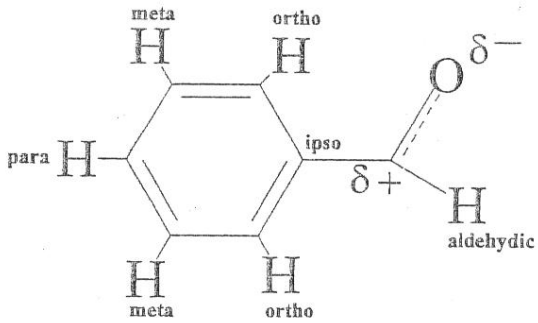
NMR SPECTRAL DATA

A. Correlation Data for ^{1}H and ^{13}C NMR Spectra
   1. For different kinds of protons.
   2. For different kinds of carbons,

B. How many kinds of **chemically nonequivalent** protons are present in benzaldehyde?
   1. This question is answered by visual inspection of structure (

BENZALDEHYDE



2. Carrying out such a visual inspection of the above structure shows four kinds of chemically nonequivalent proton. They are: 2 *meta*-protons, 1 *para*-proton, 2 *ortho*-protons, and 1 aldehyde (or formyl) proton.

C. Prediction of the **chemical shift position** and **multiplicity** for each of the different kinds of chemically nonequivalent protons present in benzaldehyde.

Table A shows that the aromatic protons come into resonance in the range 6.0-9.5 δ (**NOTE**: deshielding by the electron-withdrawing formyl group is greatest at the *ortho*-positions, then the *para*-position, and least at the *meta*-positions), and since the signals for the coupling aromatic-protons are close together, a complex absorption peakl will arise for each kind of nonequivalent aromatic-proton; Table A also shows that the aldehyde proton comes into resonance in the range 9.5-10.0 δ, and since it is not coupled with any adjacent nonequivalent protons, it will appear as a single peak.

D. How many kinds of **chemically nonequivalent** carbon atoms are present in benzaldehyde? Predict the chemical shift position for each one of the different kinds of carbon atoms.

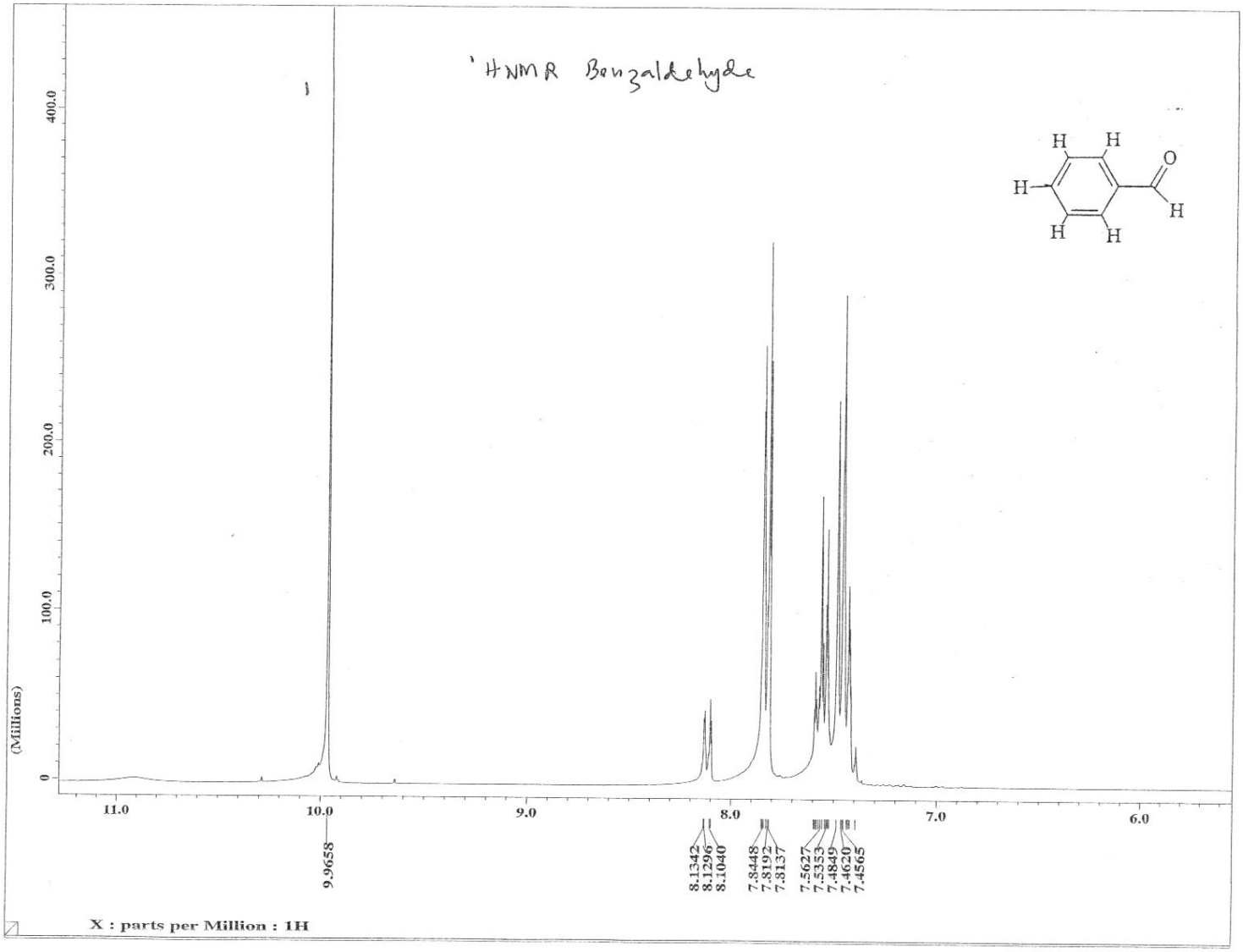
1. Visual inspection of the above structure reveals five kinds of chemically nonequivalent carbons: 2 *meta*-carbons, 2 *ortho*- carbons, 1 *para*-carbon, 1 *ipso*-carbon, and 1 carbonyl carbon.

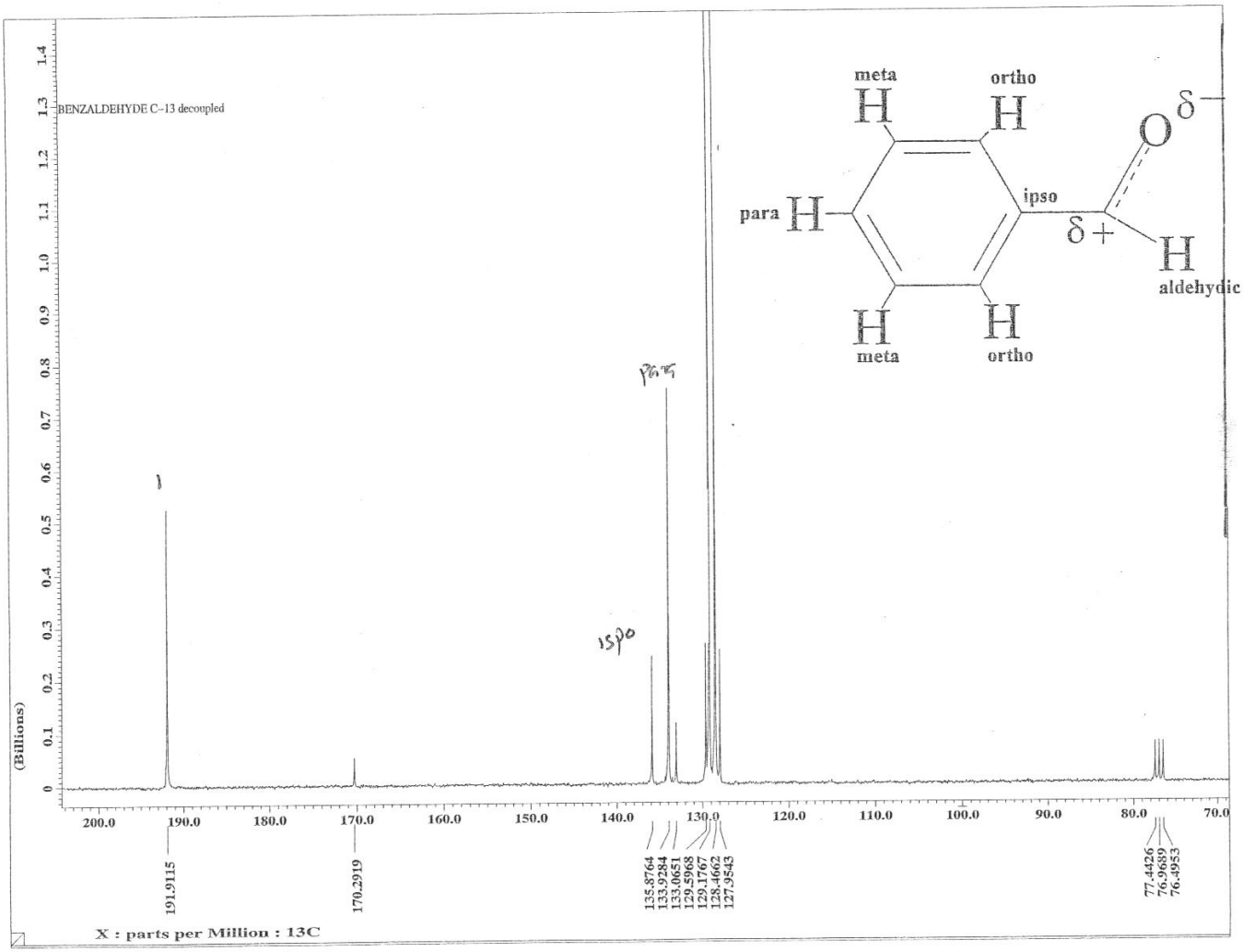
2. Table B shows that the aromatic carbons come into resonance in the range 100-170 δ, and the carbonyl carbon comes into resonance in the range 182-215 δ.

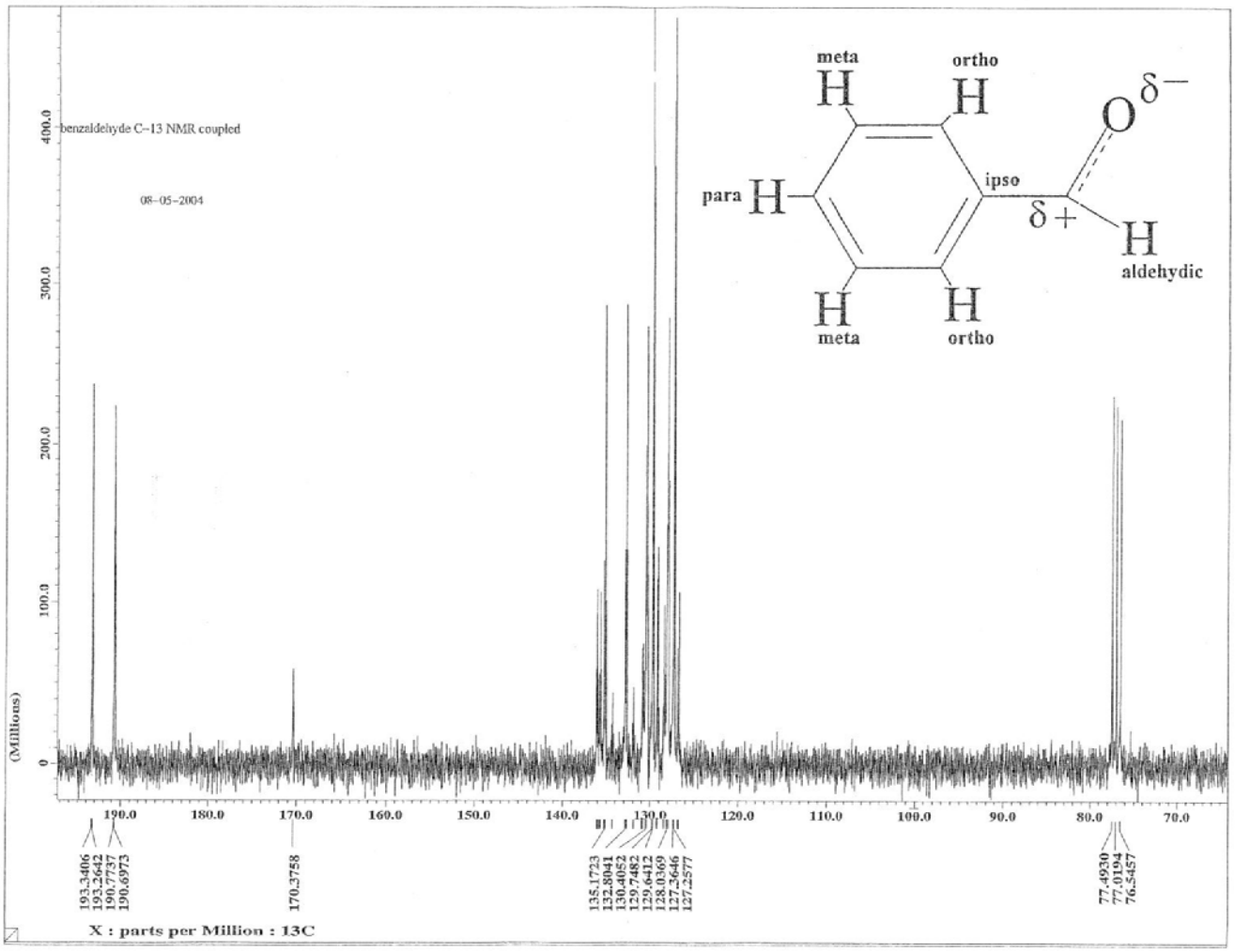
E. Observed spectral data for benzaldehyde:

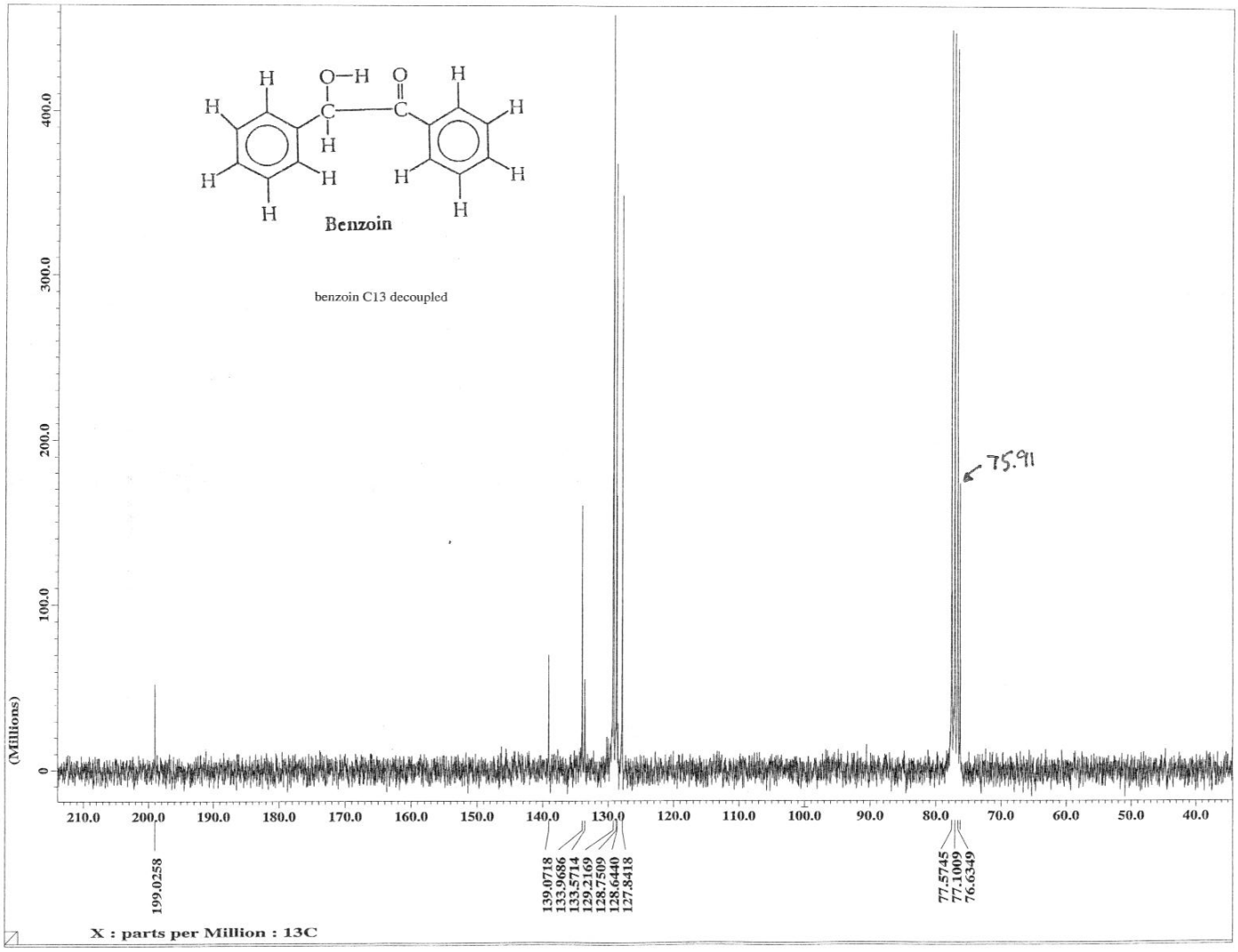
^{1}H NMR ($CDCl_3$):

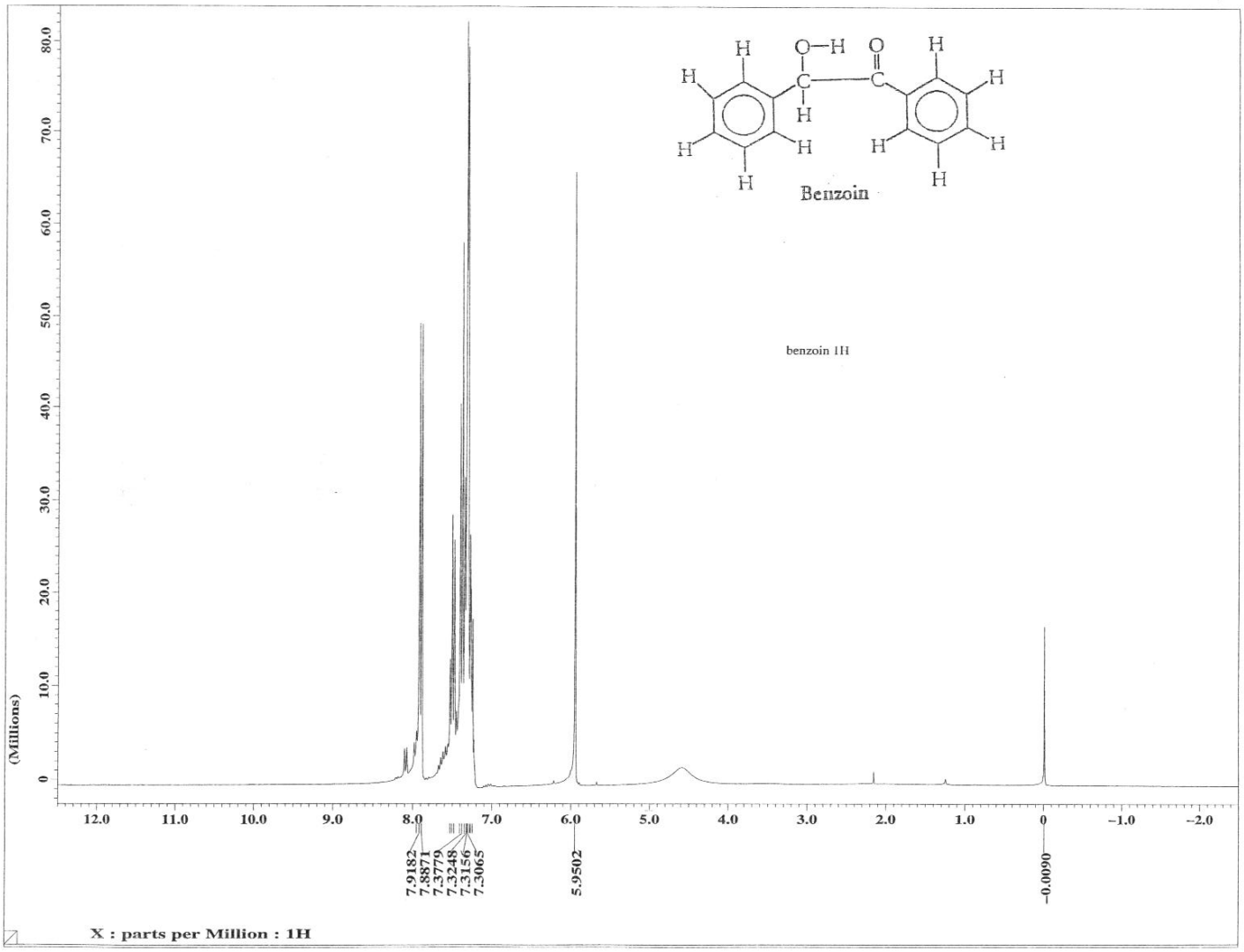
^{13}C NMR ($CDCl_3$):

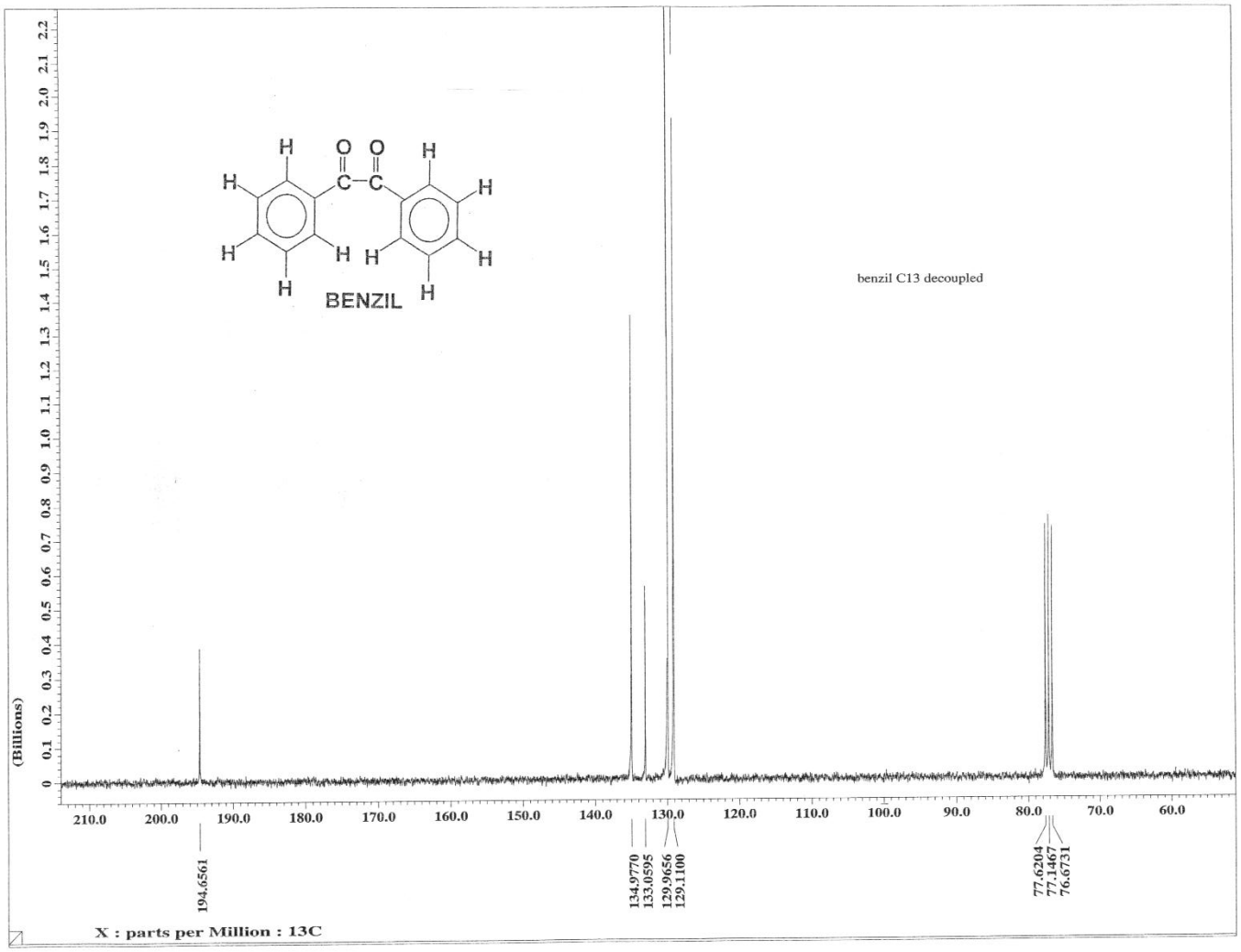

'HNMR Benzaldehyde
(Millions)
400.0
300.0
200.0
100.0
0
11.0
10.0
9.0
8.0
7.0
6.0
9.9658
8.1342
8.1296
8.1040
7.8448
7.8192
7.8137
7.5627
7.5353
7.4849
7.4620
7.4565
X : parts per Million : 1H

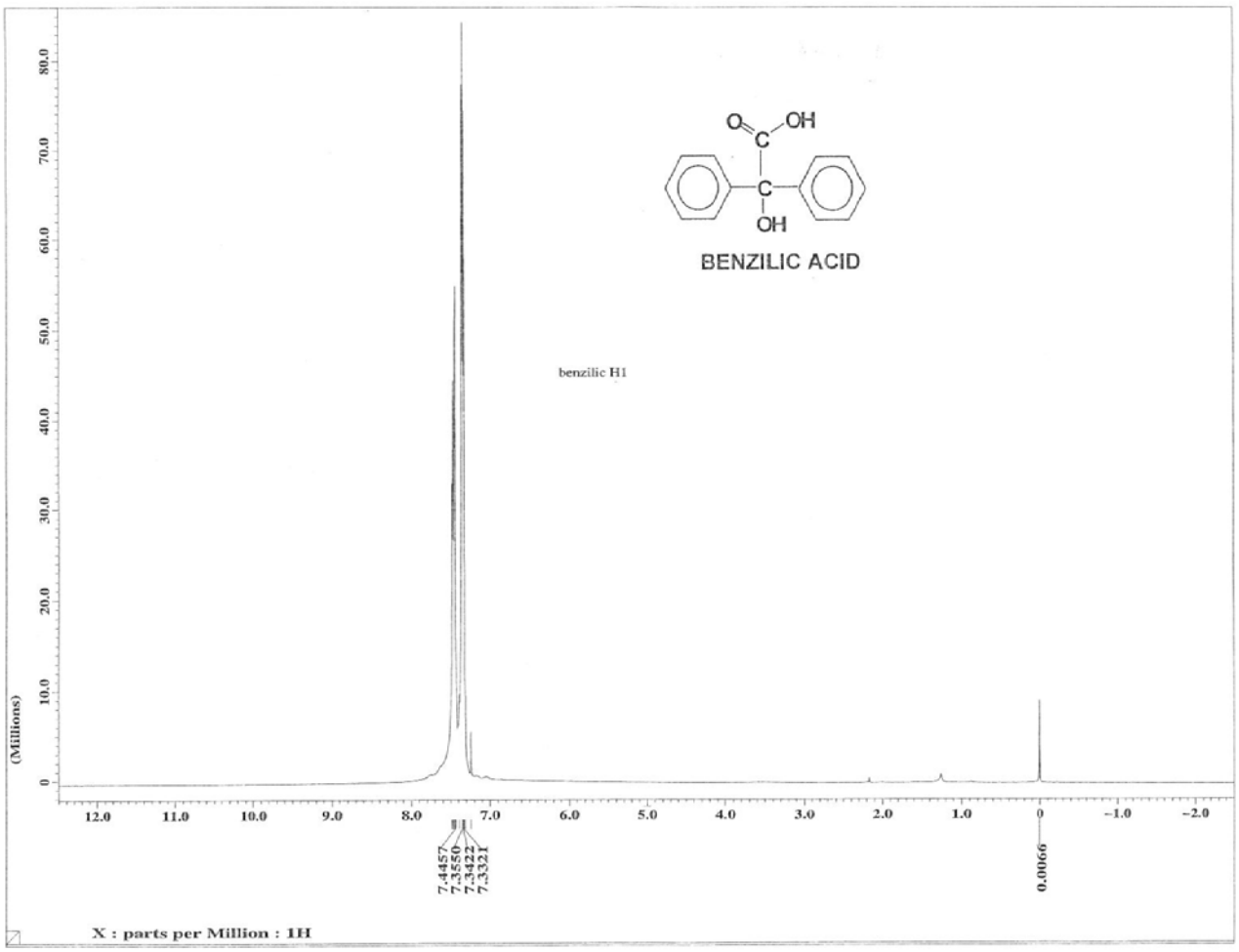

BENZALDEHYDE C-13 decoupled
(Billions)
X : parts per Million : 13C
191.9115
170.2919
135.8764
133.9284
133.0651
129.5968
129.1767
128.4662
127.9543
77.4426
76.9689
76.4953
meta
ortho
para
ipso
aldehydic
δ
δ+

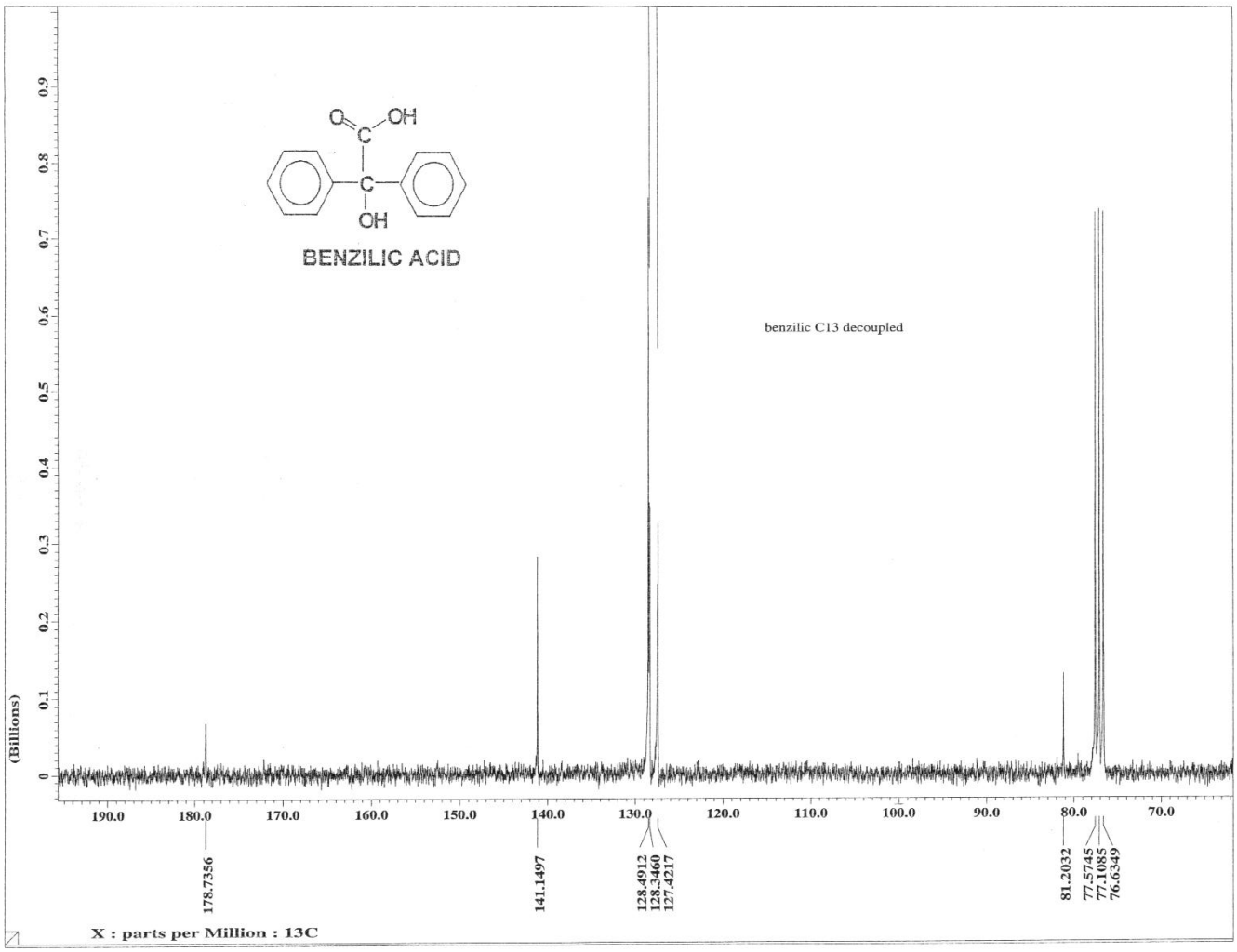

benzaldehyde C-13 NMR coupled
08-05-2004
(Millions)
400.0
300.0
200.0
100.0
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
193.3406
193.2642
190.7737
190.6973
170.3758
135.1723
132.8041
130.4052
129.7482
129.6412
128.0369
127.3646
127.2577
77.4930
77.0194
76.5457
X : parts per Million : 13C
meta
ortho
para
ipso
δ−
δ+
aldehydic
meta
ortho


Benzoin
benzoin C13 decoupled
75.91
(Millions)
400.0
300.0
200.0
100.0
0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
199.0258
139.0718
133.9686
133.5714
129.2169
128.7509
128.6440
127.3418
77.5745
77.1009
76.6349
X : parts per Million : 13C


Benzoin
benzoin 1H
(Millions)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
−2.0
7.9182
7.8871
7.3779
7.3248
7.3156
7.3065
5.9502
−0.0090
X : parts per Million : 1H


BENZIL
benzil C13 decoupled
(Billions)
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0
194.6561
134.9770
133.0595
129.9656
129.1100
77.6204
77.1467
76.6731
X : parts per Million : 13C


BENZILIC ACID
benzilic H1
(Millions)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
−1.0
−2.0
7.4457
7.3550
7.3422
7.3321
0.0066
X : parts per Million : 1H


BENZILIC ACID
benzilic C13 decoupled
(Billions)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
178.7356
141.1497
128.4912
128.3460
127.4217
81.2032
77.5745
77.1085
76.6349
X : parts per Million : 13C

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