

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

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- 3) Phosphoranes 549C-551A
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7) Benzotriazoles	694B-695C
8) Benzoxazoles	696C-699D
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3) Pyrimidines	806C-839C
4) Pyrazines	839D-845D
5) Triazines	846A-851D

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1) Quinolines	853A-873A
2) Acridines	874A-877C
3) Isoquinolines	877D-879C
4) Cinnolines, Phthalazines, Quinazolines, Quinoxalines, Phenazines, etc.	879D-887C
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6) Miscellaneous	892D-899B

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3) Phthaleins	1006B-1009D
4) Fluoresceins	1010A-1015C
5) Sulfonephthaleins	1015D-1028C
6) Miscellaneous	1027A-1045D

Steroids and Indole Alkaloids 1047-1071

1) Steroids	1047A-1064D
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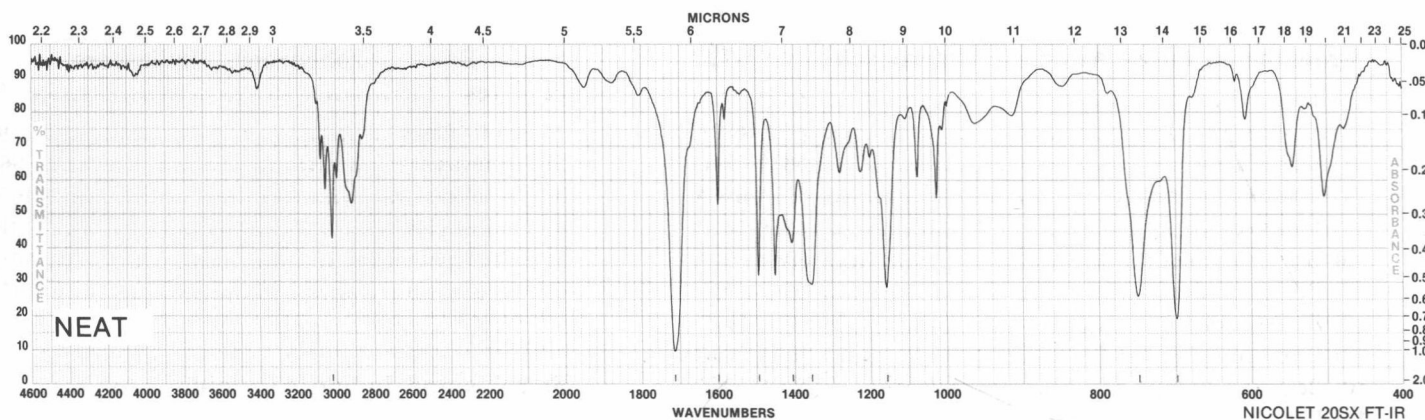
Deuterated Compounds 1073-1090**Silanes 1091-1125****Boranes 1127-1137****Organometallic and Arsenic Compounds 1139-1156**

1) Arsenic	1141A-1142D
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3) Tin	1143B-1148A
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5) Mercury	1148C-1150A
6) Organometallic Complexes	1150B-1156A

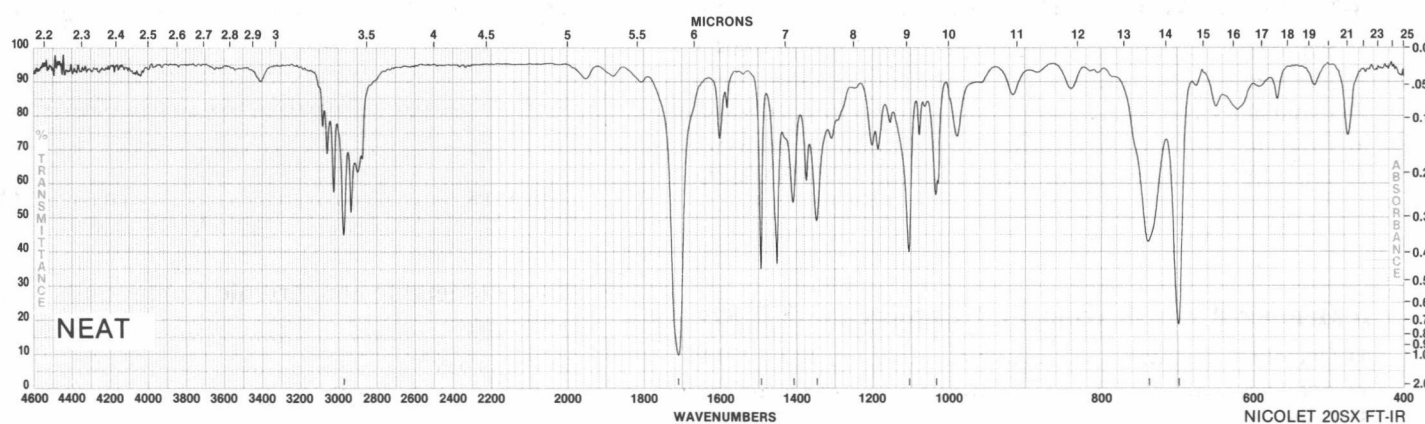
Polymers 1157-1225**Inorganics 1227-1303****Alphabetical Index 1304****Molecular Formula Index 1398****CAS Number Index 1534**

AROMATIC KETONES

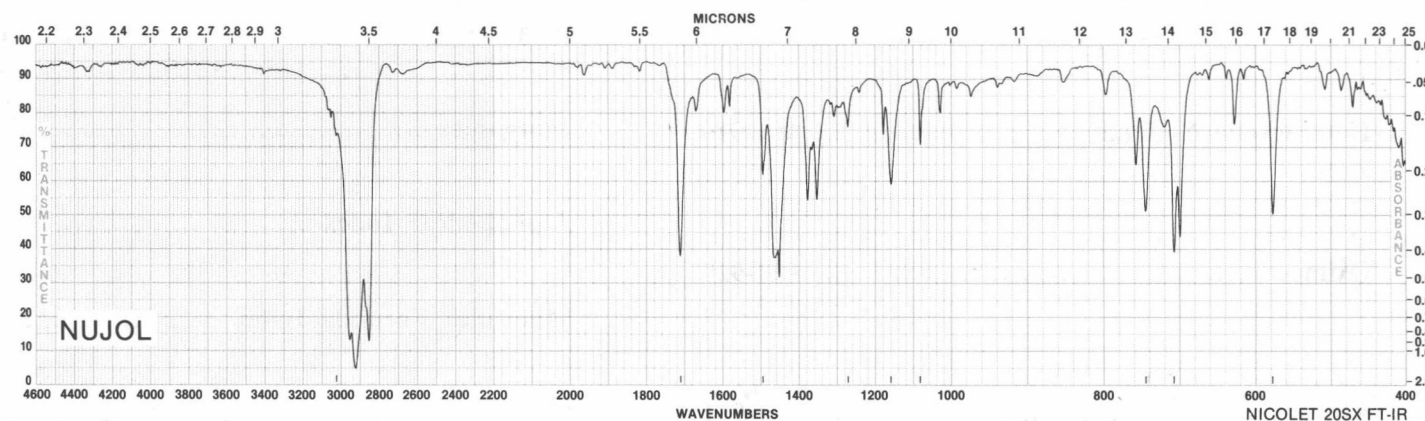
A

B1600-3 CAS [2550-26-7]
Benzylacetone, 98%FW 148.21
bp 235°C
d 0.989Fp 209°F
n_D 1.5122IR III, 848B
NMR II, 2,3A3027.3 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 0.998Fp 195°F
n_D 1.5122IR III, 848C
NMR II, 2,2D2977.5 1411.4 1037.8
1713.0 1350.1 739.1
1495.8 1108.8 699.2

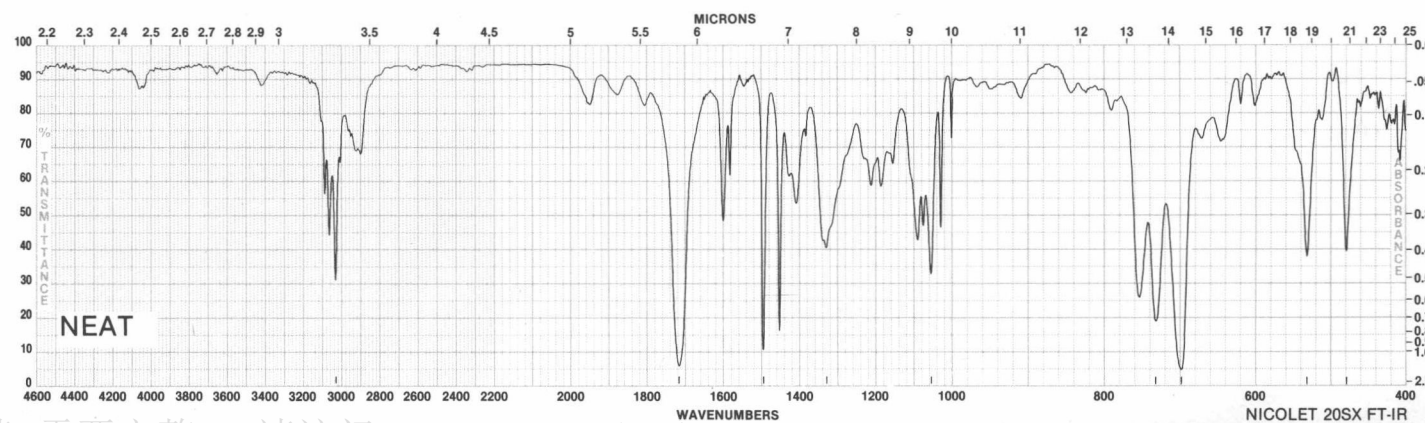
C

D20440-4 CAS [781-35-1]
1,1-Diphenylacetone, 98%FW 210.28
mp 59-63°CIR III, 848D
NMR II, 2,3C3025.3 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, 2,3D3029.0 1495.7 732.1
1715.6 1331.8 698.3
1601.8 1056.0 532.0

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AROMATIC KETONES

2

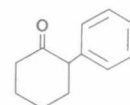
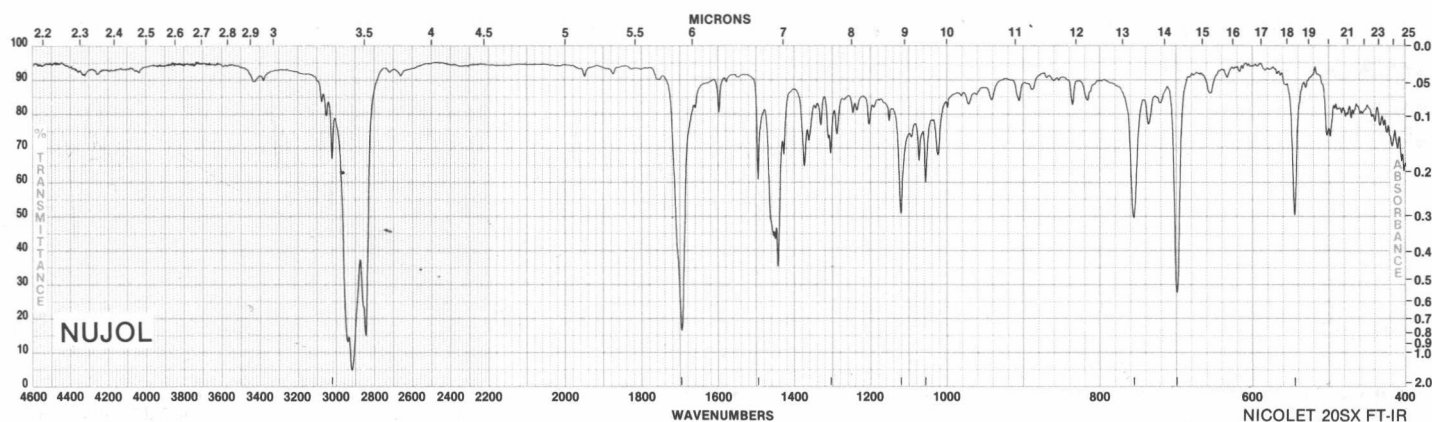
P2227-3 CAS [1444-65-1]
2-Phenylcyclohexanone, 98%

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



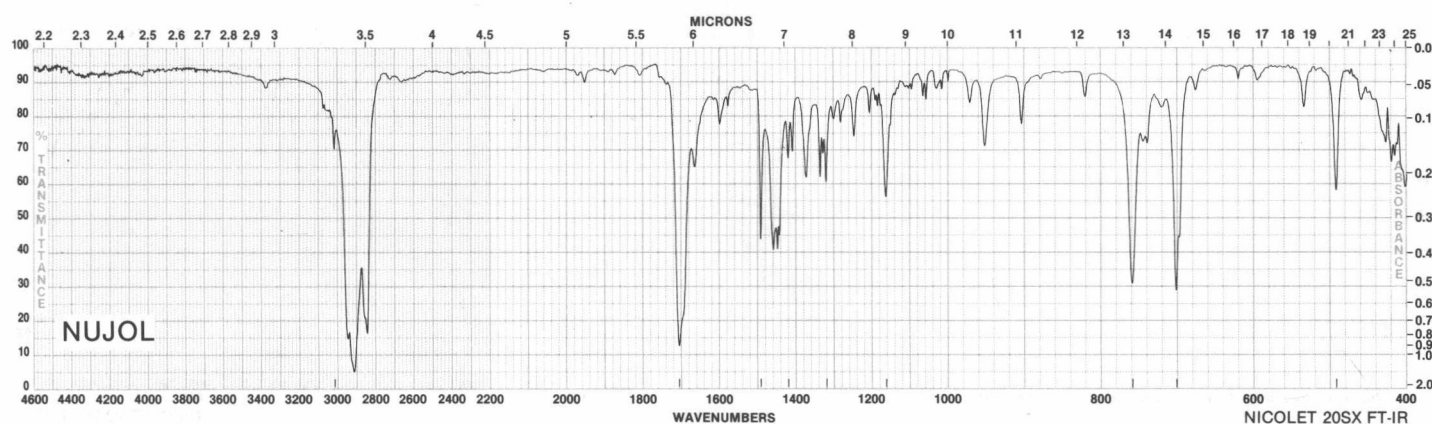
19623-1 CAS [4894-75-1]
4-Phenylcyclohexanone, 98 + %

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%

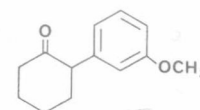
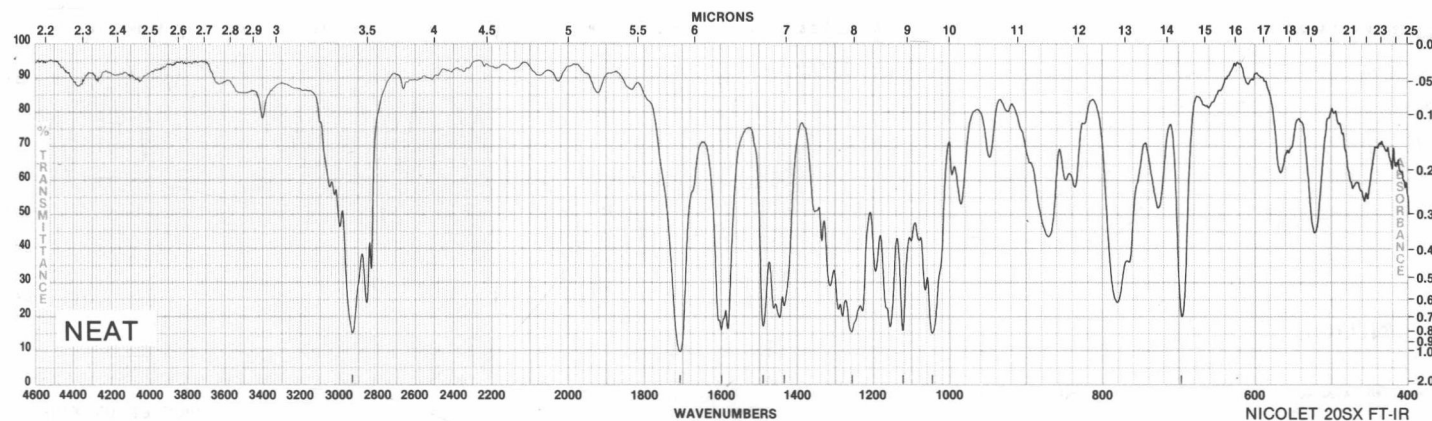
FW 204.27
d 1.100
Fp >235°F

n_D 1.5470

IR III, 848H

2936.9	1492.9	1124.9
1710.0	1437.1	1048.2
1602.1	1259.1	697.5

C



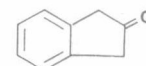
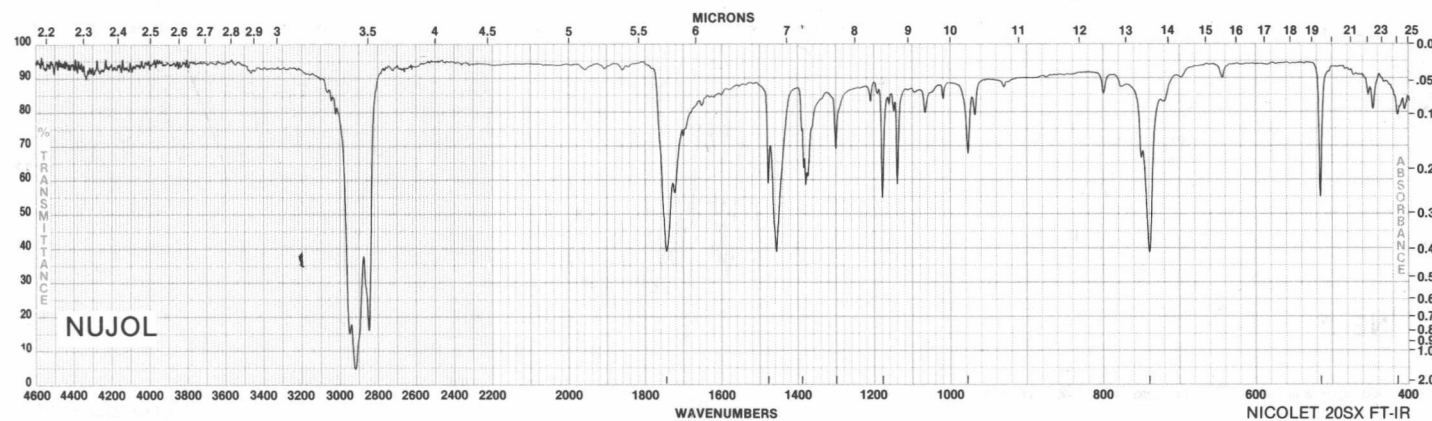
14669-2 CAS [615-13-4]
2-Indanone, 98%

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

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

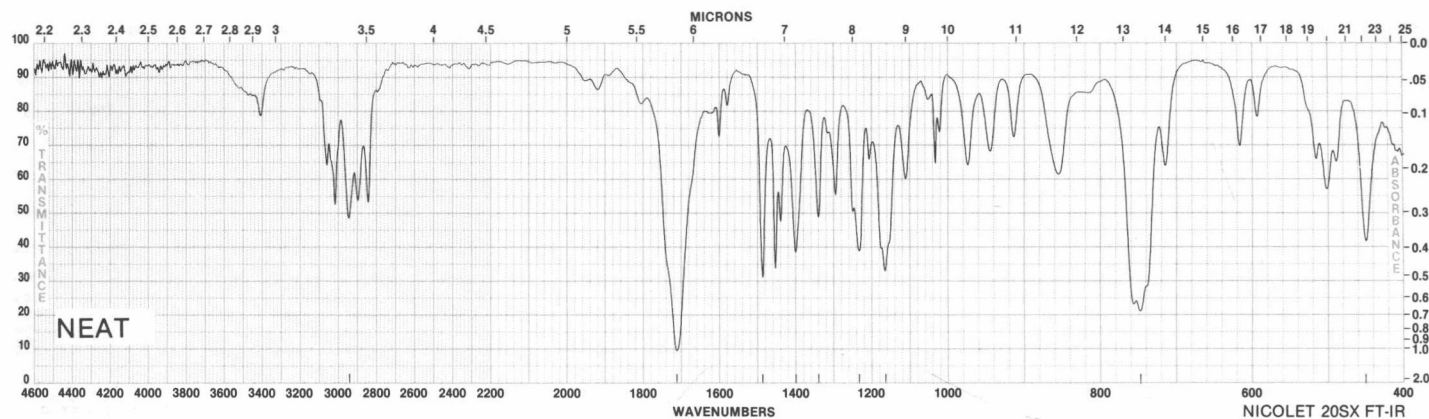
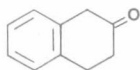
FW 146.19
 mp 18°C
 bp 131°C/11mm

d 1.106
 Fp > 235°F
 n_D 1.5598

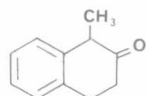
IR III, 849C
 NMR II, 2,4B

2949.8 1404.0 1169.4
 1716.3 1343.5 750.0
 1491.0 1237.5 452.5

A



B



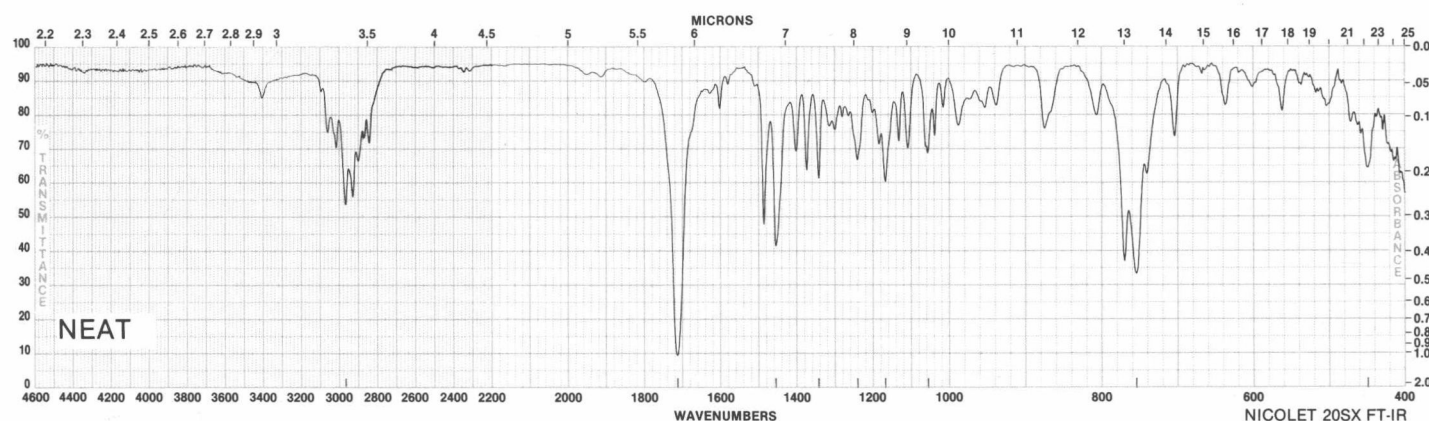
M8290-6 CAS [4024-14-0]
 1-Methyl-2-tetralone, tech., 90%

FW 160.22
 bp 261°C
 d 1.020

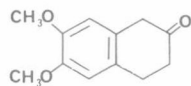
Fp > 235°F
 n_D 1.5530

IR III, 849D
 NMR II, 2,5A

2975.0 1344.6 1058.3
 1716.0 1243.4 755.0
 1457.8 1169.9 449.9



C

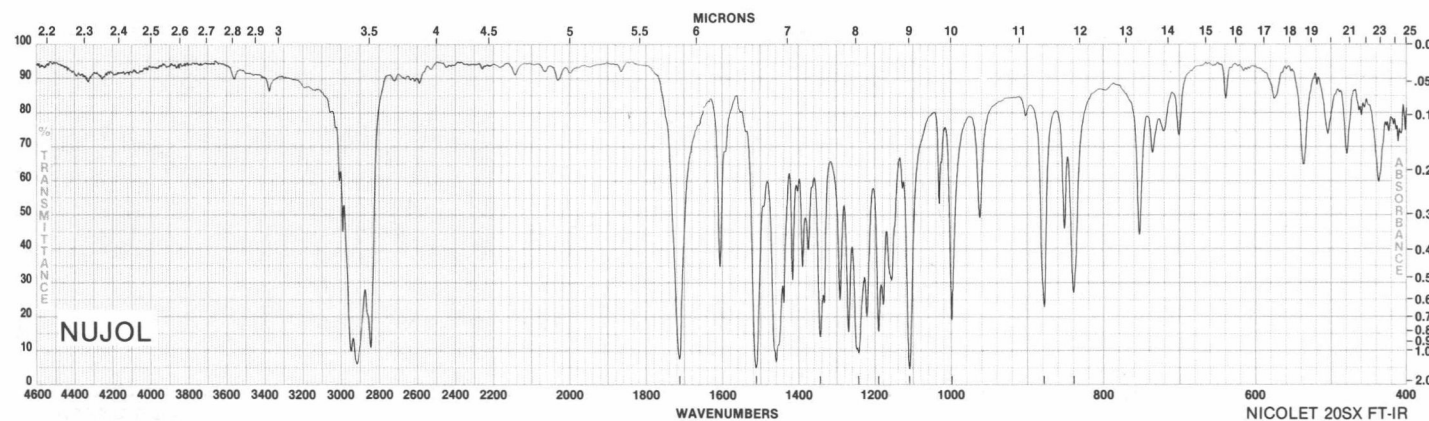


22926-1 CAS [2472-13-1]
 6,7-Dimethoxy-2-tetralone, 99%

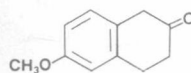
FW 206.24
 mp 87-89°C

NMR II, 2,4D

1716.0 1246.5 1002.4
 1515.1 1194.0 880.0
 1347.0 1113.3 841.4



D

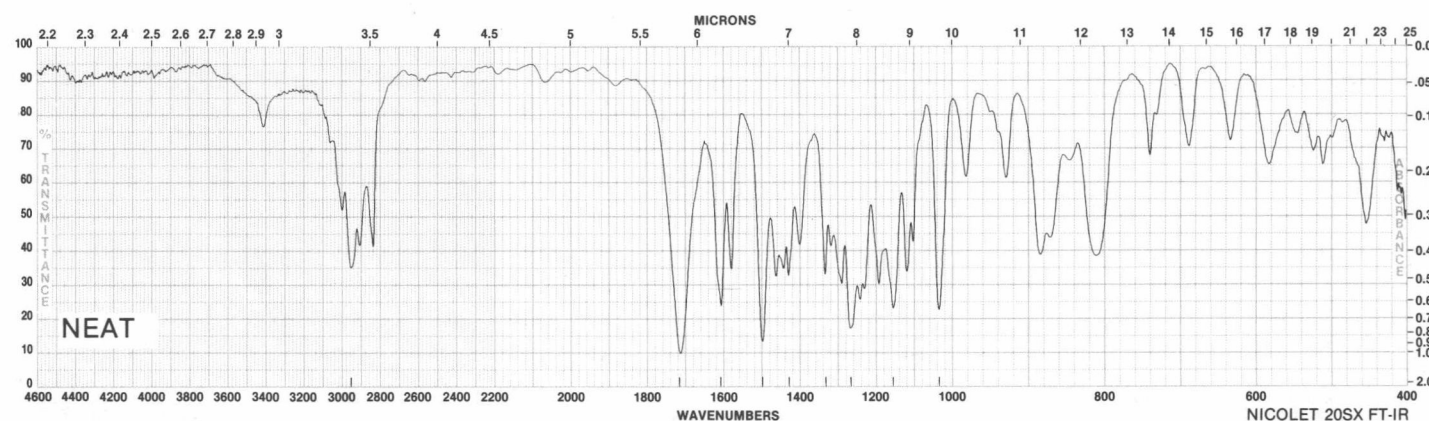


18406-3 CAS [2472-22-2]
 6-Methoxy-2-tetralone, 95%

FW 176.22
 Fp > 235°F
 n_D 1.5645

IR III, 849F

2952.9 1501.2 1269.8
 1716.5 1432.3 1157.9
 1610.0 1336.3 1037.4



AROMATIC KETONES

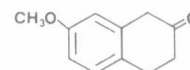
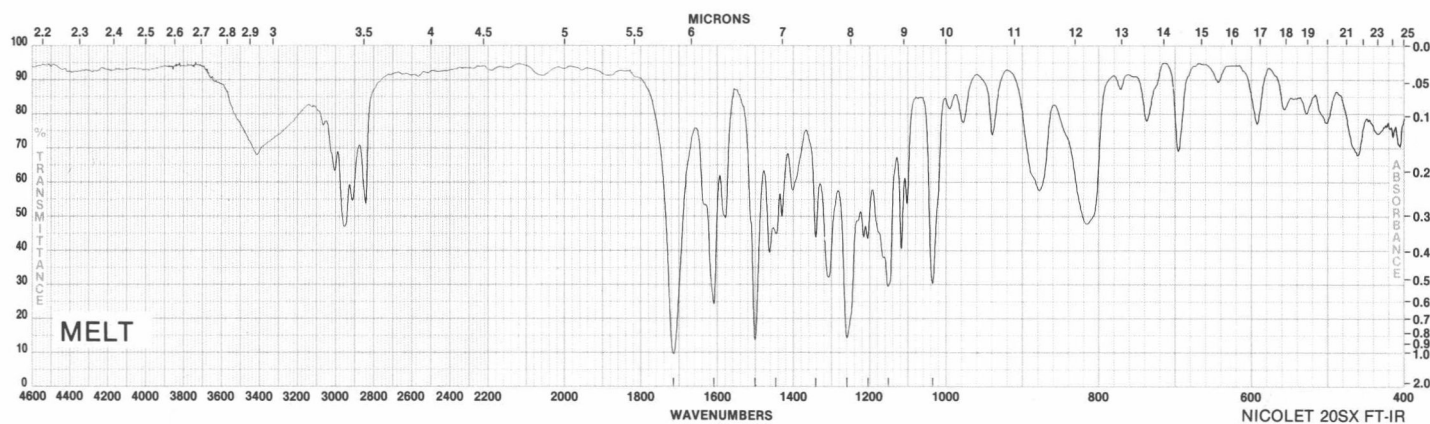
4

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 1.5595
d 1.130

1716.4 1447.6 1207.2
1610.9 1343.6 1154.3
1503.1 1261.7 1037.7

A

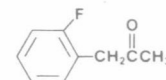
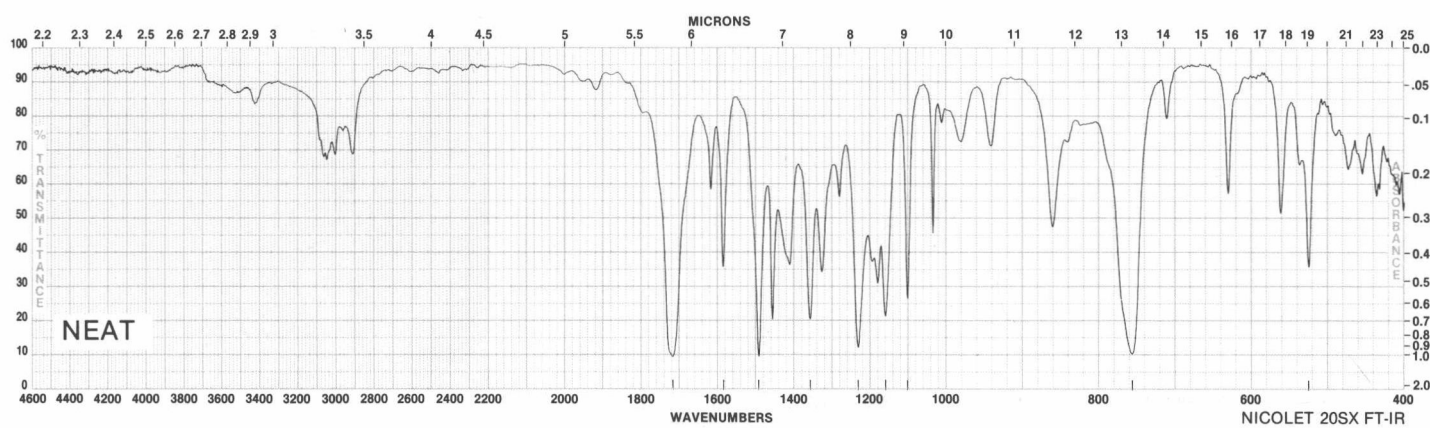


20874-4 CAS [2836-82-0]
(2-Fluorophenyl)acetone, 99%

FW 152.17 Fp 185°F IR III, 849H
bp 47°C/0.05mm n_D 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

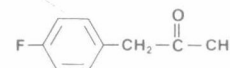
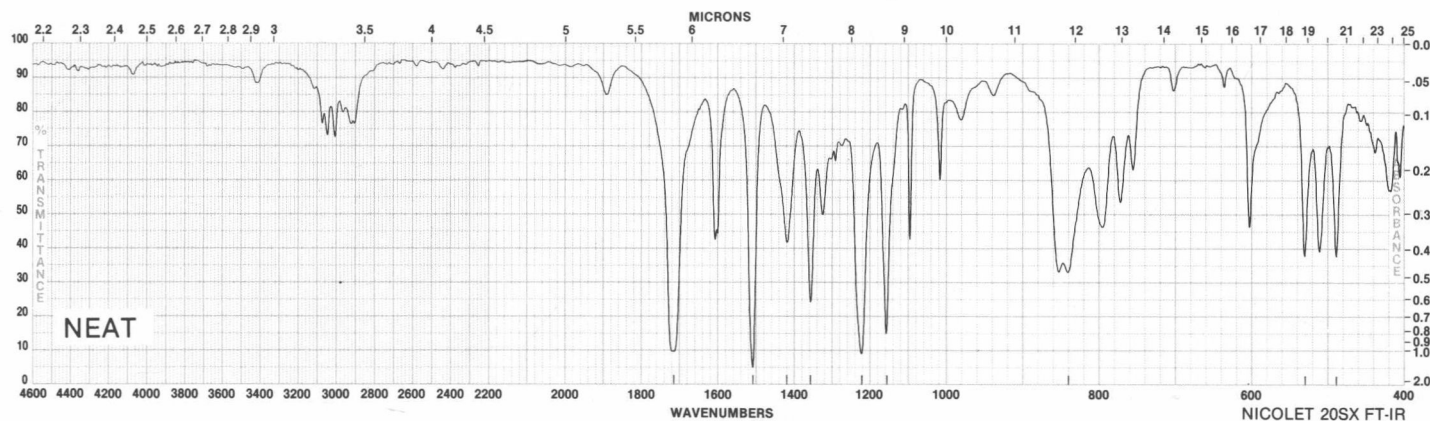


20945-7 CAS [459-03-0]
(4-Fluorophenyl)acetone, 98%

FW 152.17 Fp 197°F IR III, 850A
bp 107°C/18mm n_D 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

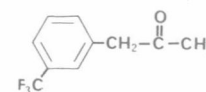
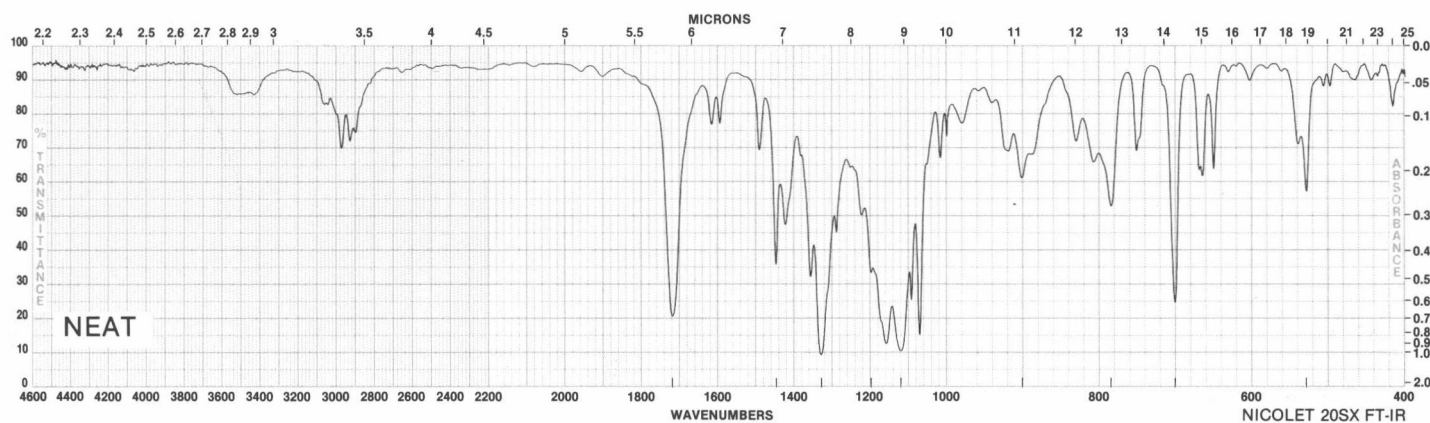


19379-8 CAS [21906-39-8]
3-(Trifluoromethyl)phenylacetone, 97%

FW 202.18 Fp 192°F IR III, 850B
bp 90°C/0.5mm n_D 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

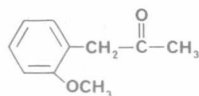
21398-5 CAS [5211-62-1]
2-Methoxyphenylacetone, 98%

FW 164.20 Fp >235°F
bp 130°C/10mm n_D 1.5250
d 1.054

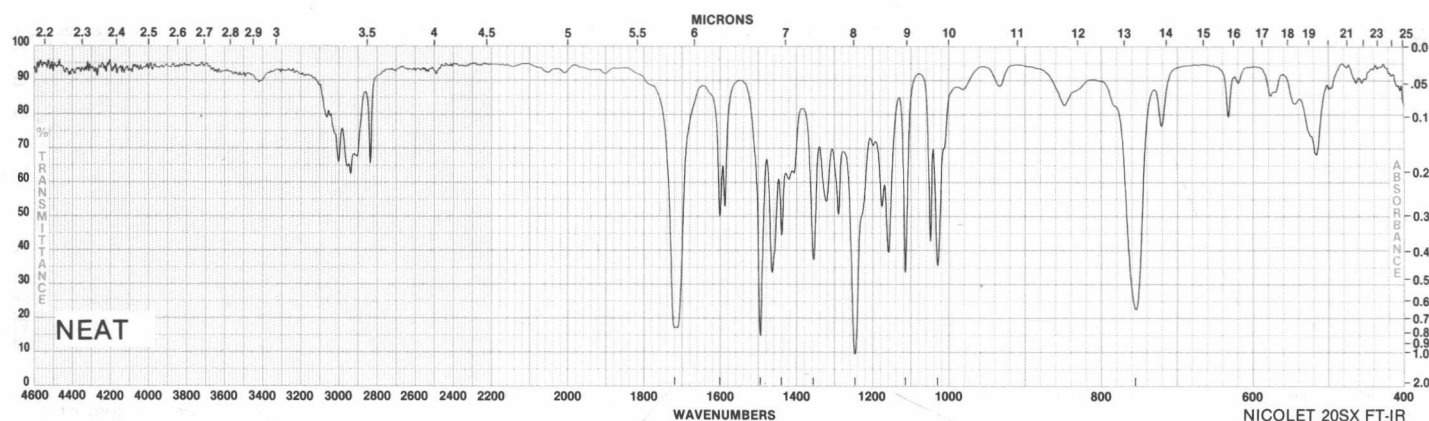
IR III, 850C

1721.1 1439.7 1115.3
1601.9 1355.9 1030.7
1496.0 1247.2 754.9

A



NEAT



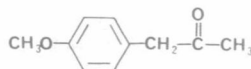
B

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

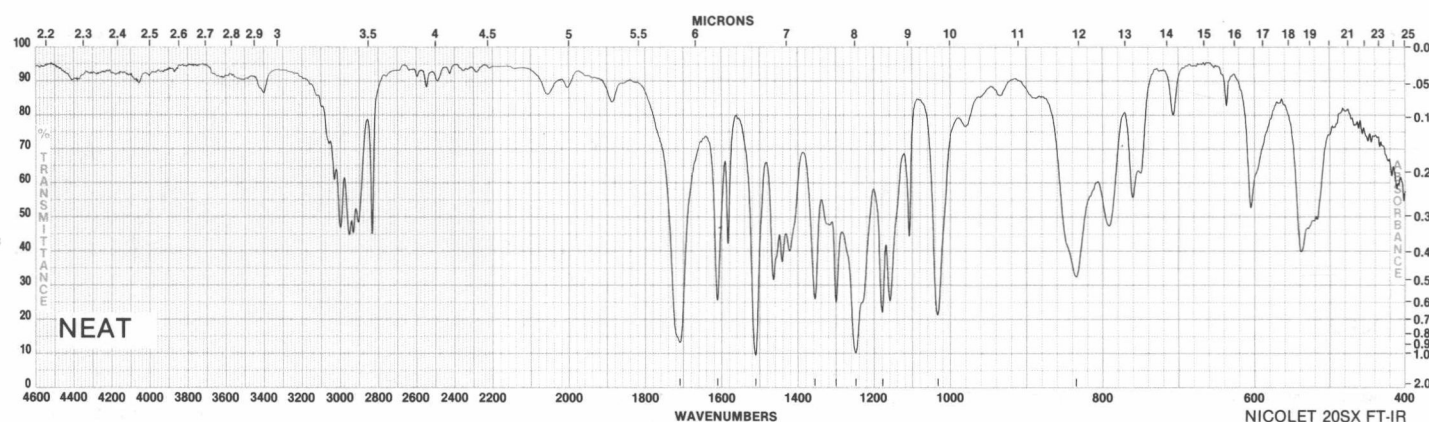
FW 164.20 Fp 215°F
bp 145°C/25mm n_D 1.5250
d 1.067

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



NEAT



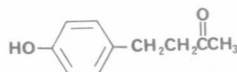
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17851-9 CAS [5471-51-2]
4-(4-Hydroxyphenyl)-2-butanone, 99%

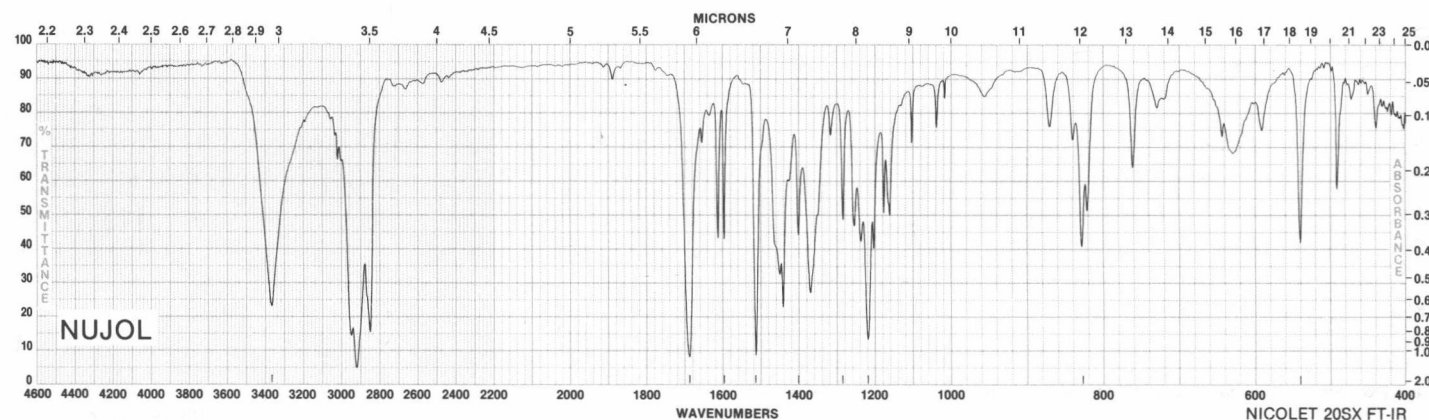
FW 164.20
mp 82-83°C

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



NUJOL



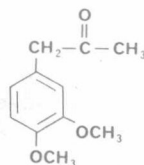
D

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

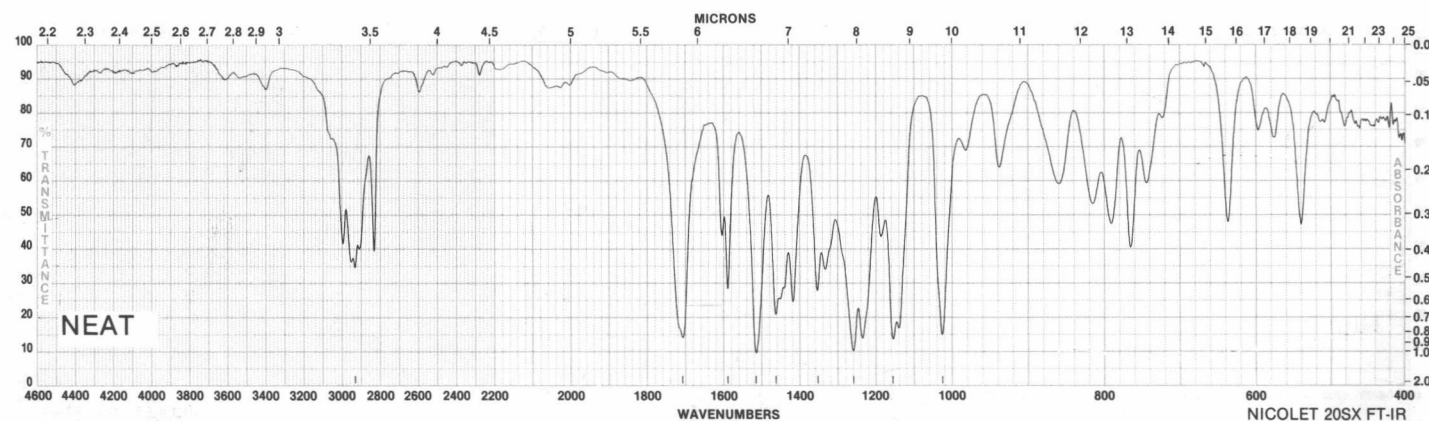
FW 194.23 n_D 1.5358
d 1.115 Fp >235°F

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



NEAT



AROMATIC KETONES

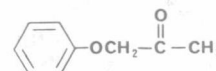
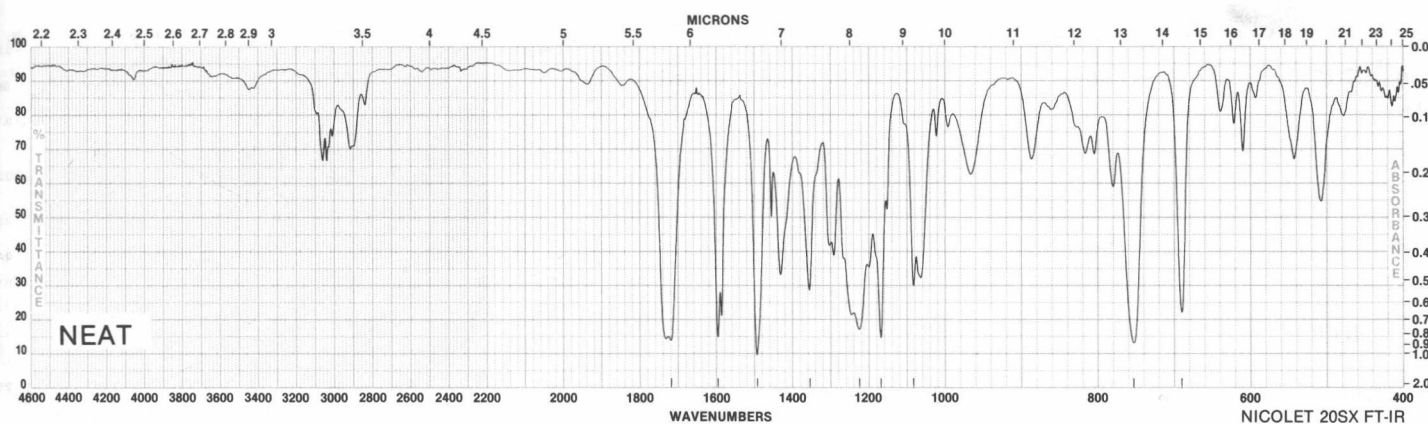
6

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

FW 150.18 Fp 185°F IR III, 851B
bp 229-230°C n_D 1.5210 NMR II, 2,5D
d 1.097

1722.3 1358.0 1085.5
1599.0 1228.4 754.9
1496.1 1171.7 691.7

A

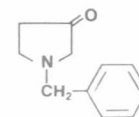
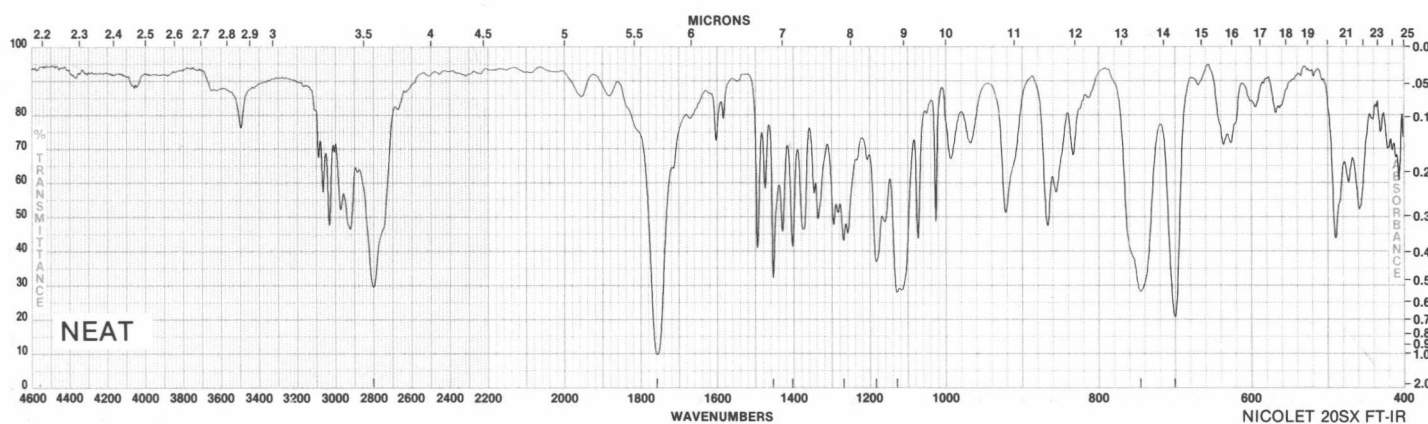


18517-5 CAS [775-16-6]
1-Benzyl-3-pyrrolidinone, 98%

FW 175.23 Fp >235°F IR III, 851E
bp 77°C/0.01mm n_D 1.5378 NMR II, 2,6A
d 1.091

2798.2 1403.6 1130.1
1756.7 1269.7 744.6
1453.9 1184.5 699.9

B

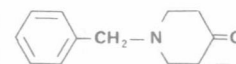
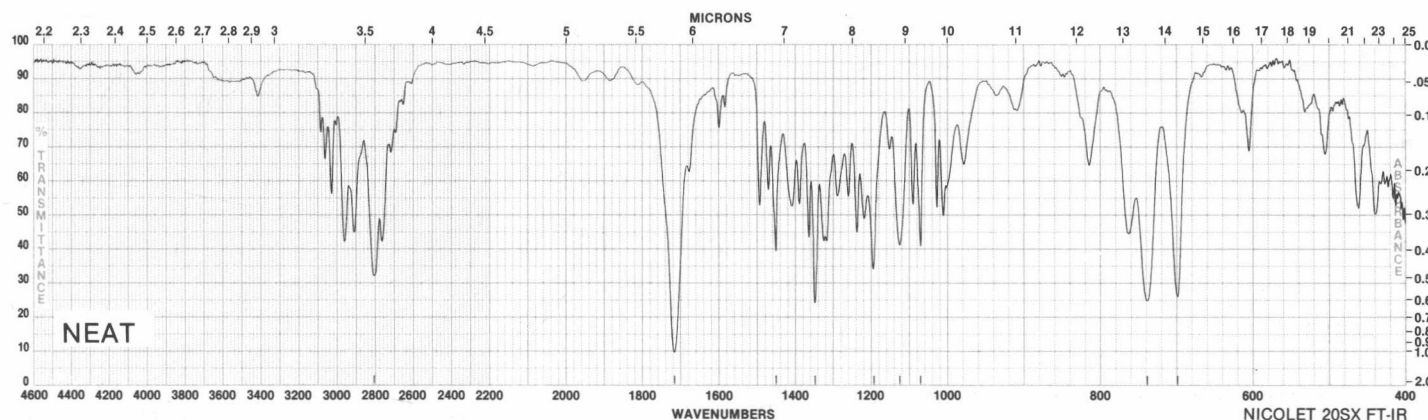


B2980-6 CAS [3612-20-2]
1-Benzyl-4-piperidone, 99 + %

FW 189.26 Fp >235°F IR III, 851F
bp 134°C/7mm n_D 1.5399 NMR II, 2,6B
d 1.021

2807.3 1349.6 1071.8
1718.4 1195.4 738.7
1453.4 1126.7 699.3

C

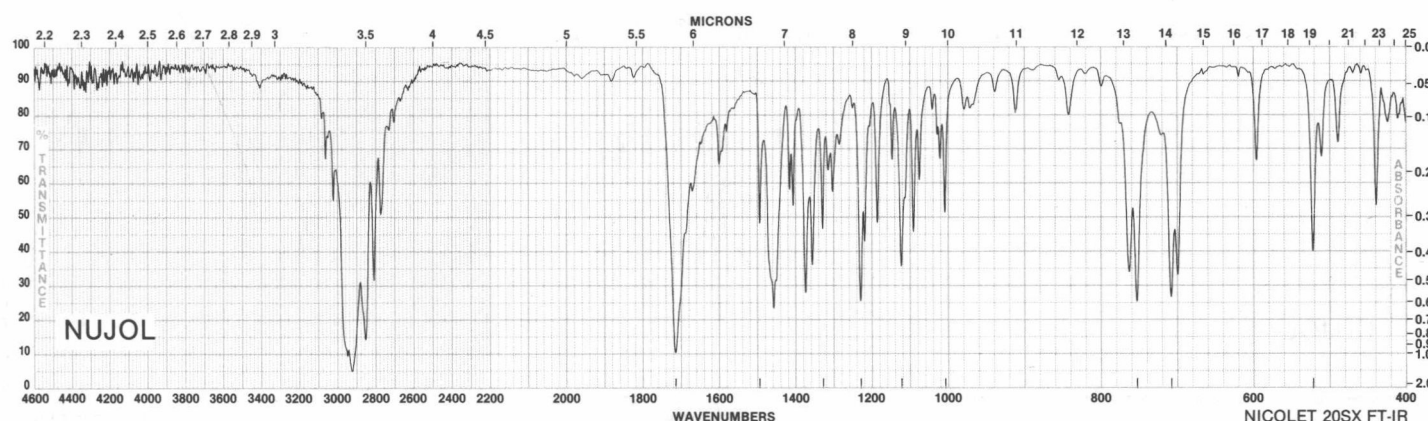


13138-5 CAS [39742-60-4]
1-Phenethyl-4-piperidone, 97%

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



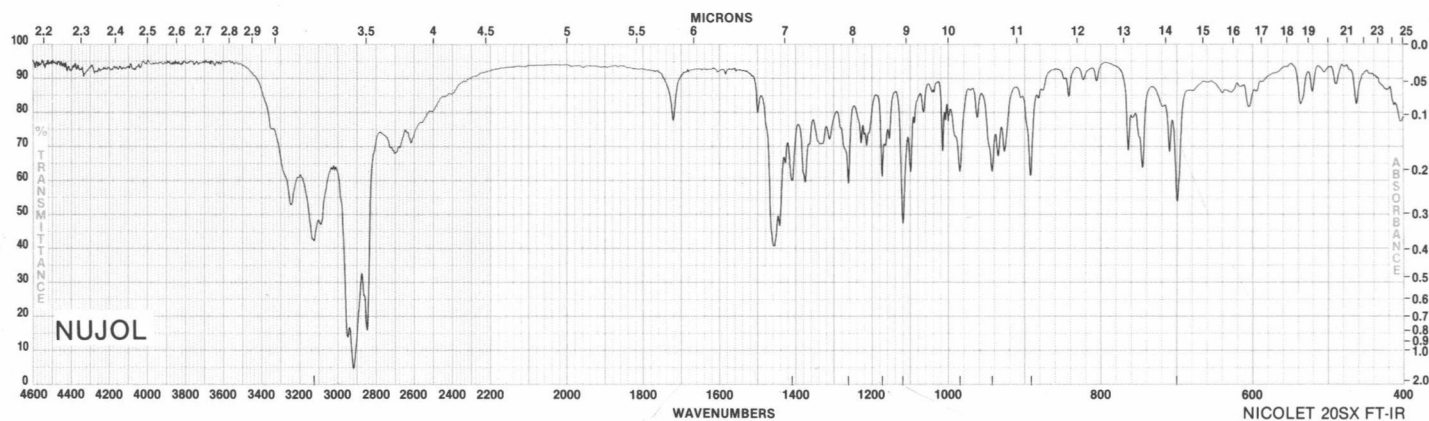
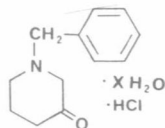
AROMATIC KETONES

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



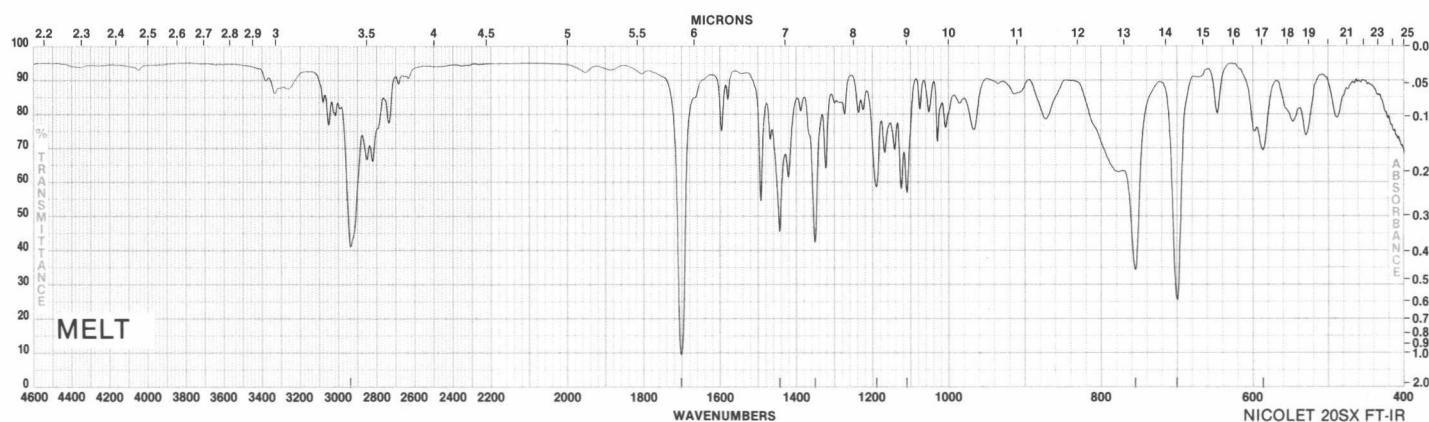
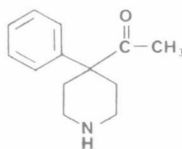
B

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

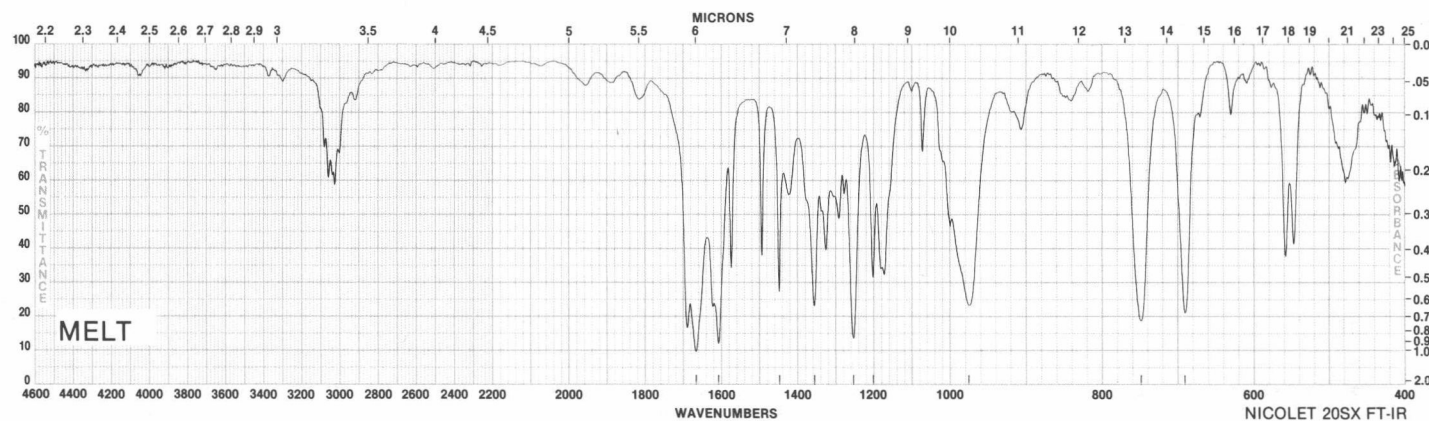
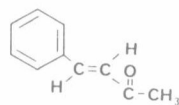
14788-5 CAS [122-57-6]
trans-4-Phenyl-3-buten-2-one, 99%

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



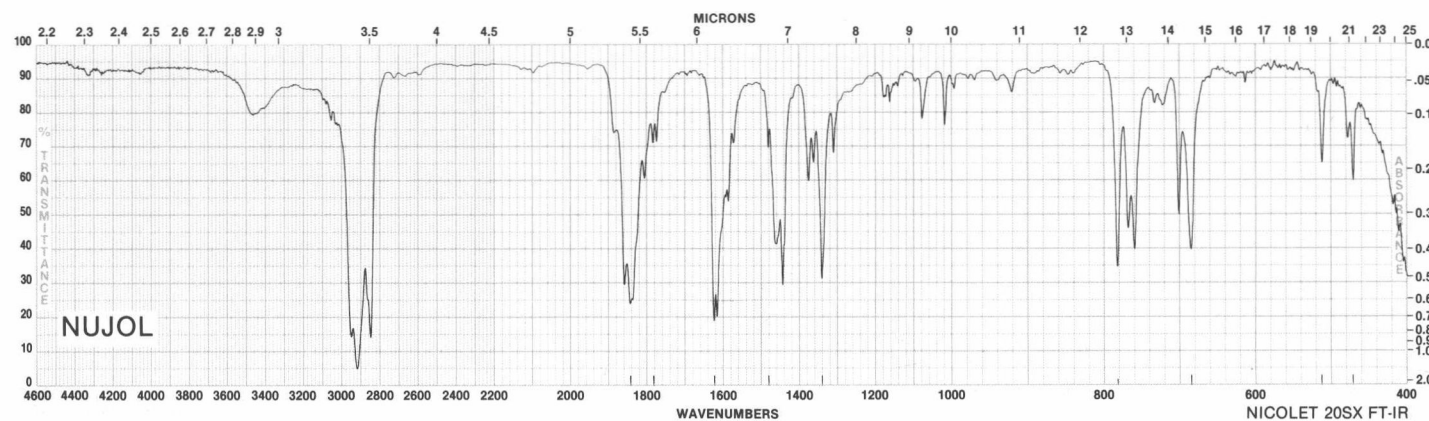
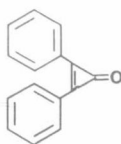
D

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

FW 206.24
mp 119-121°C

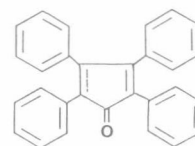
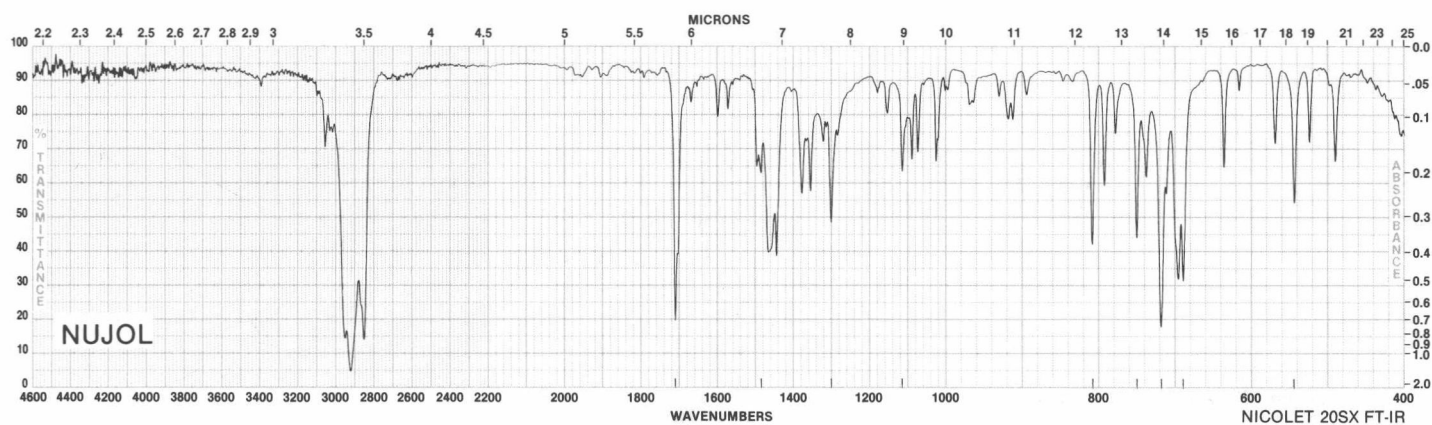
IR III, 853B
NMR II, 2,11A

1846.0	1482.7	685.2
1785.1	1343.0	512.5
1626.4	782.4	471.6



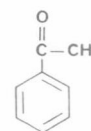
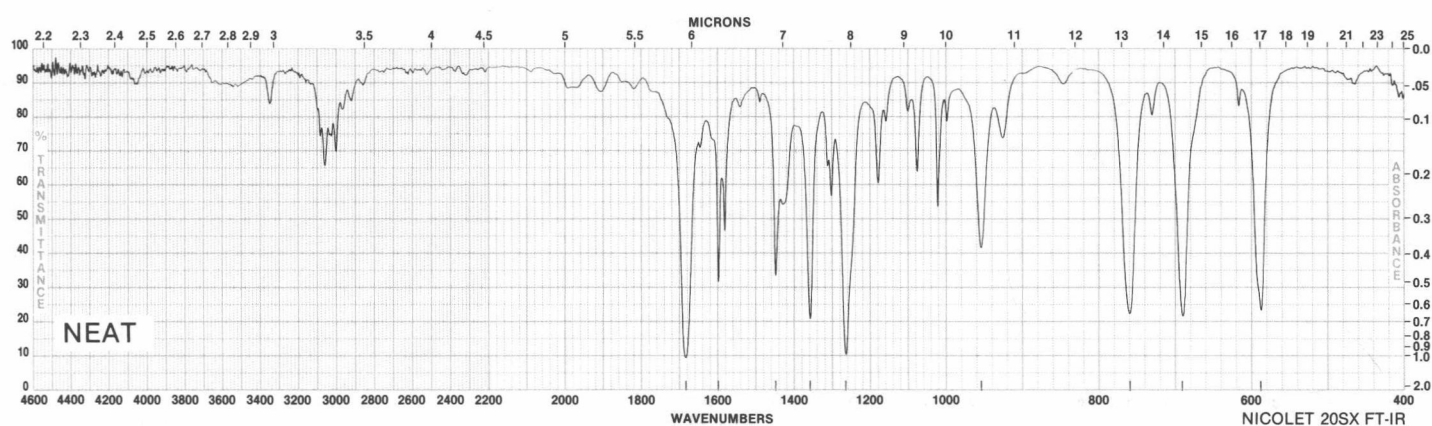
1710.5	1116.2	718.8
1485.0	809.3	689.8
1300.7	750.5	544.8

A



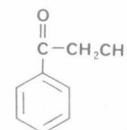
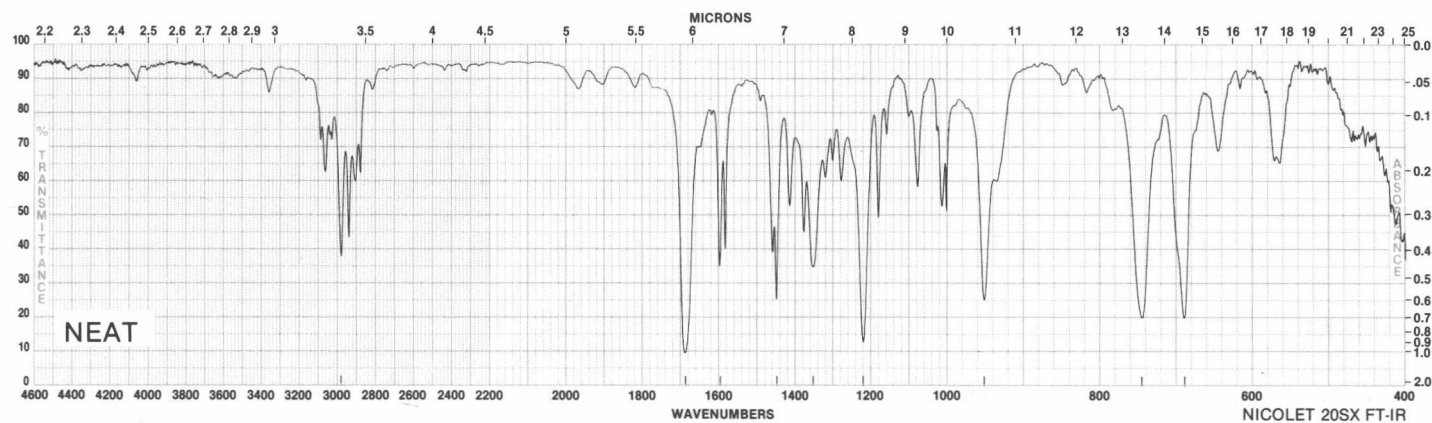
1685.2	1359.4	760.3
1599.0	1266.3	690.5
1449.3	955.4	588.3

B



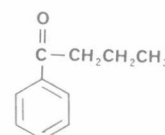
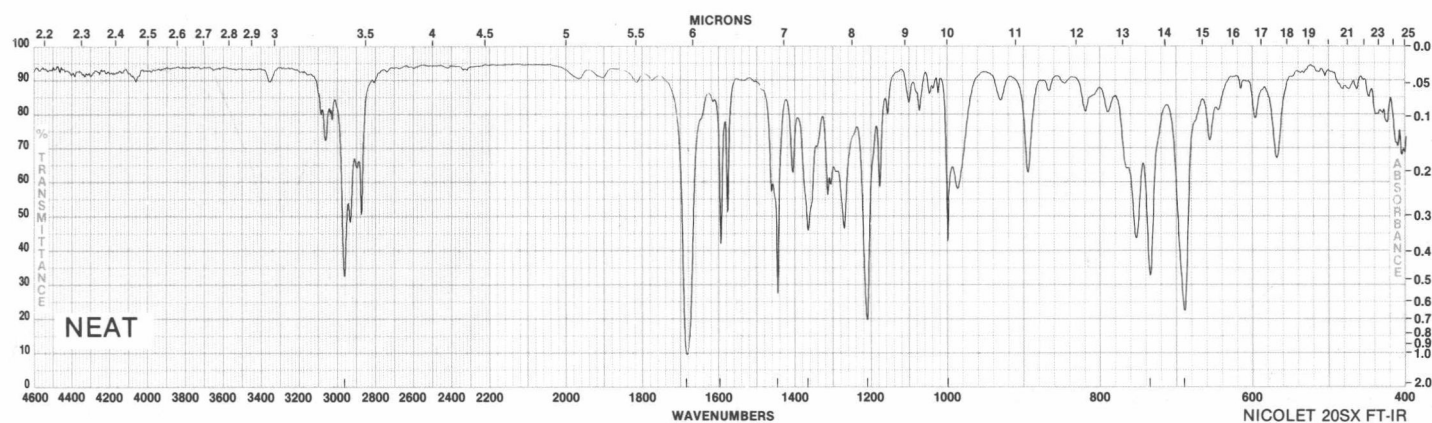
2978.5	1449.0	951.9
1688.0	1353.2	745.5
1597.3	1220.5	690.3

C



2962.9	1448.3	1002.2
1687.2	1368.7	735.5
1597.8	1213.4	690.6

D



AROMATIC KETONES

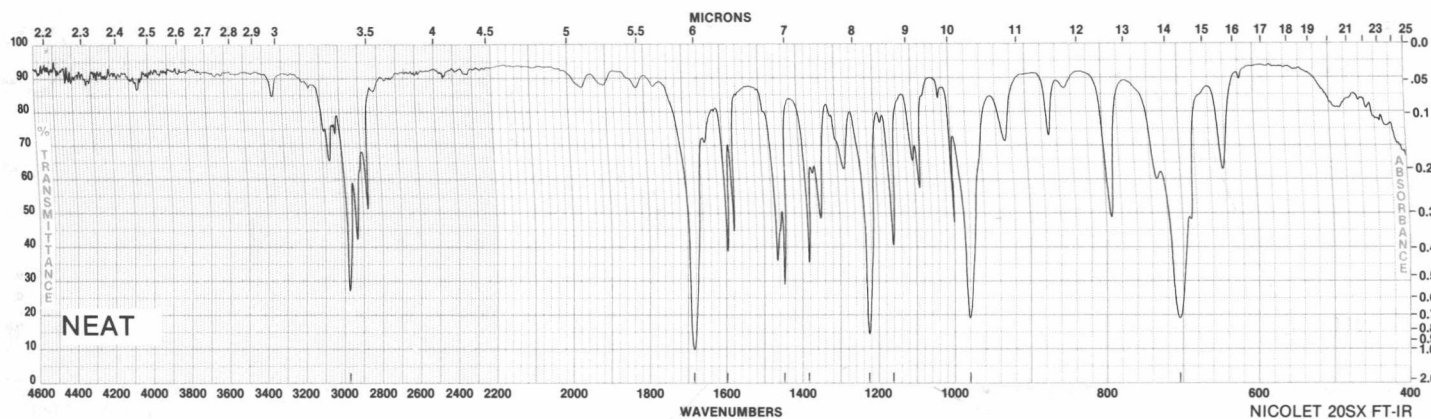
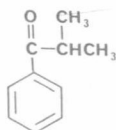
13036-2 CAS [611-70-1]
Isobutyrophenone, 97%

FW 148.21
bp 217°C
d 0.988

Fp 184°F
n_D 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



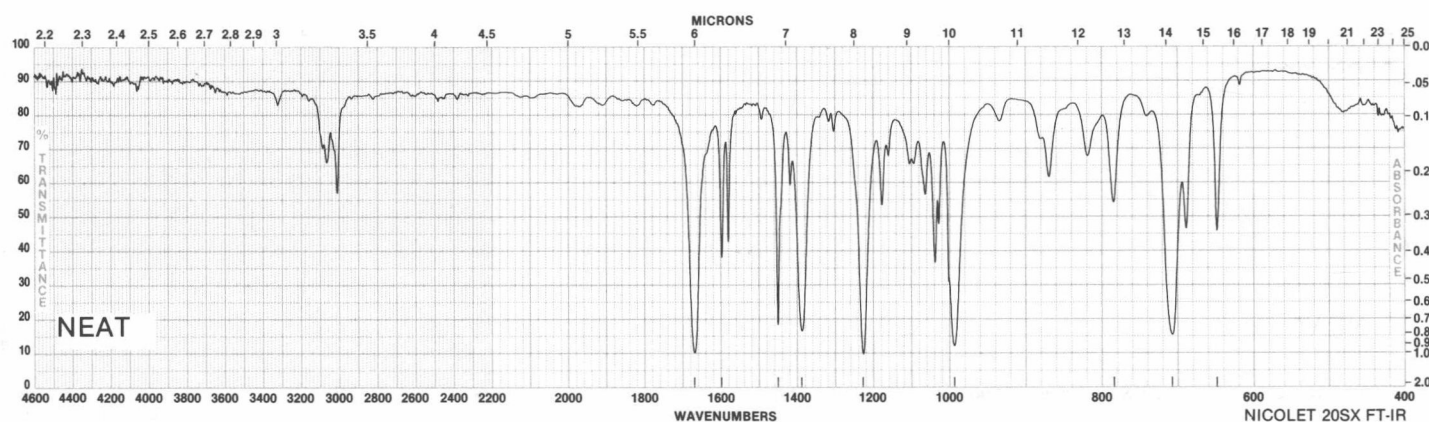
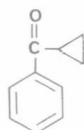
12551-2 CAS [3481-02-5]
Cyclopropyl phenyl ketone, 97%

FW 146.19
mp 7-9°C
bp 123°C/15mm

d 1.058
Fp 195°F
n_D 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



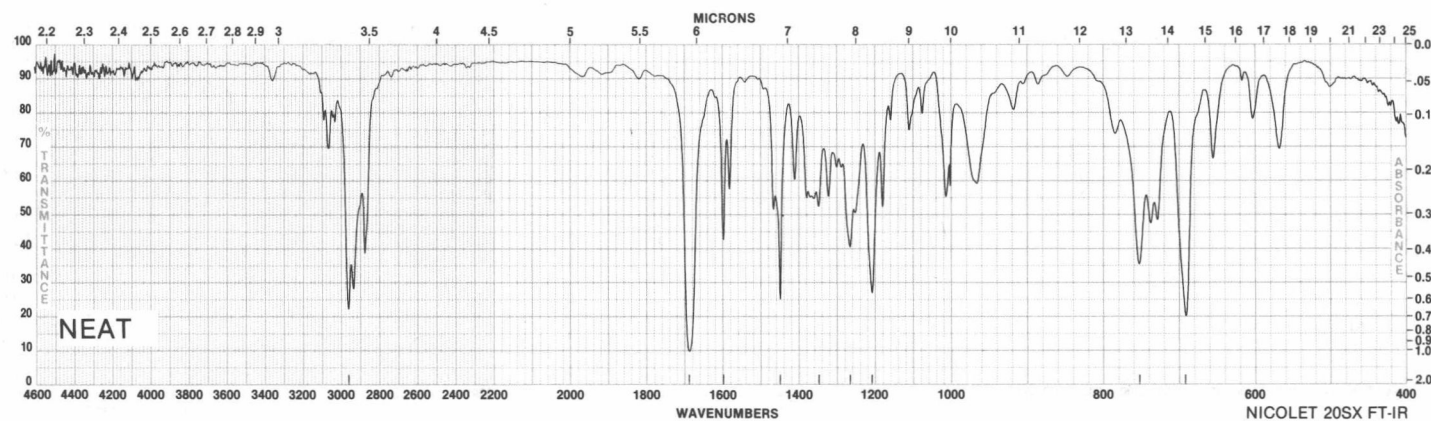
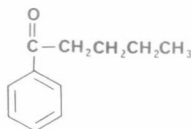
V65-9 CAS [1009-14-9]
Valerophenone, 99%

FW 162.23
bp 107°C/5mm
d 0.988

Fp 217°F
n_D 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



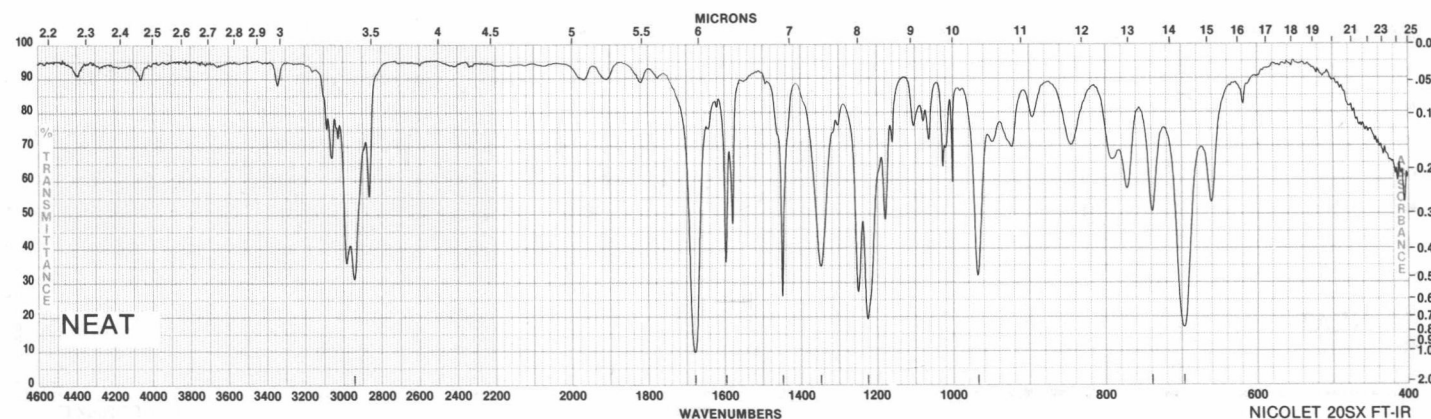
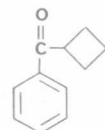
10836-7 CAS [5407-98-7]
Cyclobutyl phenyl ketone, 98%

FW 160.22
bp 118°C/7mm
d 1.050

Fp >235°F
n_D 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



AROMATIC KETONES

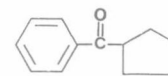
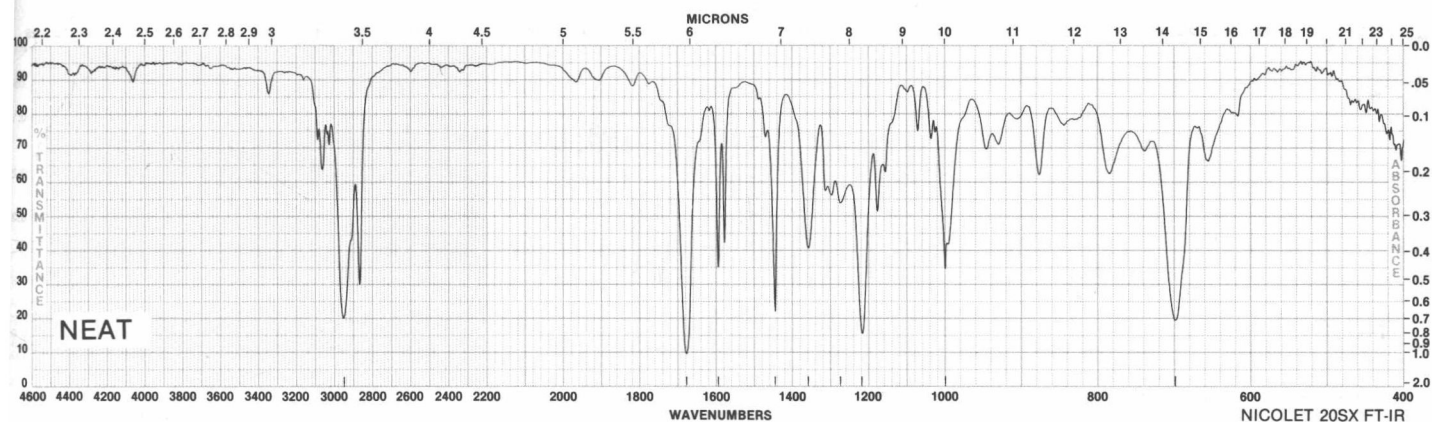
10

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

FW 174.24 n_D 1.5428 IR III, 854D
d 1.034 NMR II, 2,11D
Fp > 235°F

2954.1 1447.9 1220.7
1680.2 1360.9 1002.4
1596.7 1277.1 699.9

A

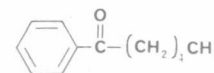
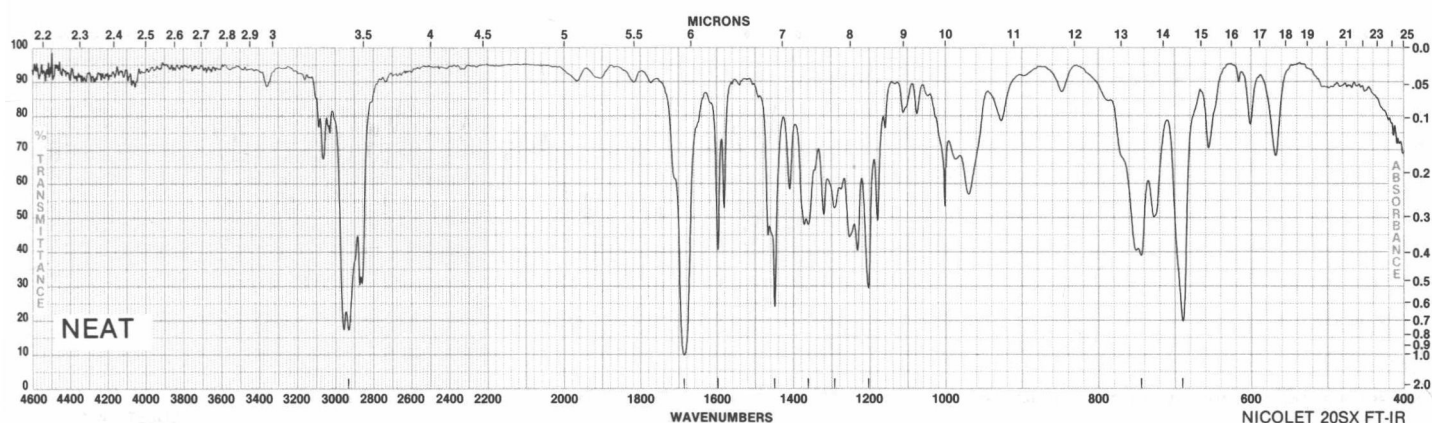


H1245-5 CAS [942-92-7]
Hexanophenone, 98%

FW 176.26 d 0.958 IR III, 854E
mp 25-26°C Fp > 235°F NMR II, 2,8D
bp 265.2°C n_D 1.5105

2930.9 1448.5 1204.3
1687.1 1361.4 745.1
1597.5 1292.3 690.5

B

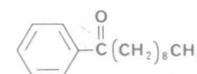
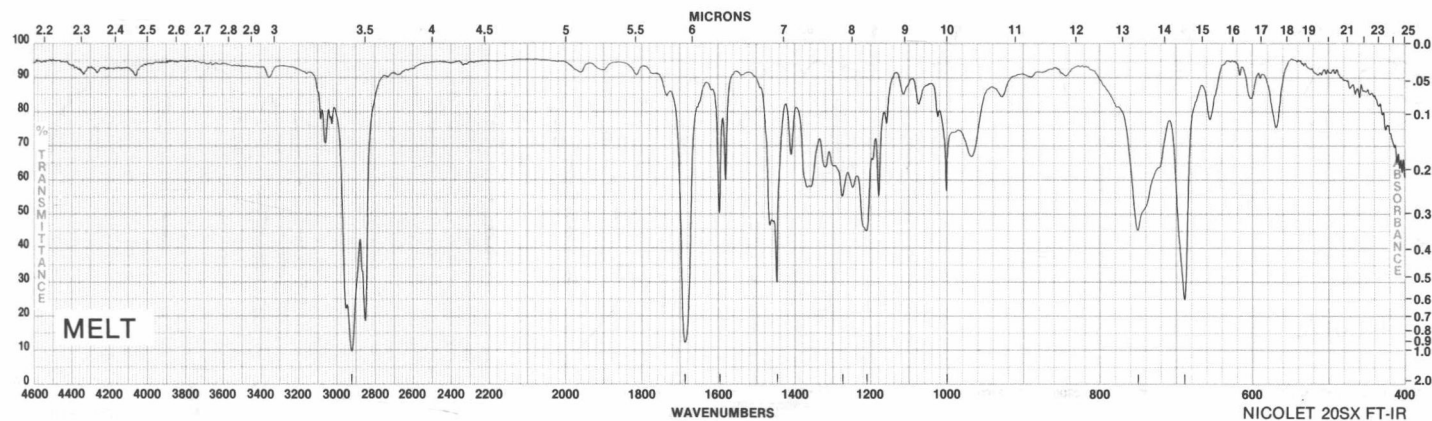


23200-9 CAS [6048-82-4]
Decanophenone, 95%

FW 232.37 Fp > 235°F NMR II, 2,9B
mp 34-36°C
bp 168°C/5mm

2926.3 1448.4 1001.9
1688.9 1275.5 751.4
1597.7 1212.2 690.2

C

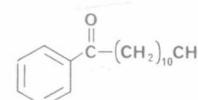
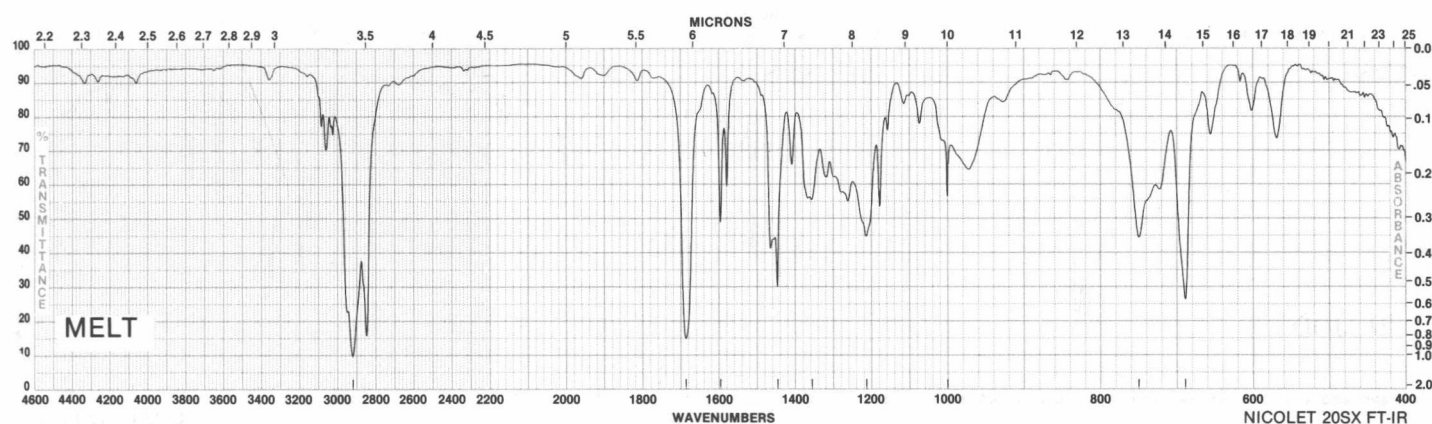


25271-9 CAS [1674-38-0]
Dodecanophenone, 98%

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

2924.7 1448.4 1001.9
1689.2 1357.7 750.5
1597.8 1215.4 690.1

D



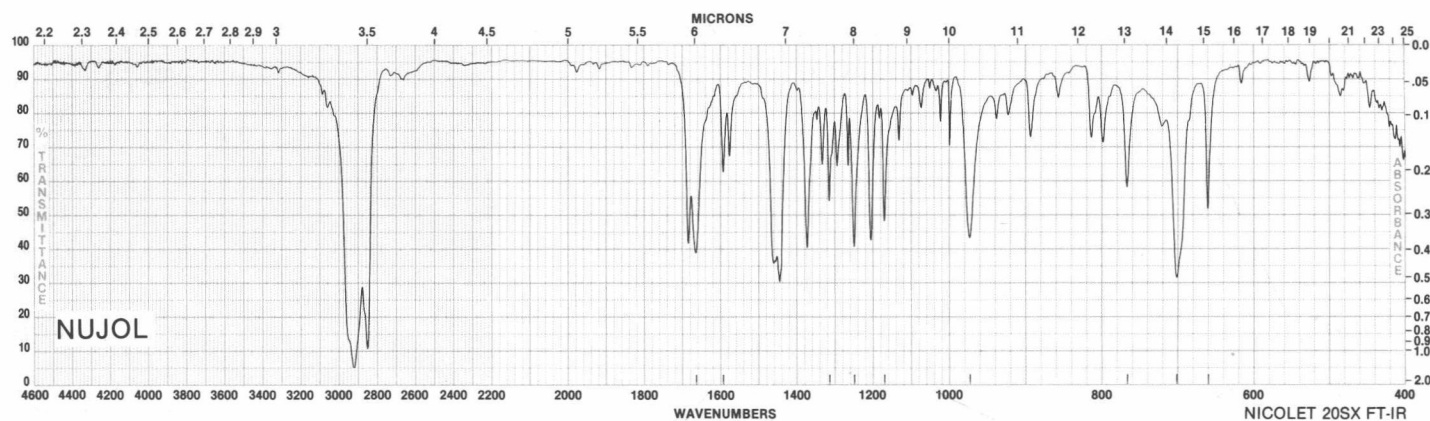
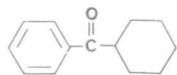
AROMATIC KETONES

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



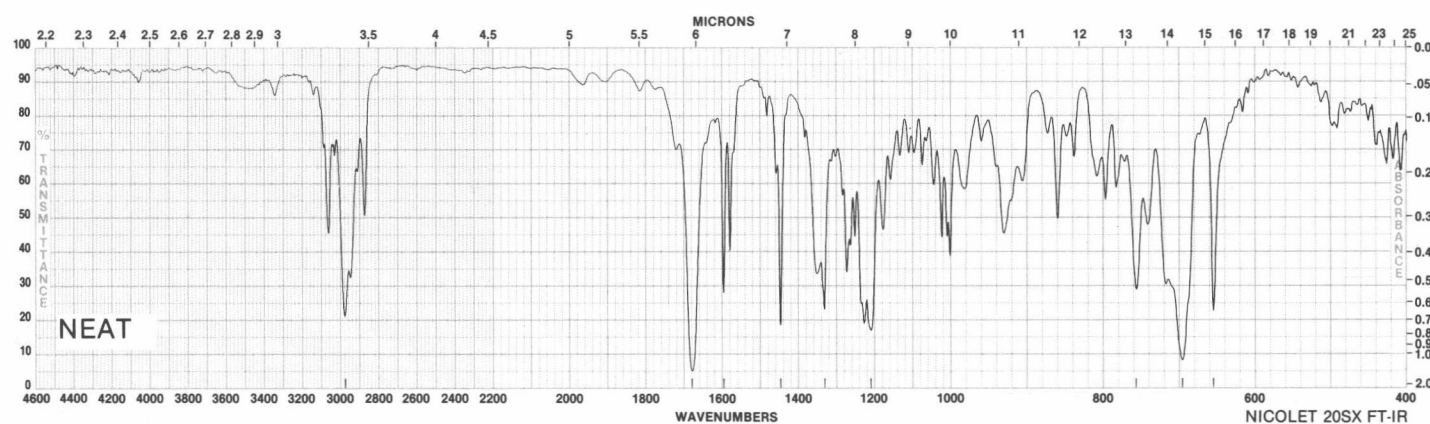
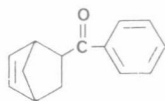
11506-1 CAS [6056-35-5]
2-Benzoyl-5-norbornene, tech., 90%

FW 198.27
bp 124°C/2mm
d 1.115

Fp > 235°F
n_D 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



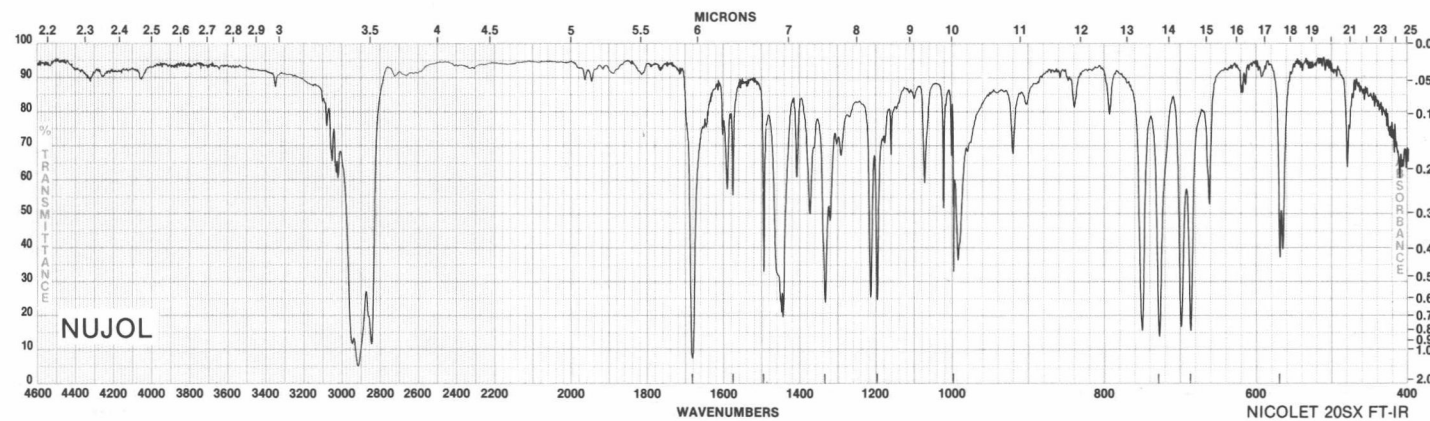
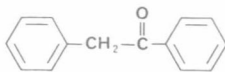
D436-9 CAS [451-40-1]
Deoxybenzoin, 97%

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

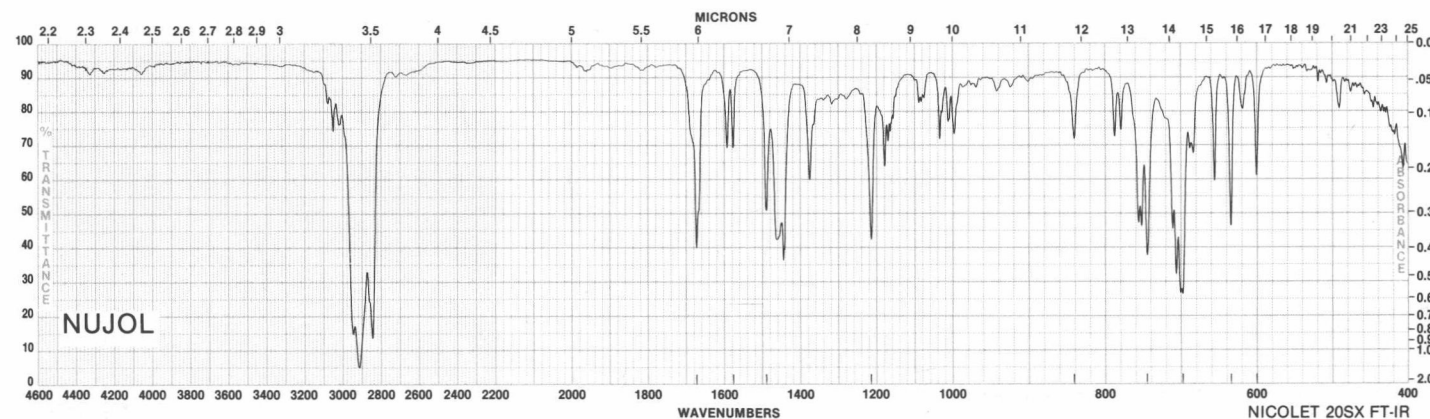
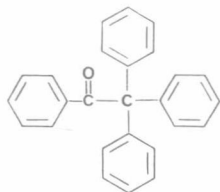


21669-0 CAS [466-37-5]
2,2,2-Triphenylacetophenone, 98%

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



AROMATIC KETONES

12

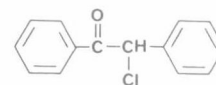
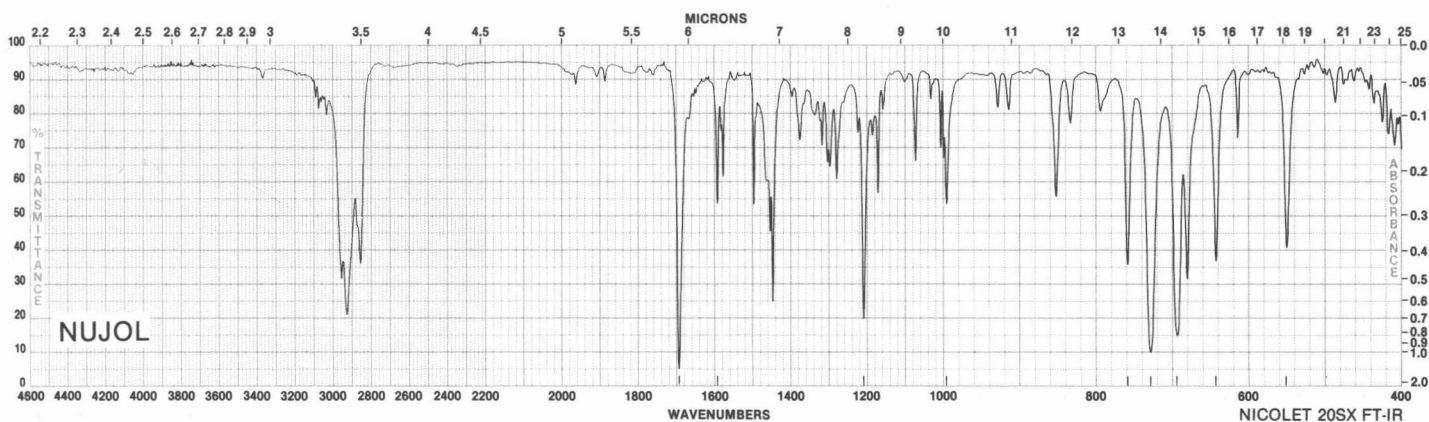
15750-3 CAS [447-31-4]
Desyl chloride, 95%

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



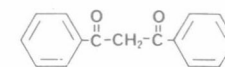
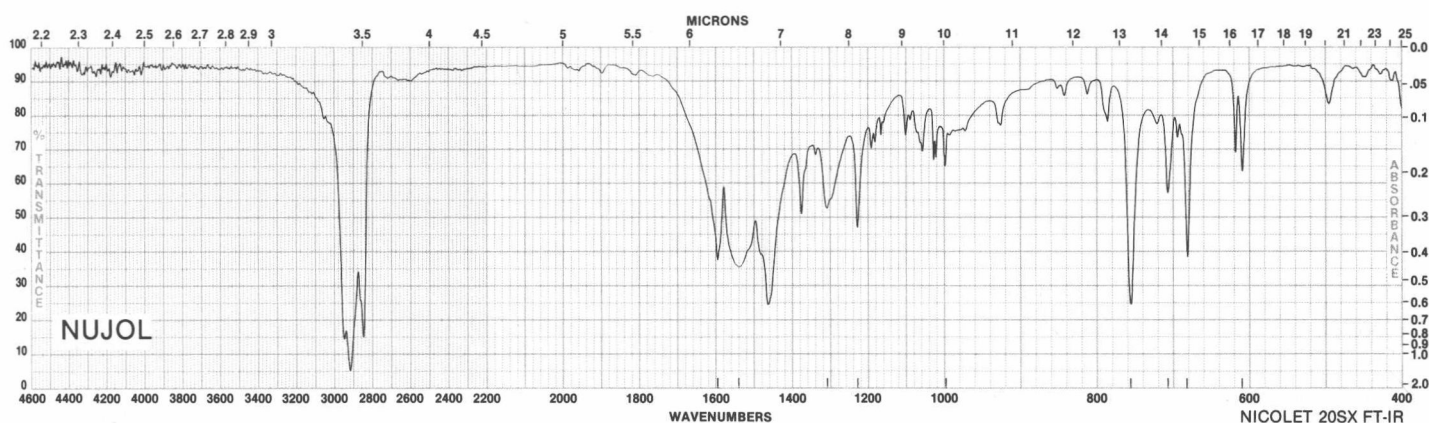
D3345-4 CAS [120-46-7]
Dibenzoylmethane, 98%

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



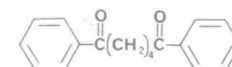
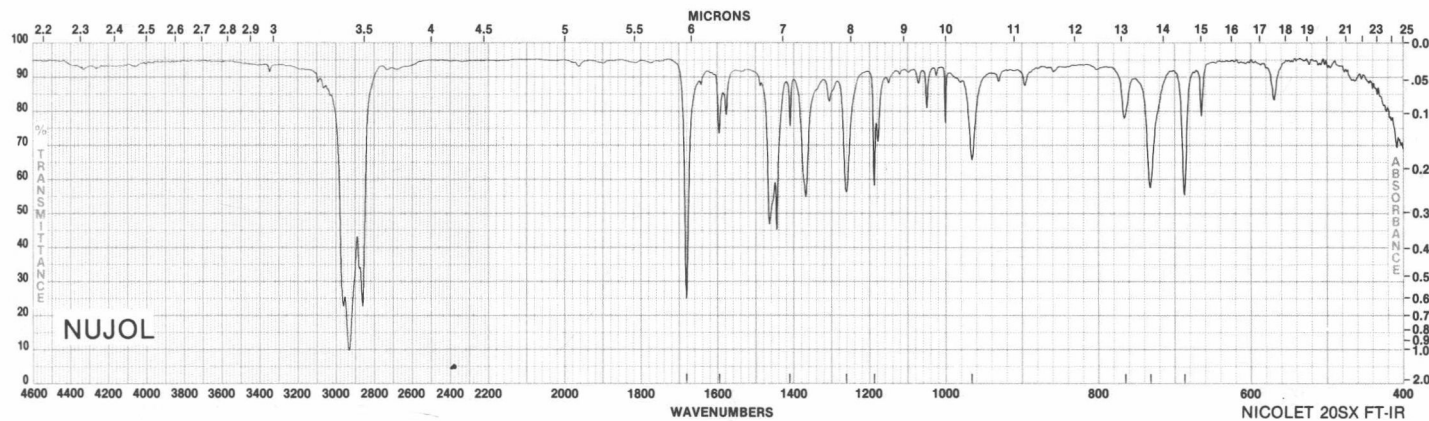
D3280-6 CAS [3375-38-0]
1,4-Dibenzoylbutane, 97%

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%

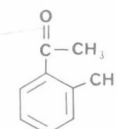
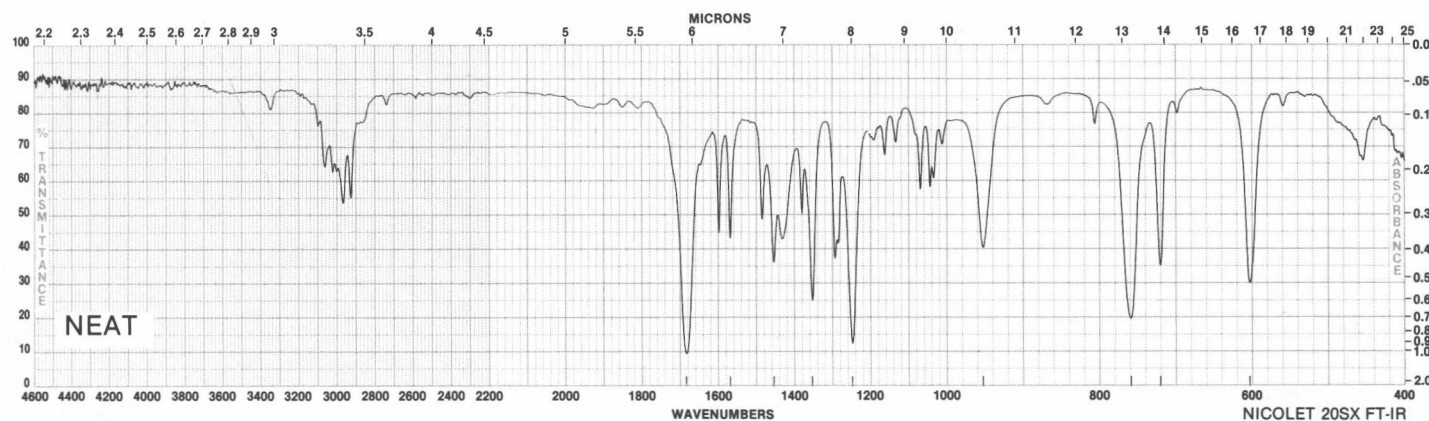
FW 134.18
bp 214°C
d 1.026

Fp 168°F
n_D 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



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

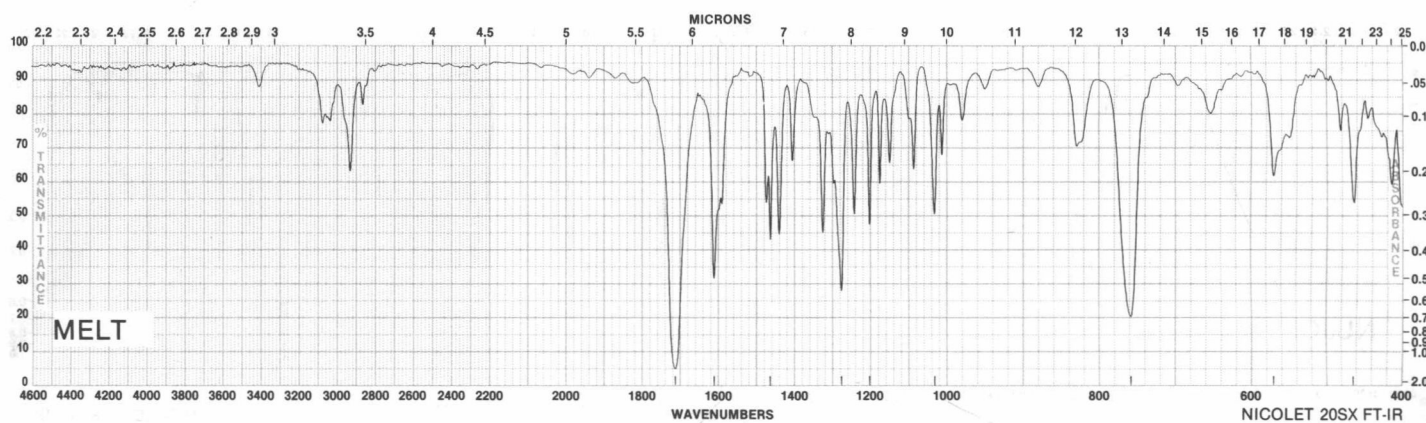
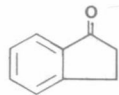
NMR II, 2,13B

2925.2 1462.9 1033.0

1713.0 1277.0 758.2

1610.2 1202.8 464.0

A



B

22035-3

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

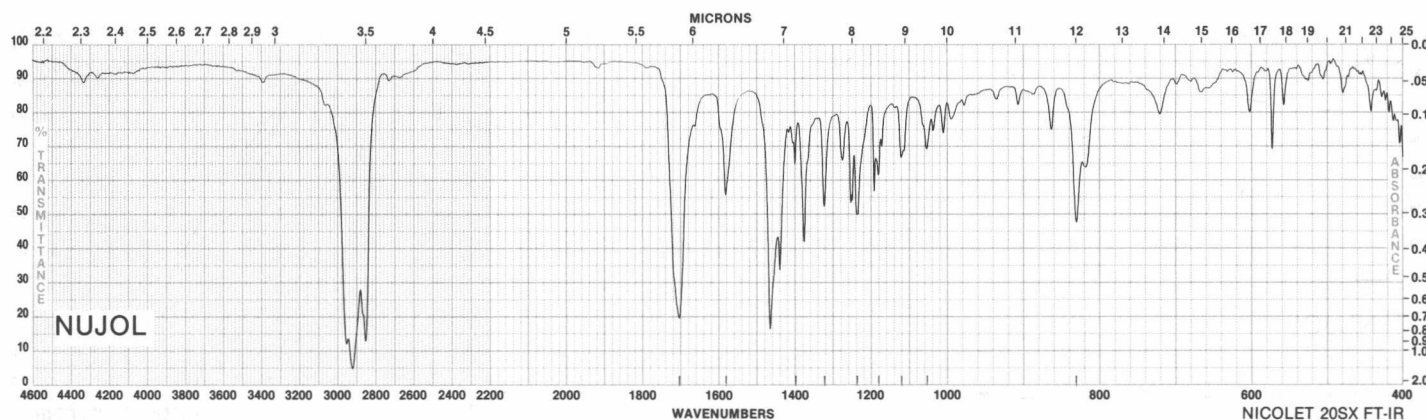
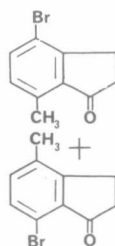
FW 225.09

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

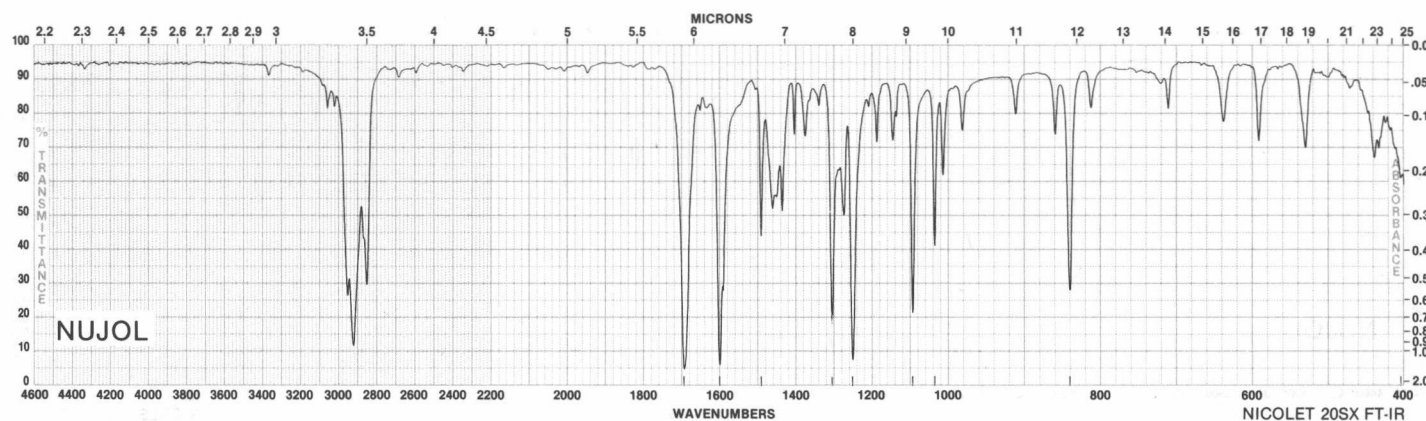
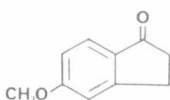
IR III, 856F

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 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

