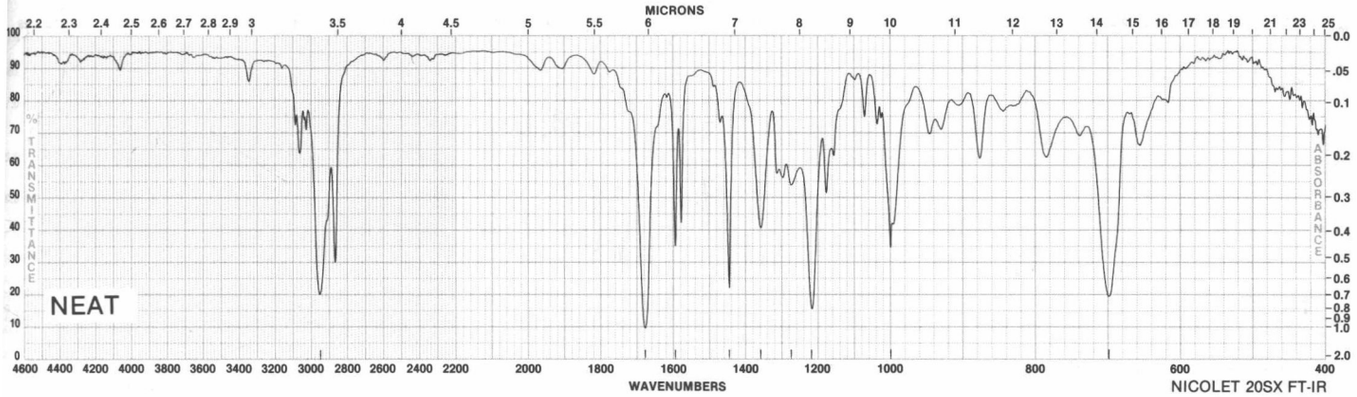
18993-6 *CAS [5422-88-8]*
Cyclopentyl phenyl ketone, 98%

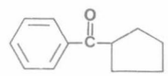
FW 174.24 | d 1.034 | Fp >235°F | nᴅ 1.5428

IR III, 854D | NMR II, 2,11D

2954.1 1447.9 1220.7 | 1680.2 1360.9 1002.4 | 1596.7 1277.1 699.9

A





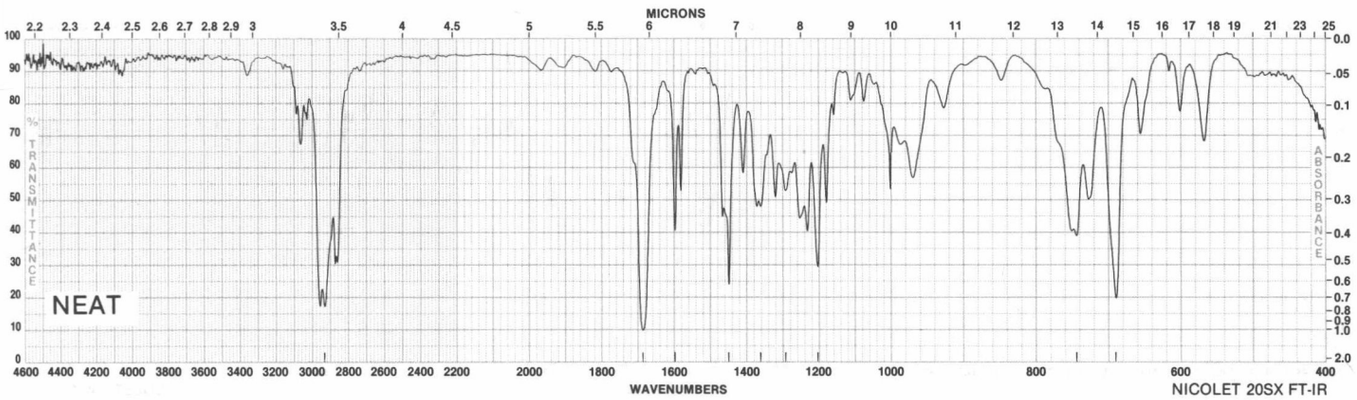
H1245-5 *CAS [942-92-7]*
Hexanophenone, 98%

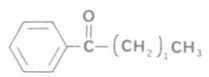
FW 176.26 | mp 25-26°C | bp 265.2°C | d 0.958 | Fp >235°F | nᴅ 1.5105

IR III, 854E | NMR II, 2,8D

2930.9 1448.5 1204.3 | 1687.1 1361.4 745.1 | 1597.5 1292.3 690.5

B





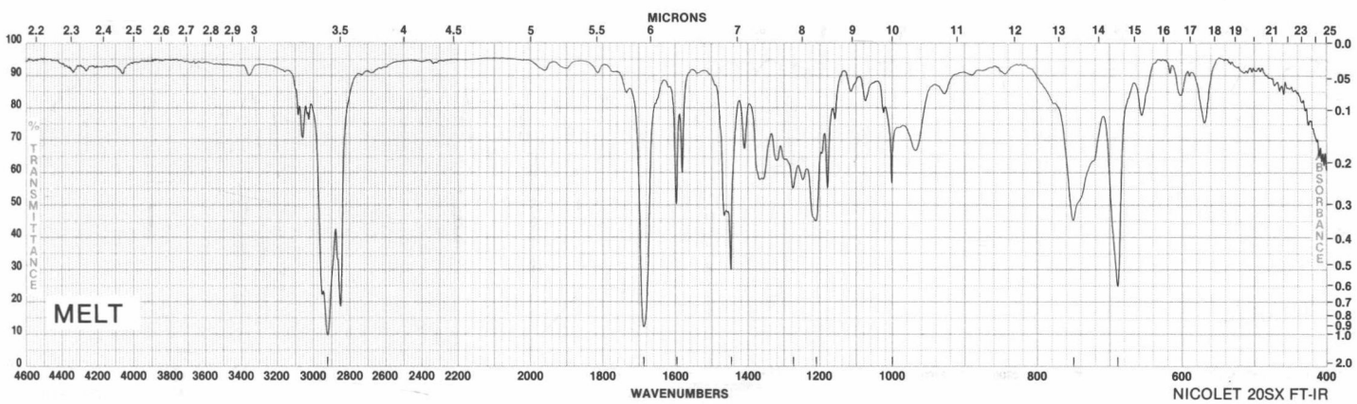
23200-9 *CAS [6048-82-4]*
Decanophenone, 95%

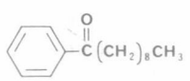
FW 232.37 | mp 34-36°C | bp 168°C/5mm | Fp >235°F

NMR II, 2,9B

2926.3 1448.4 1001.9 | 1688.9 1275.5 751.4 | 1597.7 1212.2 690.2

C



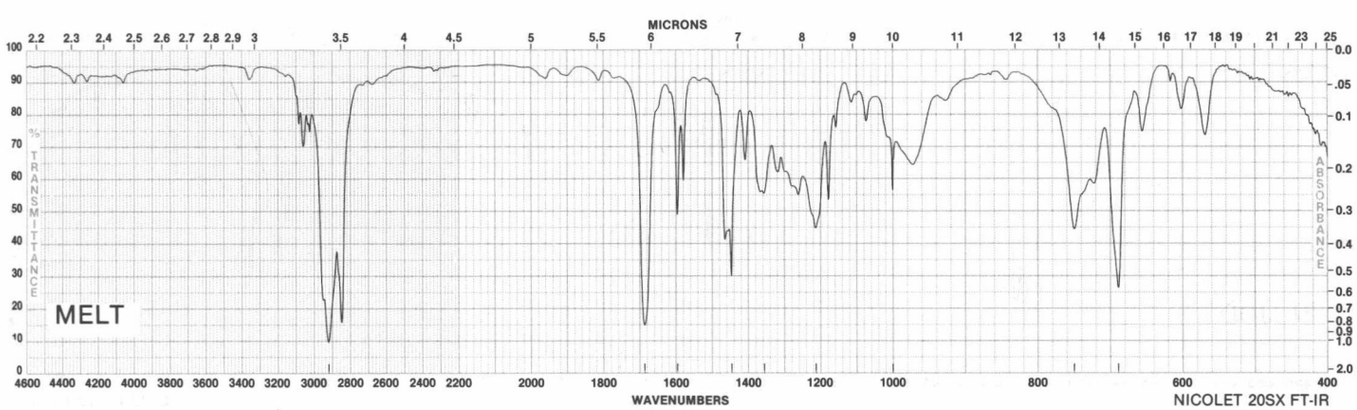


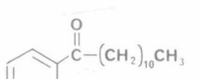
25271-9 *CAS [1674-38-0]*
Dodecanophenone, 98%

FW 260.42 | mp 45-47°C | bp 215°C/16mm | Fp >235°F

2924.7 1448.4 1001.9 | 1689.2 1357.7 750.5 | 1597.8 1215.4 690.1

D





AROMATIC KETONES

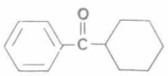
A

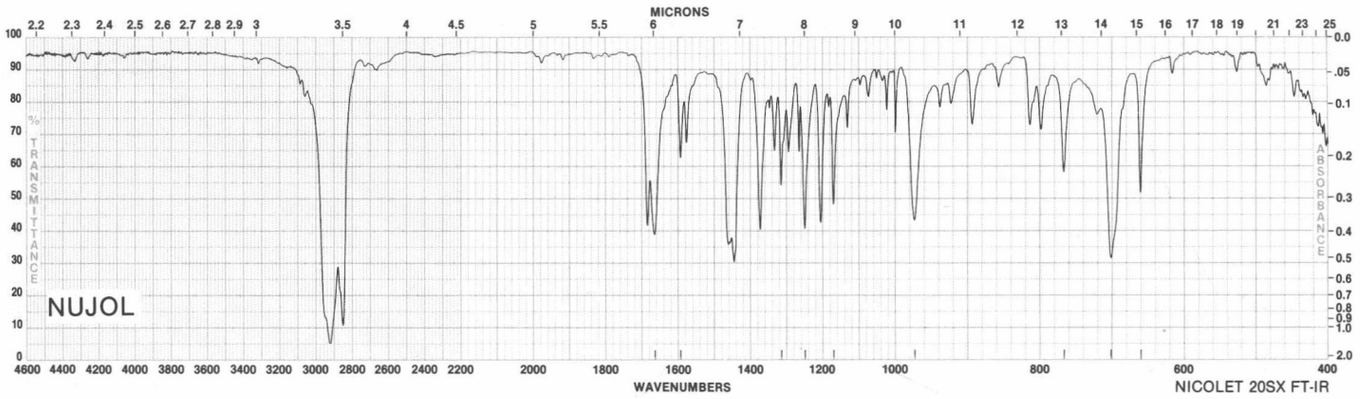
13921-1 *CAS [712-50-5]*
Cyclohexyl phenyl ketone, 98%

FW 188.27
mp 55-57°C
Fp >235°F

IR III, 854H
NMR II, 2,12A

1667.3 1251.8 768.1
1595.6 1172.6 703.0
1316.5 974.4 661.4





B

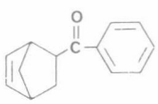
11506-1 *CAS [6056-35-5]*
2-Benzoyl-5-norbornene, tech., 90%

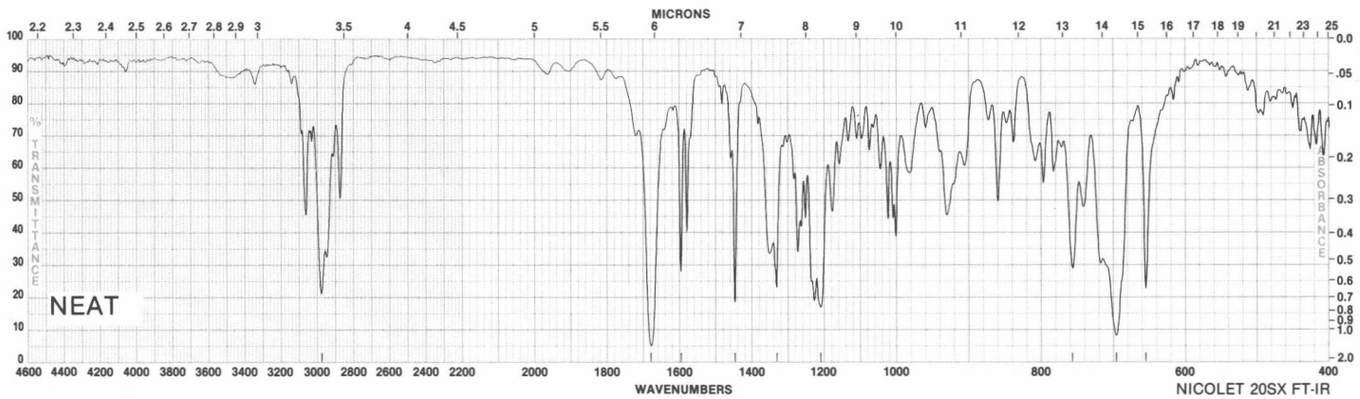
FW 198.27
bp 124°C/2mm
d 1.115

Fp >235°F
n_D^{20} 1.5680

IR III, 855A
NMR II, 2,12B

2973.8 1447.6 756.6
1680.3 1332.4 696.3
1597.1 1210.6 654.8





C

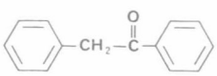
D436-9 *CAS [451-40-1]*
Deoxybenzoin, 97%

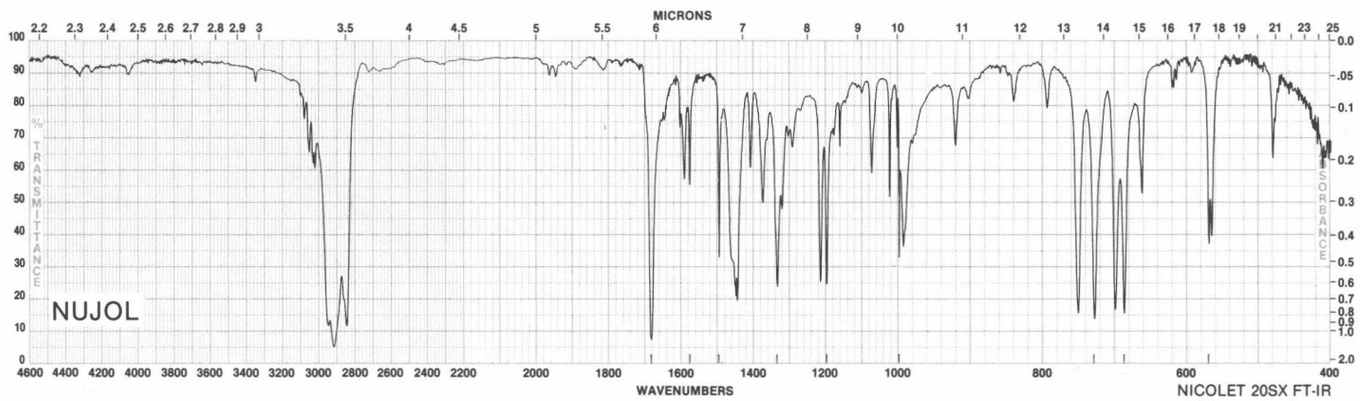
FW 196.25
mp 55-56.5°C
bp 320°C

Fp >235°F

IR III, 855C
NMR II, 2,12C

1685.7 1337.7 729.5
1579.3 1201.3 688.1
1498.9 1000.6 570.9





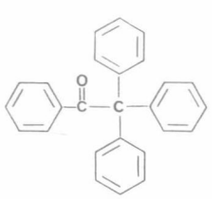
D

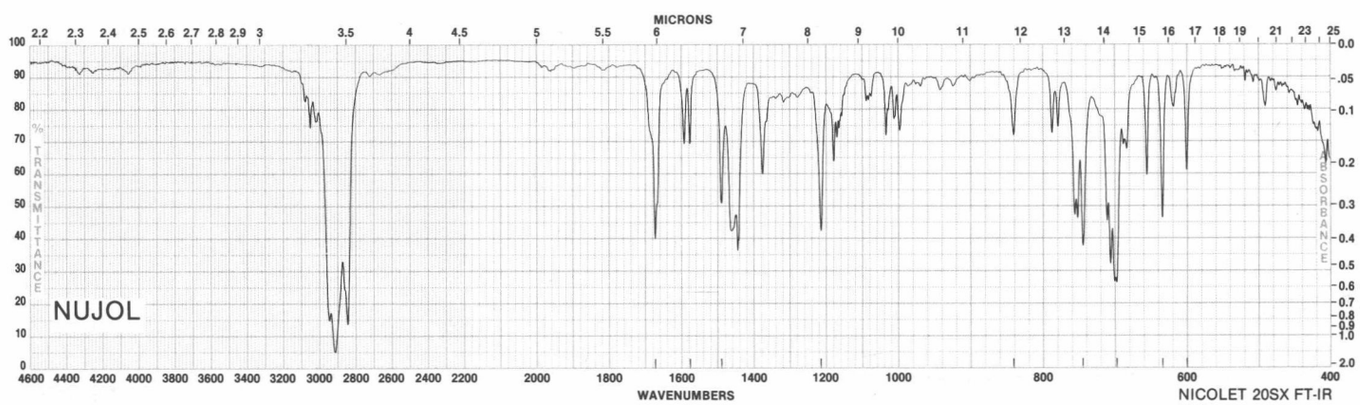
21669-0 *CAS [466-37-5]*
2,2,2-Triphenylacetophenone, 98%

FW 348.45
mp 182-184°C

IR III, 855D
NMR II, 2,45C

1675.6 1216.8 698.8
1579.3 841.7 635.2
1491.6 745.6 601.3





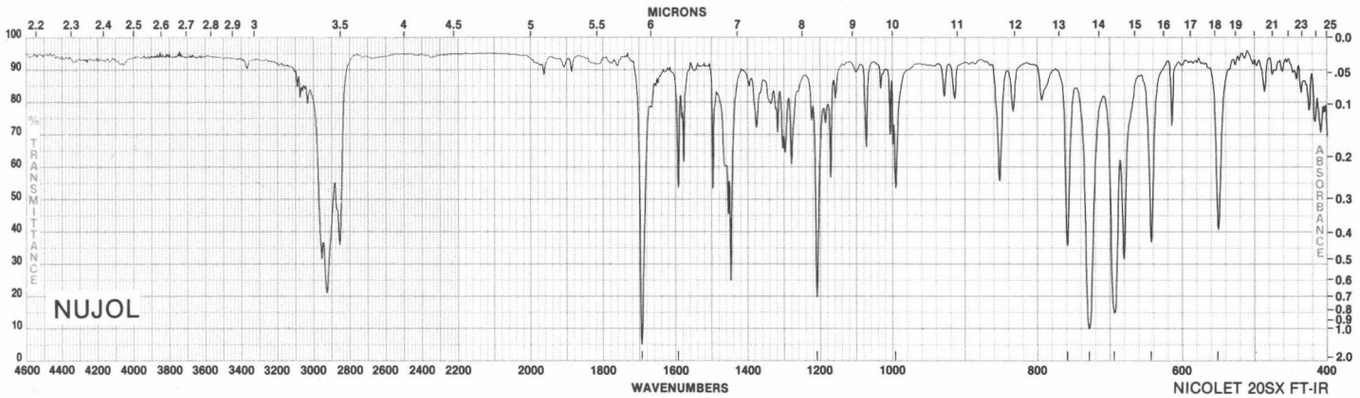
15750-3 *CAS [447-31-4]*
Desyl chloride, 95%

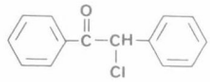
FW 230.69
mp 62-63°C

IR III, 855E
NMR II, 2,45B

3410.9 1211.1 694.4
1695.1 758.9 643.6
1497.3 729.3 550.9

A





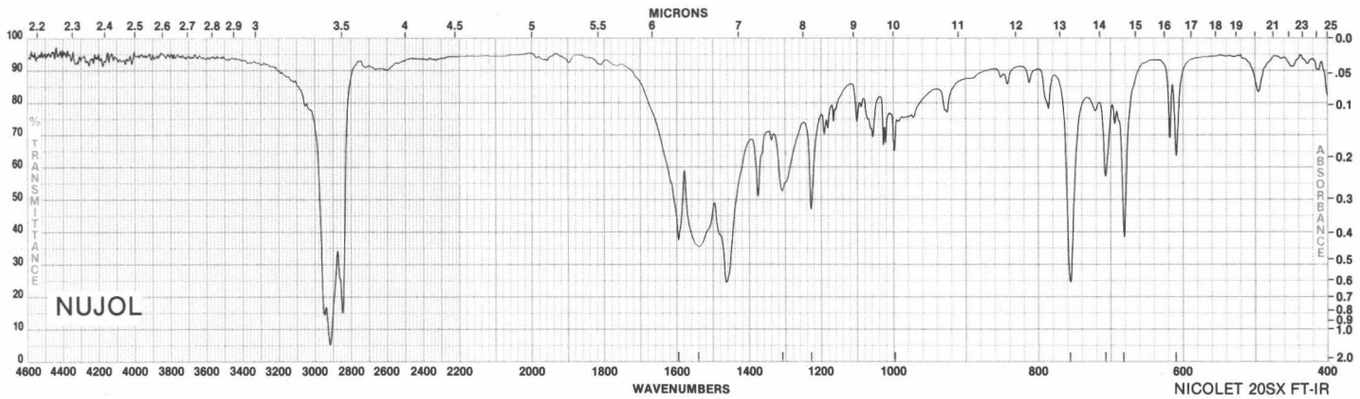
D3345-4 *CAS [120-46-7]*
Dibenzoylmethane, 98%

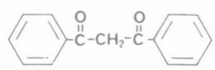
FW 224.26
mp 77.5-79°C
bp 221°C/18mm

IR III, 855H
NMR II, 2,12D
Merck 10,2980

1597.6 1229.7 707.4
1541.9 999.3 681.6
1310.2 756.0 609.7

B





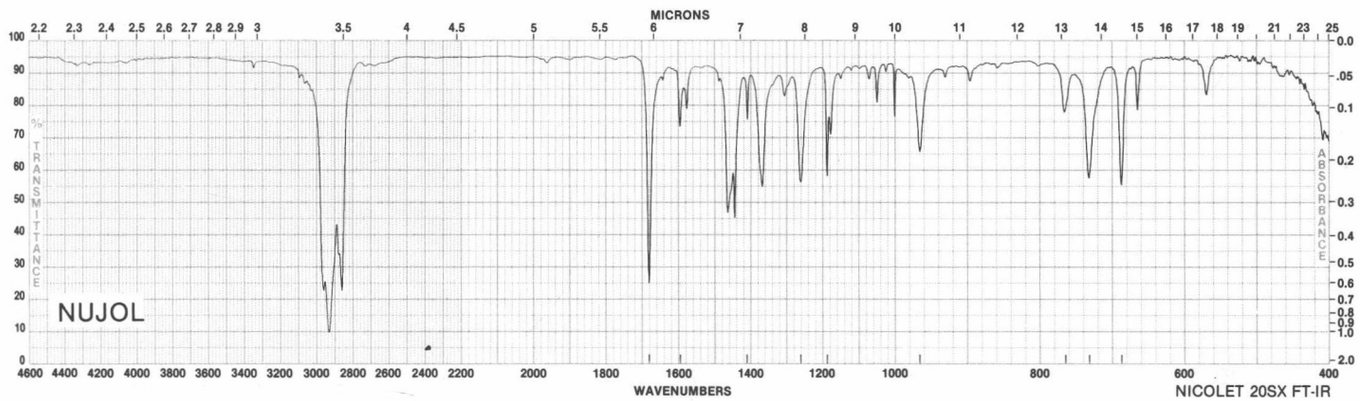
D3280-6 *CAS [3375-38-0]*
1,4-Dibenzoylbutane, 97%

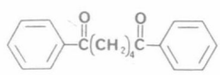
FW 266.34
mp 106-108°C

IR III, 856A
NMR II, 2,13A

1681.2 1262.4 765.4
1596.3 1189.3 731.8
1412.0 966.5 687.2

C





M2659-3 *CAS [577-16-2]*
2′-Methylacetophenone, 98%

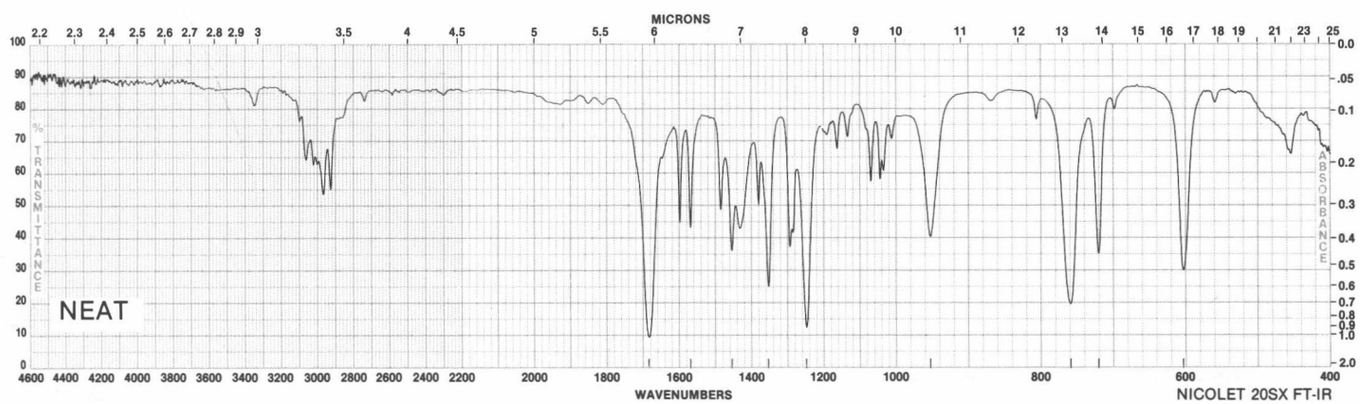
FW 134.18
bp 214°C
d 1.026

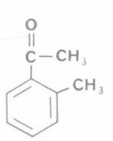
Fp 168°F
n_D^{25} 1.5302

IR III, 856C
NMR II, 2,24C

1685.5 1354.6 759.7
1570.1 1250.2 721.0
1455.5 953.6 603.5

D





AROMATIC KETONES

A

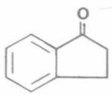
I-230-4 *CAS [83-33-0]*
1-Indanone, 99 + %

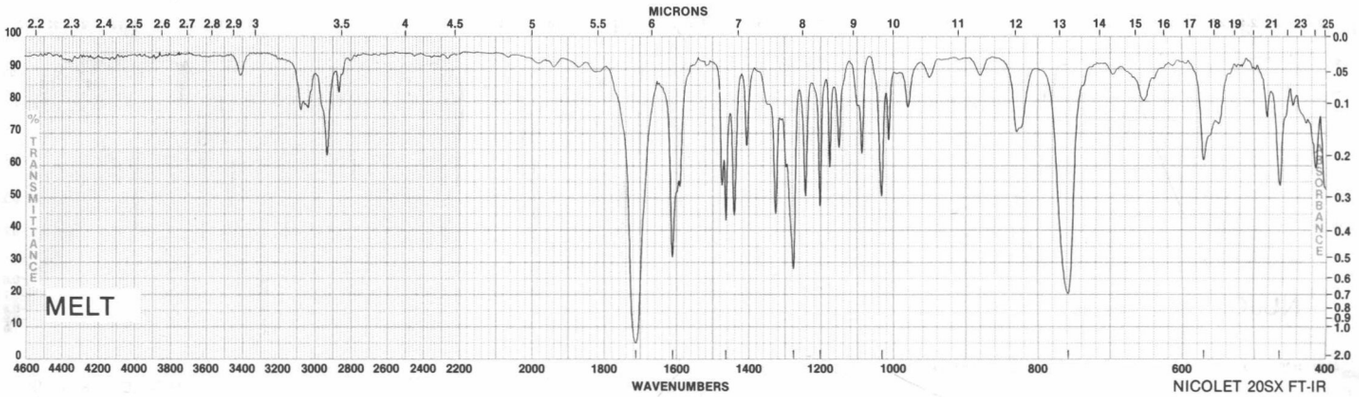
FW 132.16
mp 40-42°C
bp 243-245°C

d 1.103
Fp 233°F

IR III, 856D
NMR II, 2,13B

2925.2 1462.9 1033.0
1713.0 1277.0 758.2
1610.2 1202.8 464.0





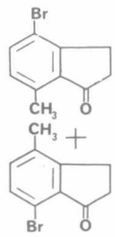
B

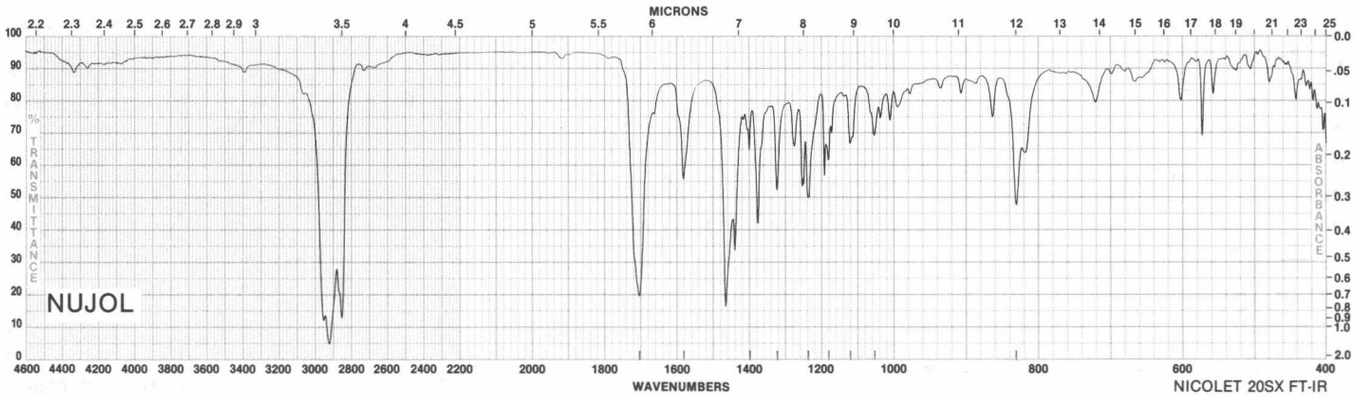
22035-3
4(7)-Bromo-7(4)-methyl-1-indanone, mixture of isomers

FW 225.09

IR III, 856E

1705.7 1323.5 1122.0
1582.8 1238.6 1055.0
1400.4 1181.5 831.5





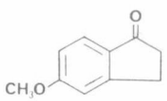
C

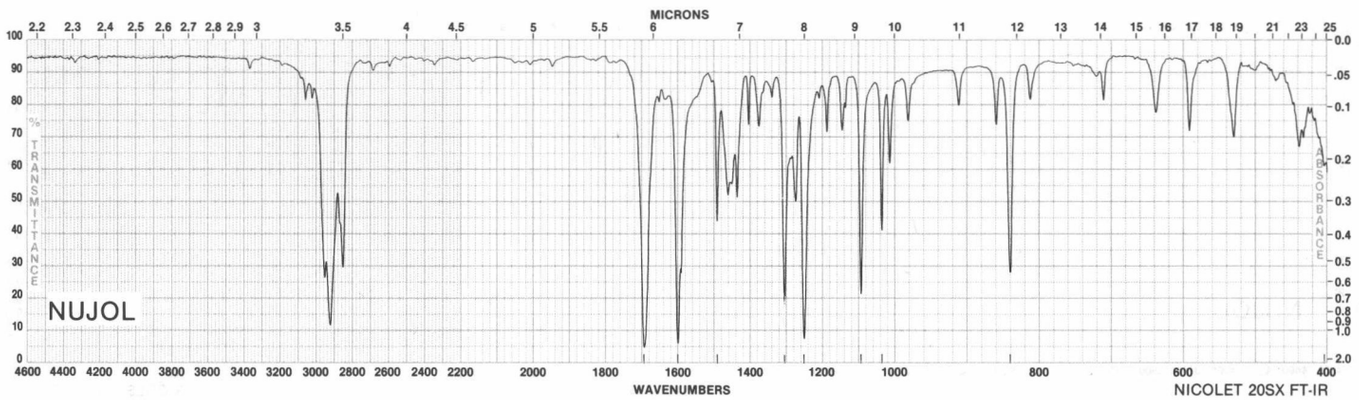
18353-9 *CAS [5111-70-6]*
5-Methoxy-1-indanone, 98%

FW 162.19
mp 108-110°C

IR III, 856F
NMR II, 2,13C

1695.7 1308.2 1038.1
1601.9 1254.2 841.9
1493.1 1096.0 404.9





D

T1900-3 *CAS [529-34-0]*
α-Tetralone, 98%

FW 146.19
mp 5.3-6°C
bp 116°C/6mm

d 1.099
Fp >235°F
n_D^{20} 1.5685

IR III, 856H
NMR II, 2,14B

2944.9 1454.4 764.1
1682.5 1286.5 734.7
1601.5 1225.4 553.6