

ELECTRONIC SUPPLEMENTARY INFORMATION

Solvent free selective oxidation of alcohols catalyzed by trinuclear complex with dicopper(II)–monozinc(II) centre using hydrogen peroxide as an oxidant

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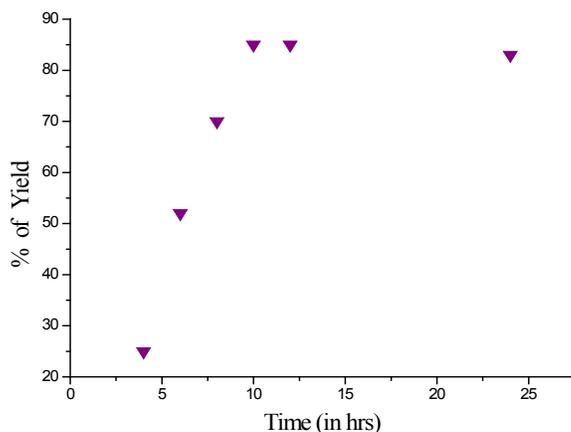
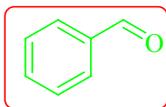


Fig. S1: Influence of reaction time on isolated yield

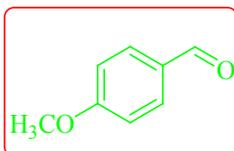
Spectral data of compounds 2a-j

1. Benzaldehyde (2a)¹



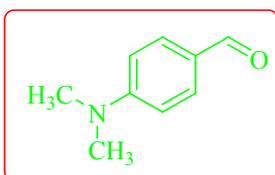
Ir (KBr): 2852, 2743, 1687 cm^{-1} . ^1H (CDCl_3 , 300 MHz): δ = 10.00 (s, 1H), 8.17 (d, J = 7.5 Hz, 1H), 7.88 (d, J = 6.9 Hz, 2H), 7.64-7.43(m, 2H).

2. 4-methoxy benzaldehyde (2b)¹



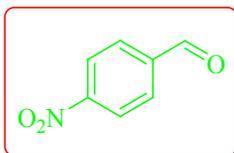
Ir (KBr): 2833, 2746, 1699 cm^{-1} . ^1H (CDCl_3 , 400 MHz): δ = 9.87 (s, 1H), 7.84 (d, J = 8.8 Hz, 2H), 7.01 (d, J = 8.8 Hz, 2H), 3.87 (s, 3H). ^{13}C (CDCl_3 , 100 MHz): δ = 190.9, 164.6, 131.9, 129.8, 114.3, 55.5.

3. 4-(N,N-Dimethylamino)benzaldehyde (2c)²



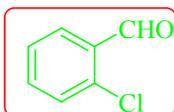
Yellowish white powder; m.p.- 72-74°C; Ir (KBr): 2795, 2714, 1661 cm^{-1} . ^1H (CDCl_3 , 300 MHz): $\delta = 9.73$ (s, 1H), 7.74 (d, $J = 8.7$ Hz, 2H), 6.71 (d, $J = 8.7$ Hz, 2H), 3.08 (s, 6H). ^{13}C (CDCl_3 , 75 MHz): $\delta = 189.6, 153.8, 131.4, 124.5, 110.5, 39.5$.

4. **4-Nitro benzaldehyde (2d)**³



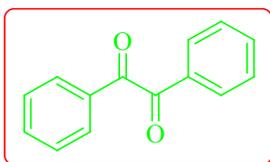
Yellow crystalline solid; mp- 104-106°C; Ir (KBr): 2854, 2726, 1697 cm^{-1} . ^1H (CDCl_3 , 400 MHz): $\delta = 10.17$ (s, 1H), 8.41 (d, $J = 8.8$ Hz, 2H), 8.10 (d, $J = 8.8$ Hz, 2H). ^{13}C (CDCl_3 , 100 MHz): $\delta = 190.3, 151.1, 140.0, 130.3, 124.3$.

5. **2-Chloro benzaldehyde (2e)**³



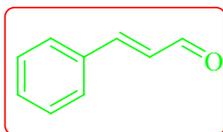
Ir (KBr): 2896, 1689 cm^{-1} . ^1H (CDCl_3 , 300 MHz): $\delta = 10.47$ (s, 1H), 7.92 (d, $J = 7.5$ Hz, 1H), 7.54-7.32 (m, 3H). ^{13}C (CDCl_3 , 75 MHz): $\delta = 189.6, 137.7, 134.9, 132.2, 130.4, 129.2, 127.1$.

6. **Benzil (2f)**⁴



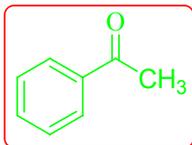
Yellow powder; m.p.- 95-97°C; Ir (KBr): 3224, 1666 cm^{-1} . ^1H (CDCl_3 , 400 MHz): $\delta = 7.98$ (d, $J = 8.0$ Hz, 4H), 7.68-7.49 (m, 6H). ^{13}C (CDCl_3 , 100 MHz): $\delta = 194.5, 134.9, 132.9, 129.9, 129.0$.

7. **Cinnamaldehyde (2g)**¹



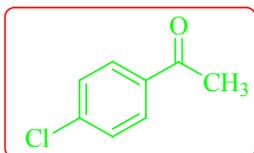
Ir (KBr): 2816, 2743, 1679 cm^{-1} . ^1H (CDCl_3 , 300 MHz): $\delta = 9.71$ (d, $J = 7.5$ Hz, 1H), 7.57-7.43 (m, 6H), 6.76-6.68 (m, 1H). ^{13}C (CDCl_3 , 75 MHz): $\delta = 193.7, 152.8, 146.4, 133.8, 130.5, 129.0, 128.4$.

8. Acetophenone (2h)⁵



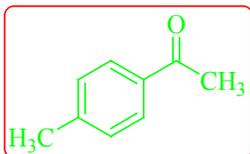
Ir (KBr): 2928, 1686 cm^{-1} . ^1H (CDCl_3 , 300 MHz): $\delta = 7.95$ (d, $J = 7.2$ Hz, 2H), 7.56-7.41 (m, 3H), 2.58 (s, 3H). ^{13}C (CDCl_3 , 75 MHz): $\delta = 197.9, 136.9, 133.0, 128.2, 26.5$.

9. 4-Chloroacetophenone (2i)²



Ir (KBr): 2926, 1687 cm^{-1} . ^1H (CDCl_3 , 300 MHz): $\delta = 7.91$ (t, $J = 9.0$ Hz, 2H), 7.44 (t, $J = 9.1$ Hz, 2H), 2.57 (s, 3H). ^{13}C (CDCl_3 , 75 MHz): $\delta = 196.4, 139.2, 135.1, 129.4, 128.5, 26.2$.

10. 4-methyl acetophenone (2j)⁶



Ir (KBr): 2923, 1682 cm^{-1} . ^1H (CDCl_3 , 300 MHz): $\delta = 7.82$ (d, $J = 8.4$ Hz, 2H), 7.20 (d, $J = 7.8$ Hz, 2H), 2.50 (s, 3H), 2.45 (s, 3H). ^{13}C (CDCl_3 , 75 MHz): $\delta = 197.1, 143.3, 134.2, 128.7, 127.9, 26.0, 21.0$.

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^1H and ^{13}C NMR spectra of compounds 2a-j

1. Benzaldehyde(2a)

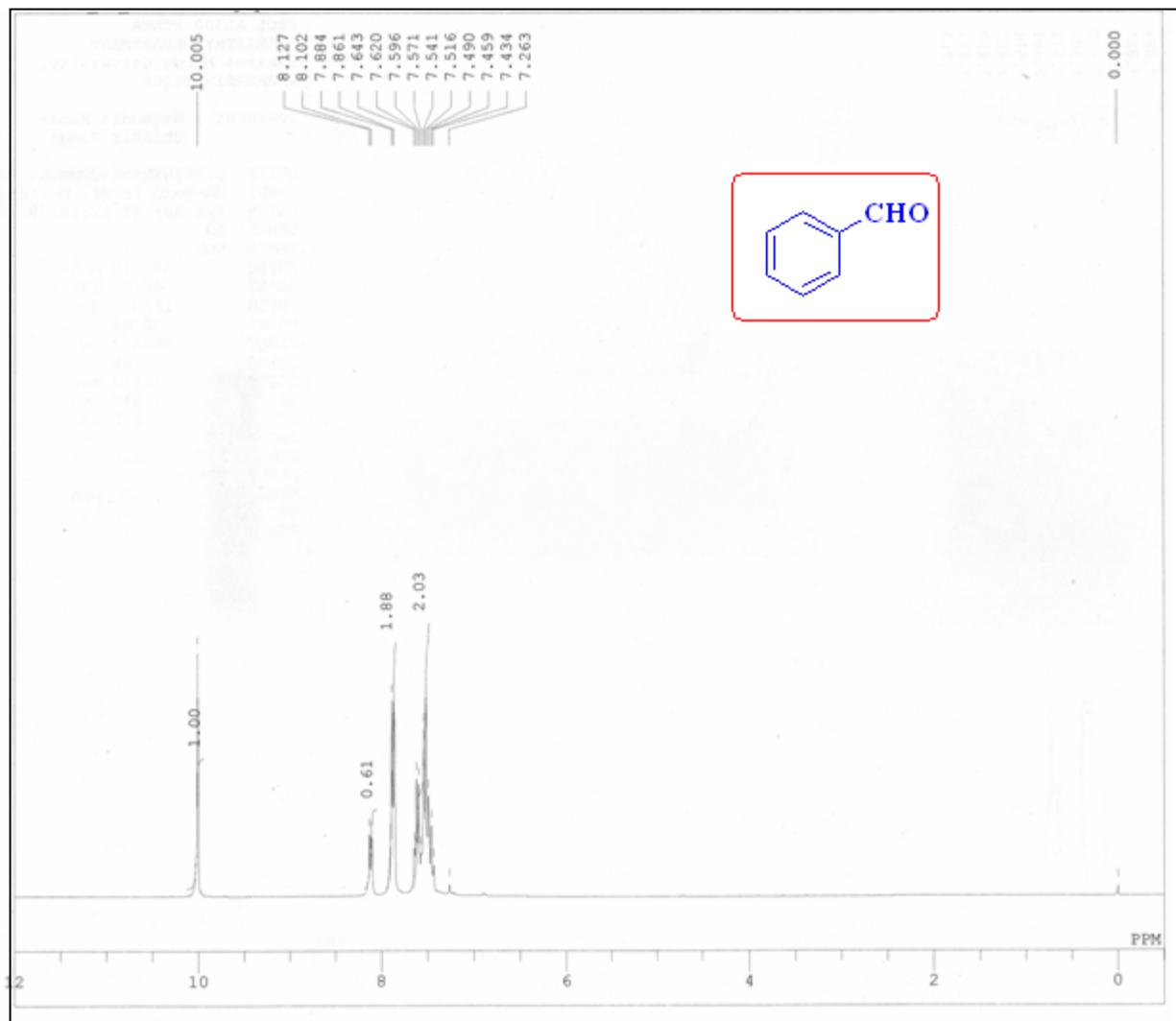


Figure 1. ^1H NMR Spectra of Benzaldehyde

2. 4-methoxy benzaldehyde (2b)

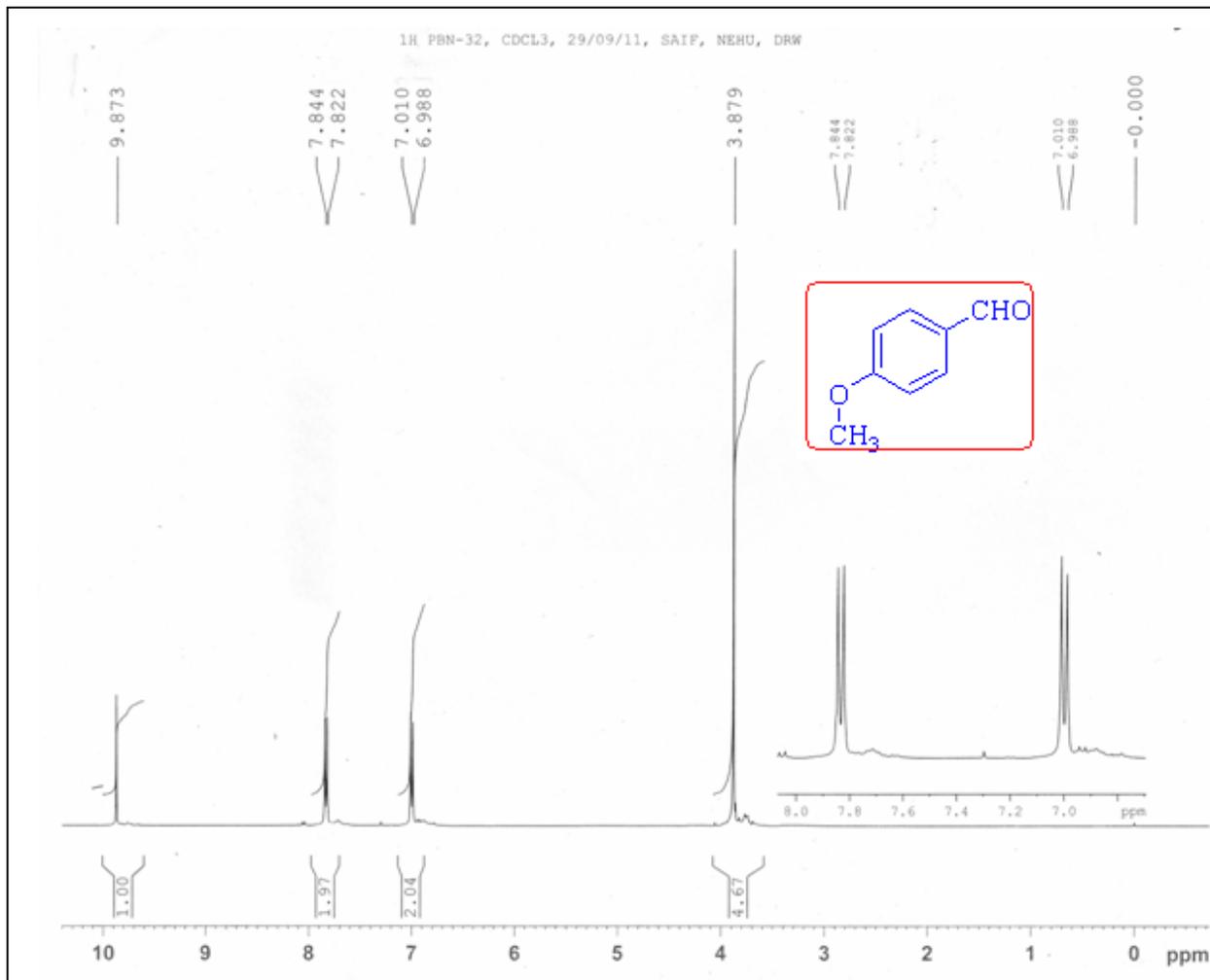


Figure 2. ¹H NMR Spectra of 4-methoxy benzaldehyde

3. 4-methoxy benzaldehyde (2b)

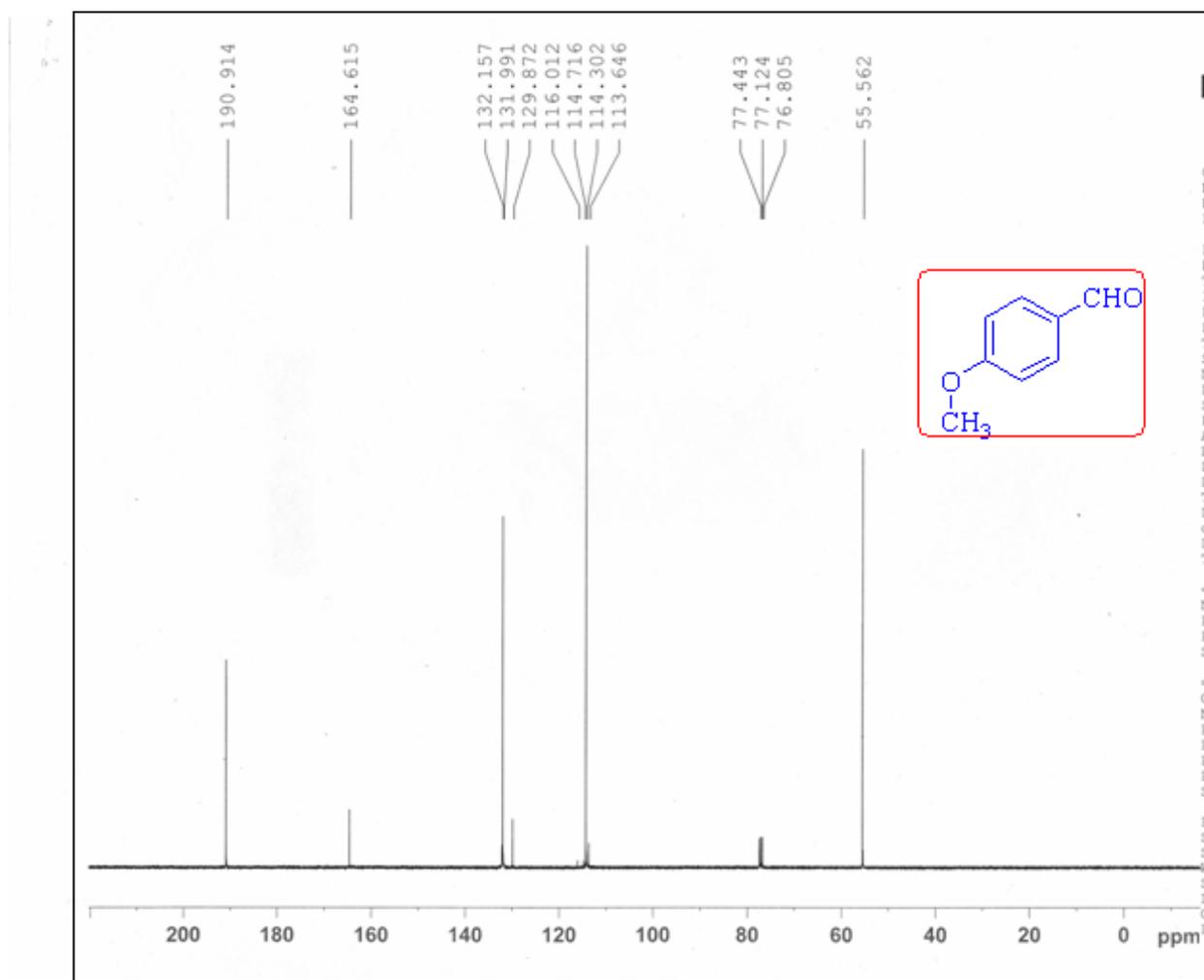


Figure 3. ^{13}C NMR Spectra of 4-methoxy benzaldehyde

4. 4-(N,N-Dimethylamino)benzaldehyde (2c)

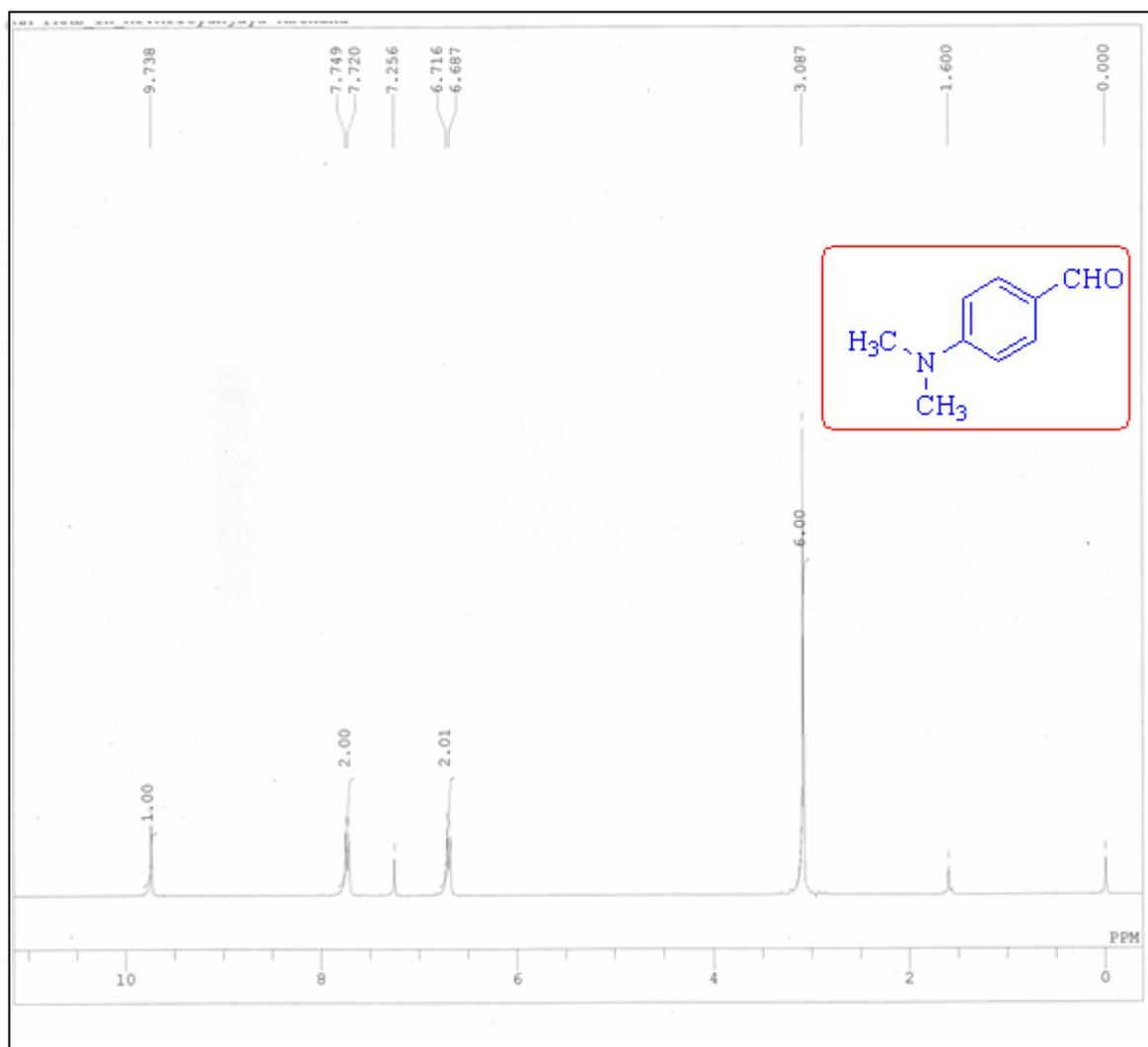


Figure 4. ¹H NMR Spectra of 4-(N,N-Dimethylamino)benzaldehyde

5. 4-(N,N-Dimethylamino)benzaldehyde (2c)

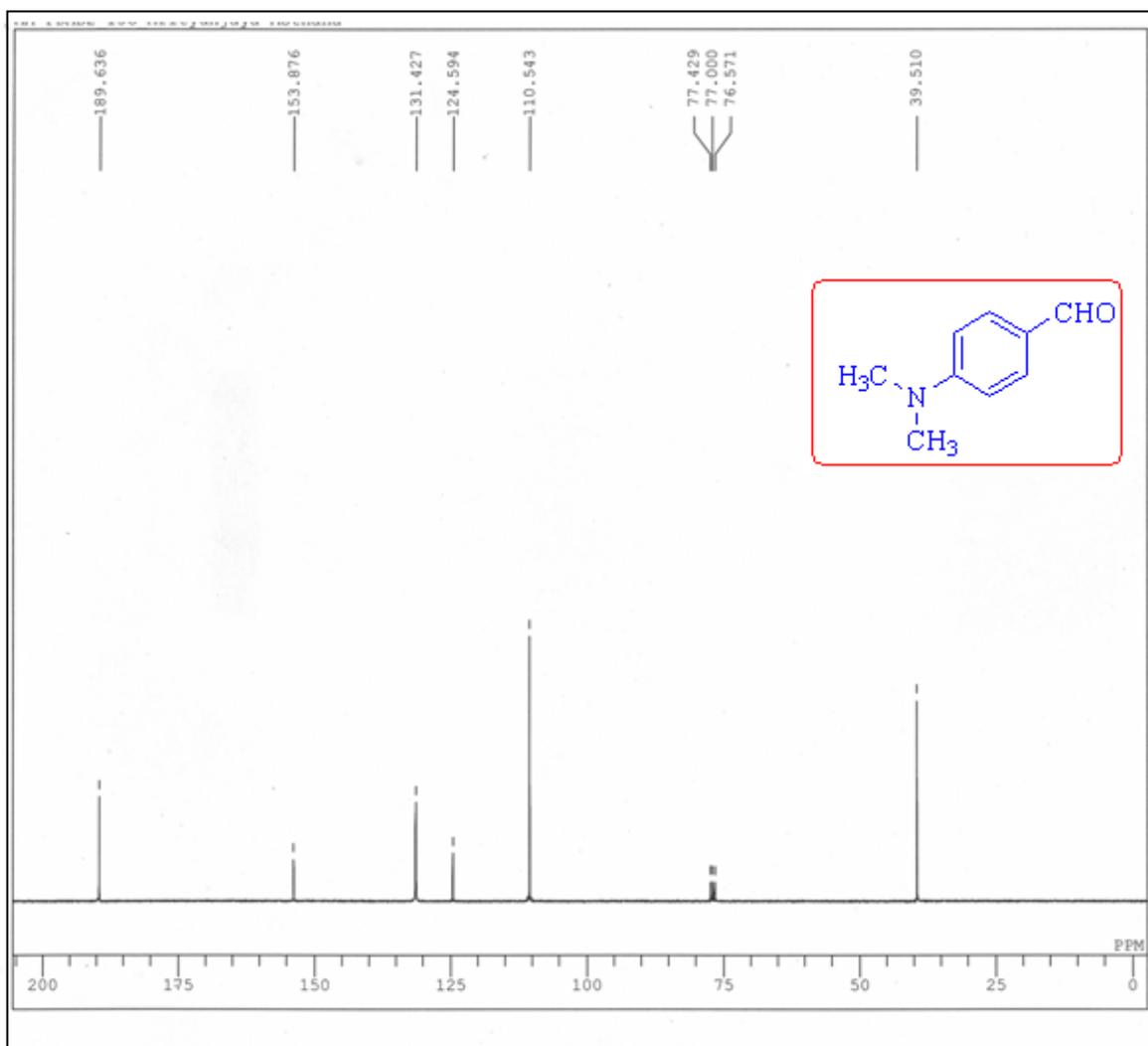


Figure 5. ^{13}C NMR Spectra of 4-(N,N-Dimethylamino)benzaldehyde

6. 4-nitro benzaldehyde (2d)

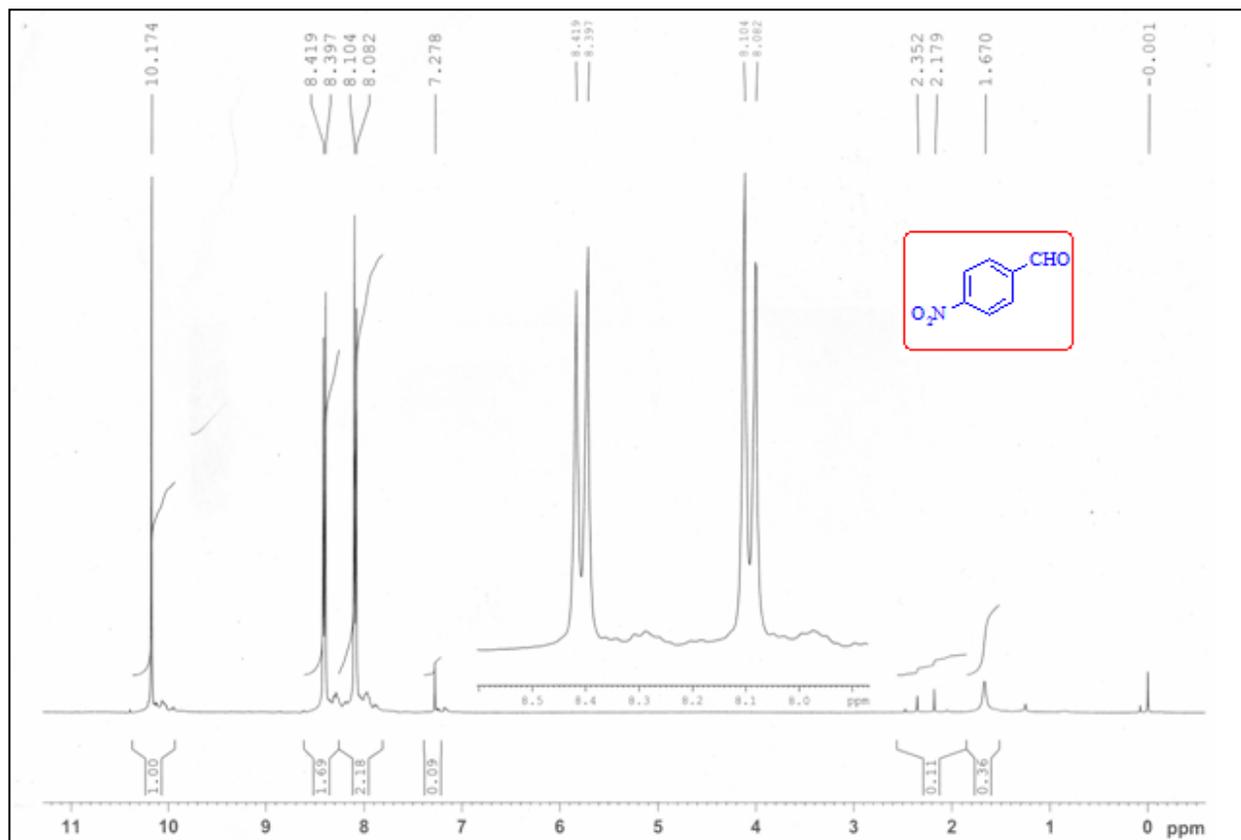


Figure 6. ¹H NMR Spectra of 4-nitro benzaldehyde

7. 4-nitro benzaldehyde (2d)

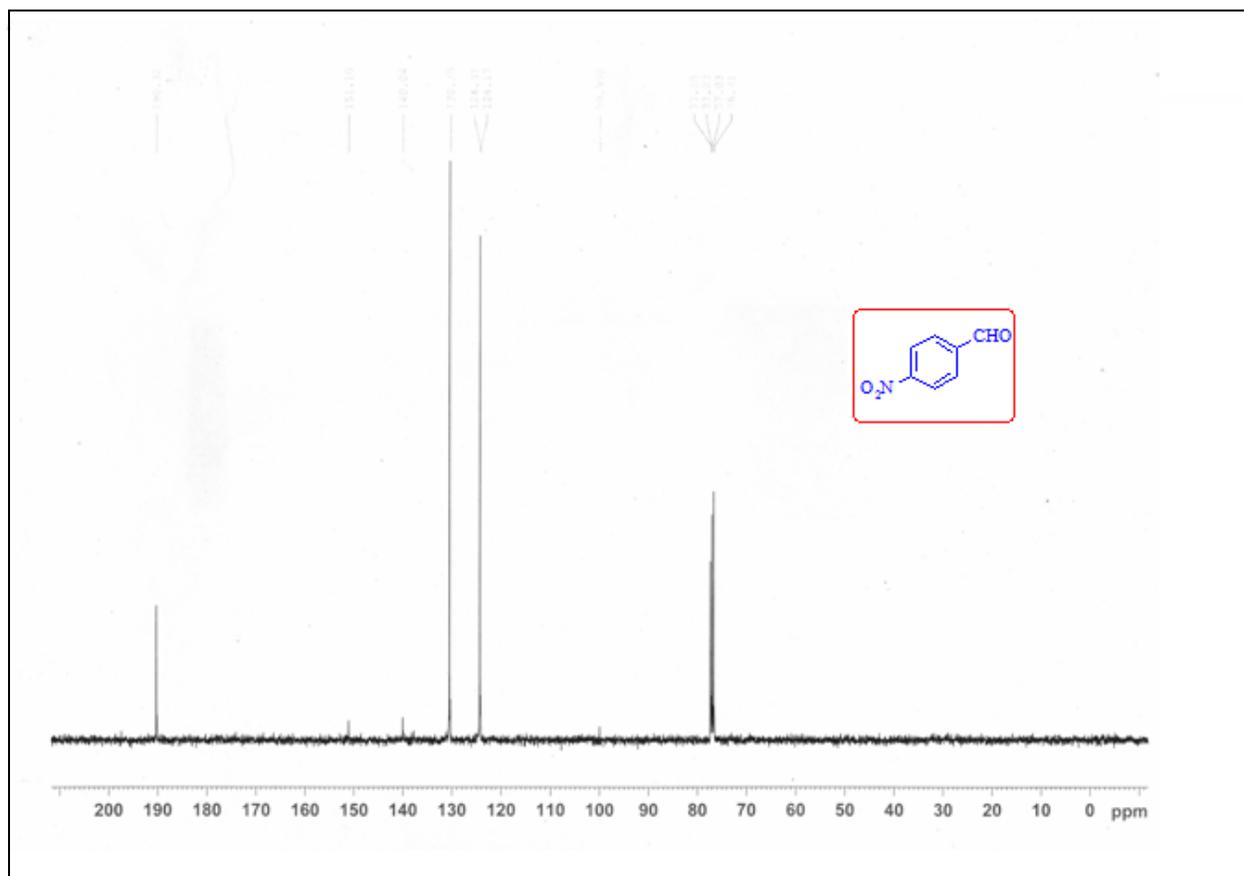


Figure 7. ^{13}C NMR Spectra of 4-nitro benzaldehyde

8. 2-chloro benzaldehyde (2e)

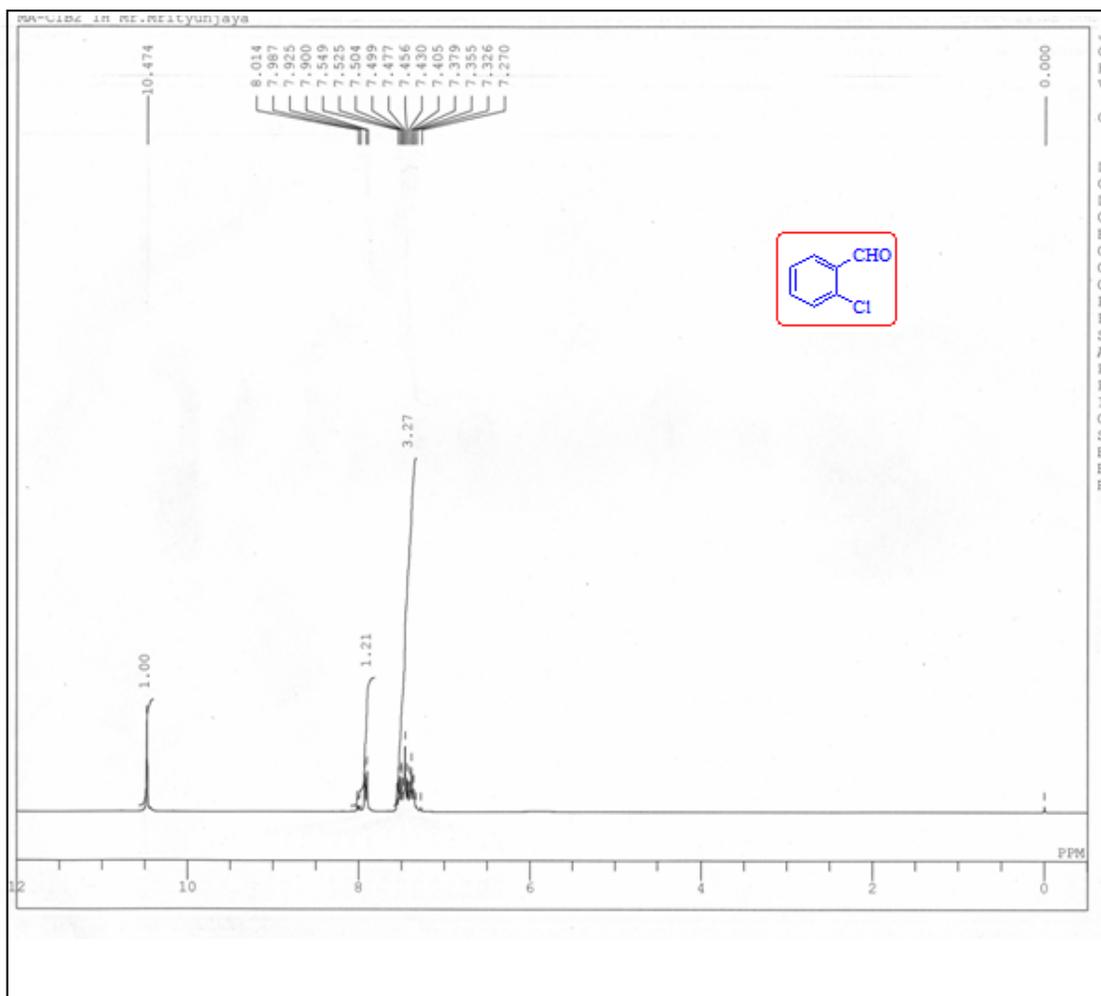


Figure 8. ^1H NMR Spectra of 2-chloro benzaldehyde

9. 2-chloro benzaldehyde (2e)

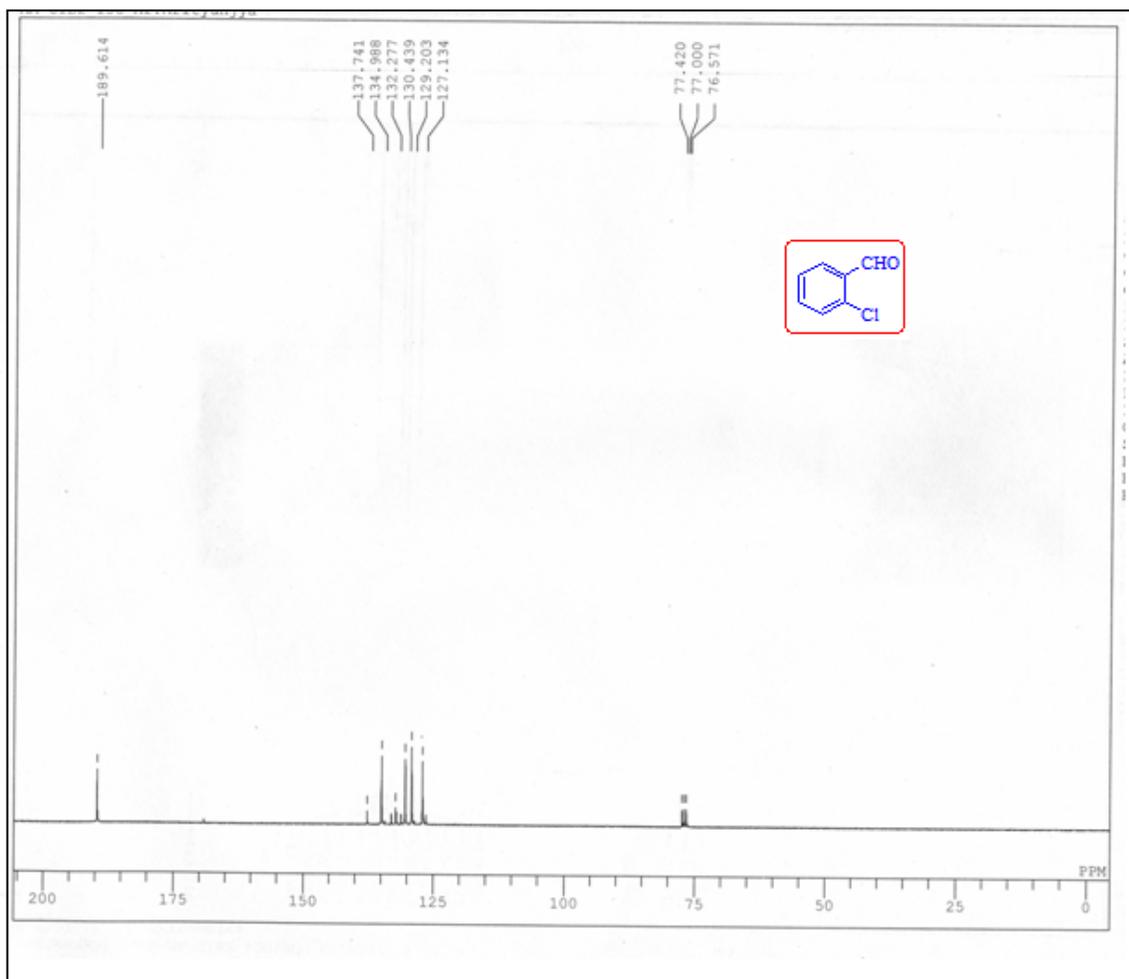


Figure 9. ^{13}C NMR Spectra of 2-chloro benzaldehyde

10. Benzil (2f)

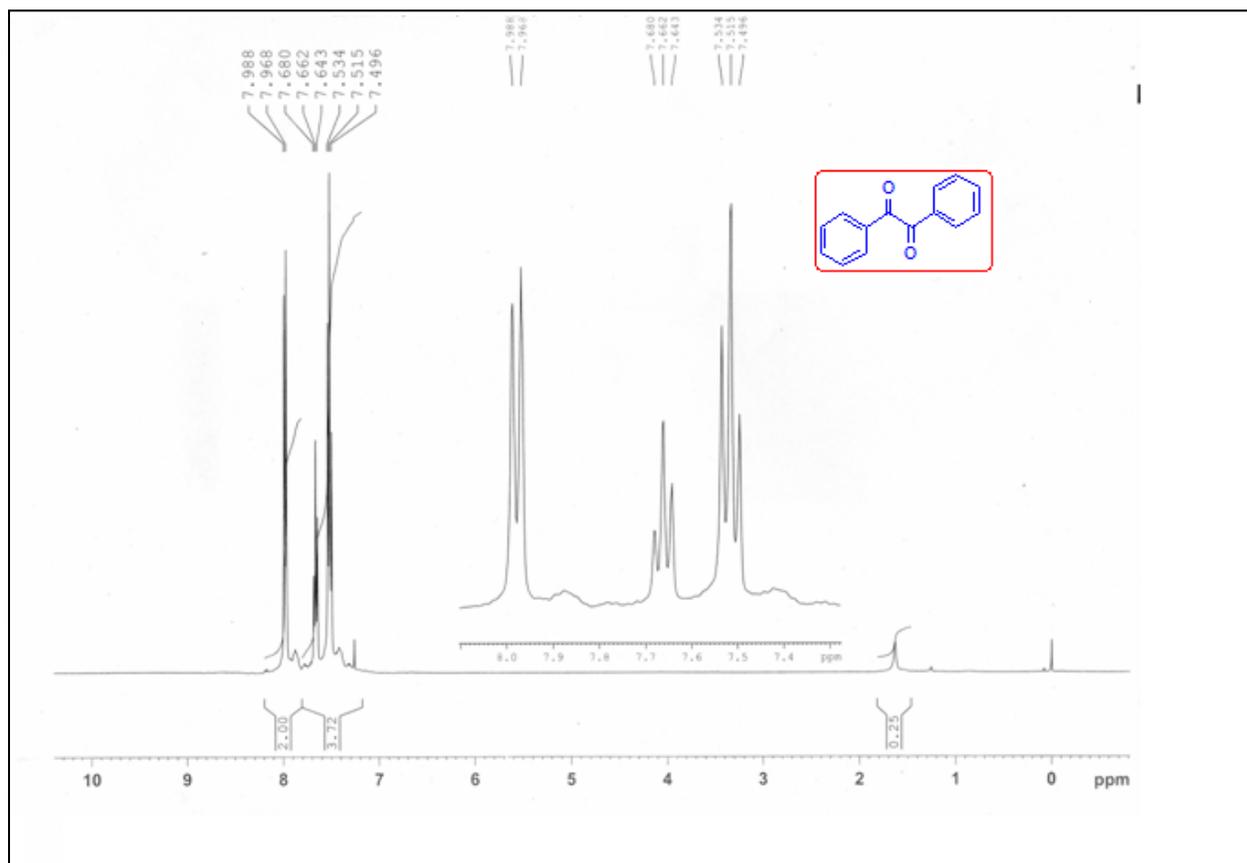


Figure 10. ¹H NMR Spectra of Benzil

11. Benzil (2f)

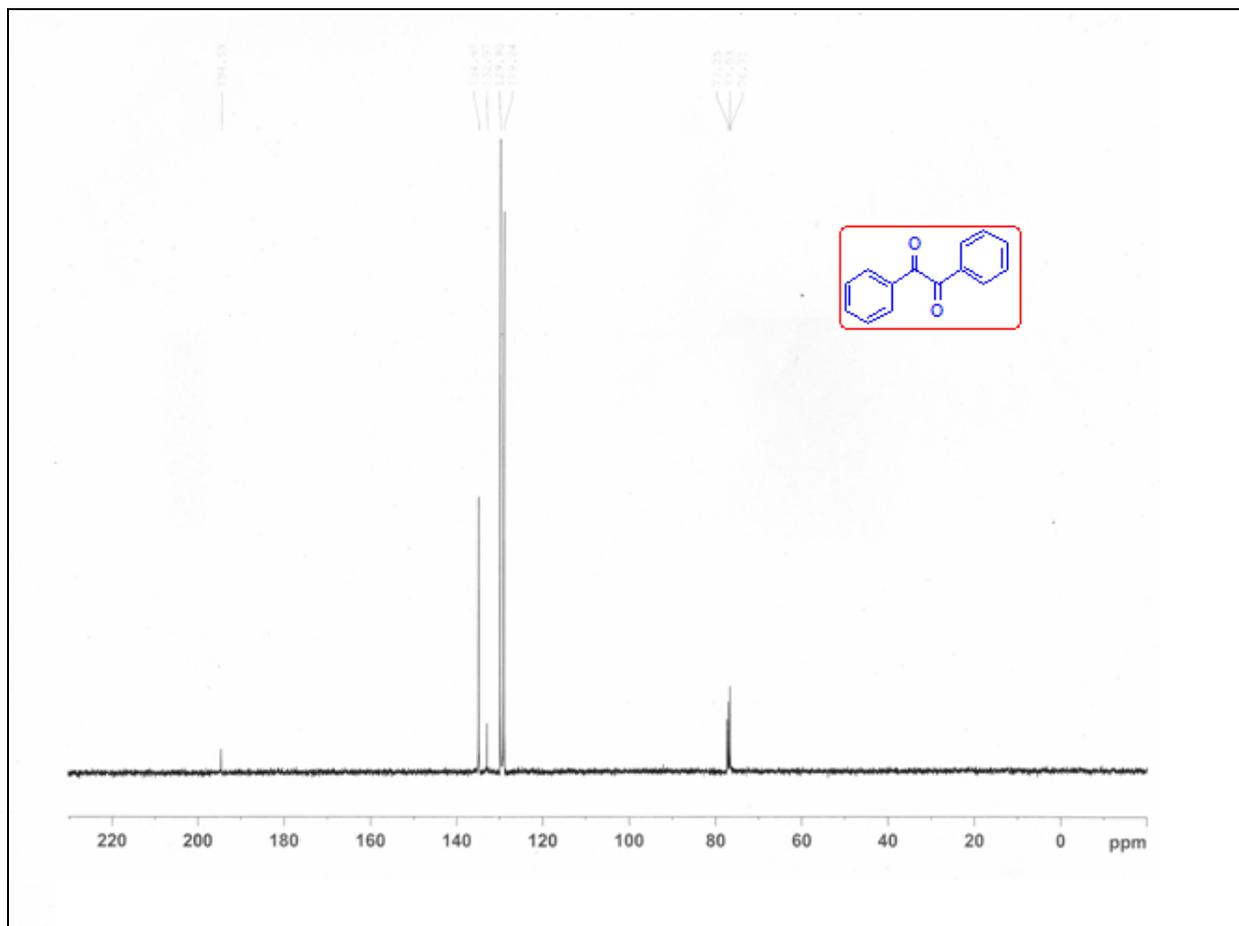


Figure 11. ^{13}C NMR Spectra of Benzil

12. Cinnamaldehyde (2g)

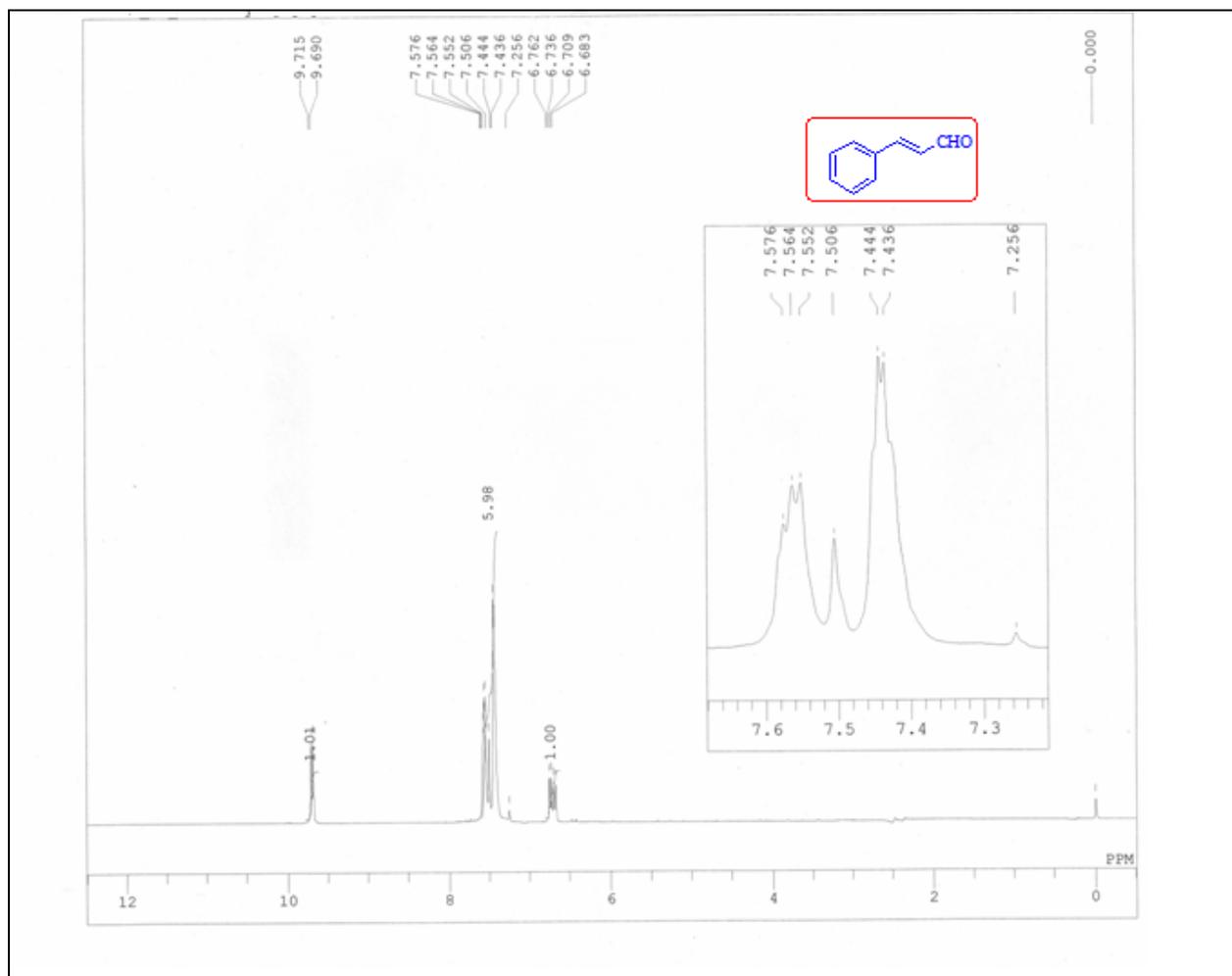


Figure 12. ^1H NMR Spectra of Cinnamaldehyde

13. Cinnamaldehyde (2g)

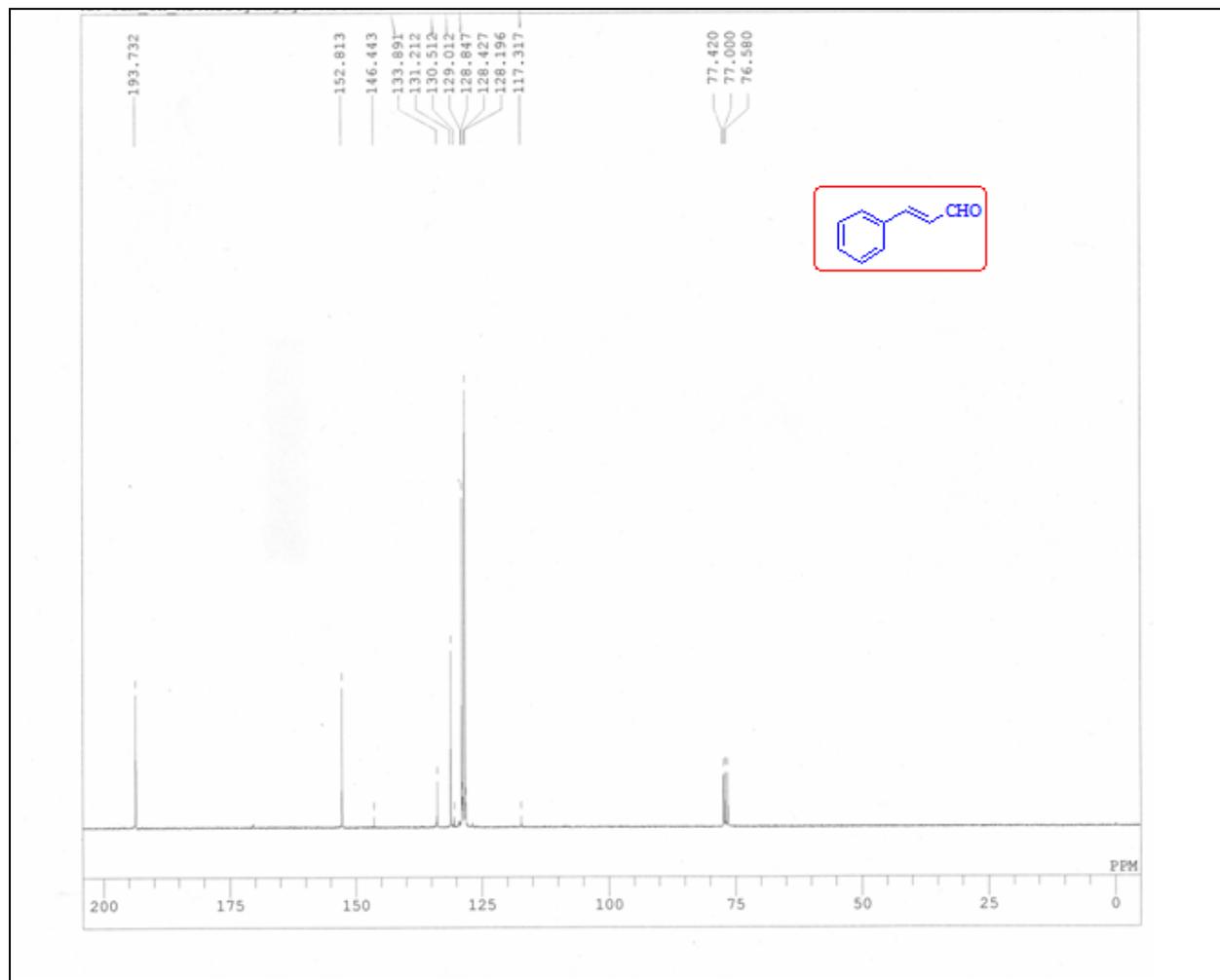


Figure 13. ^{13}C NMR Spectra of Cinnamaldehyde

14. Acetophenone (2h)

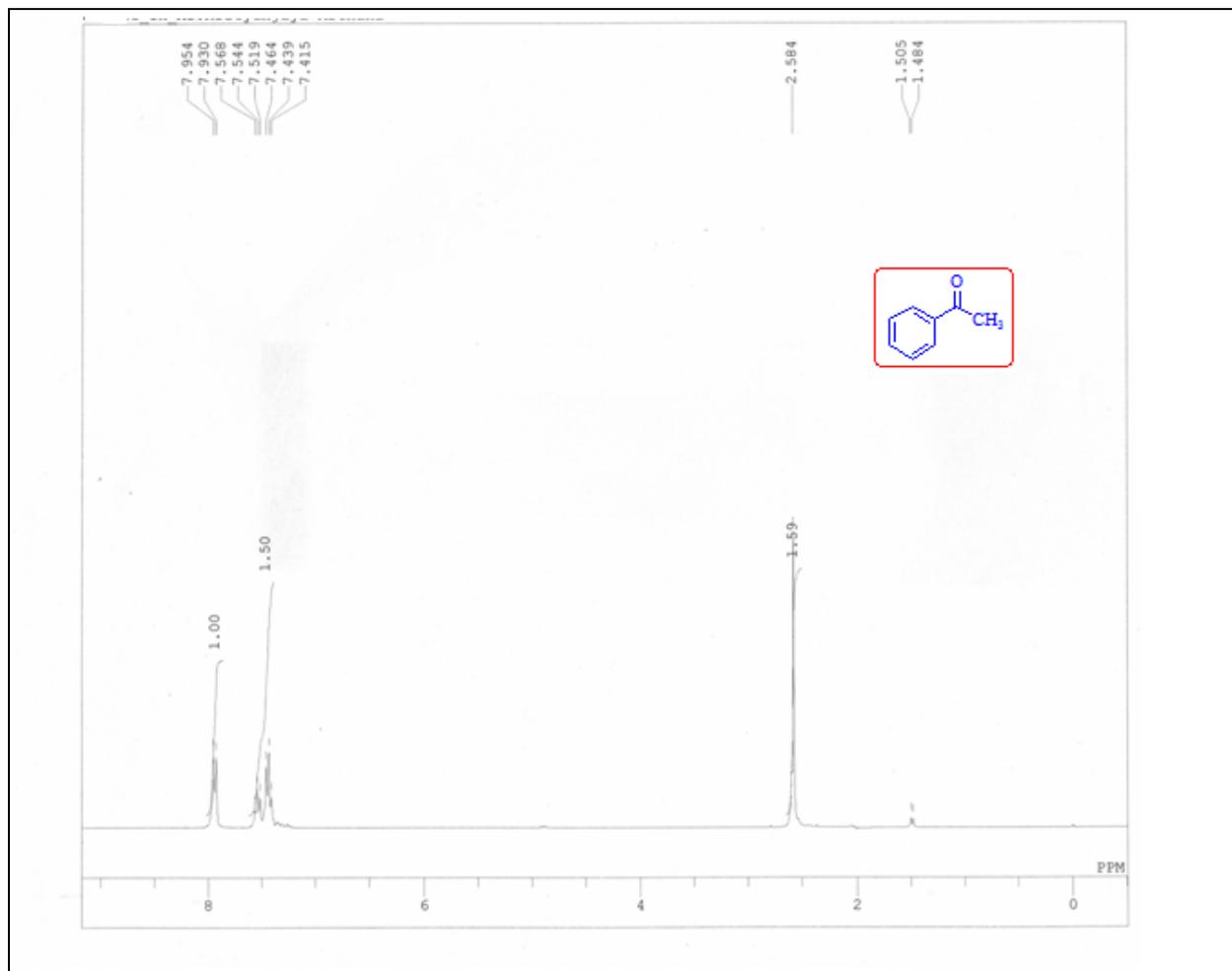


Figure 14. ¹H NMR Spectra of acetophenone

15. Acetophenone (2h)

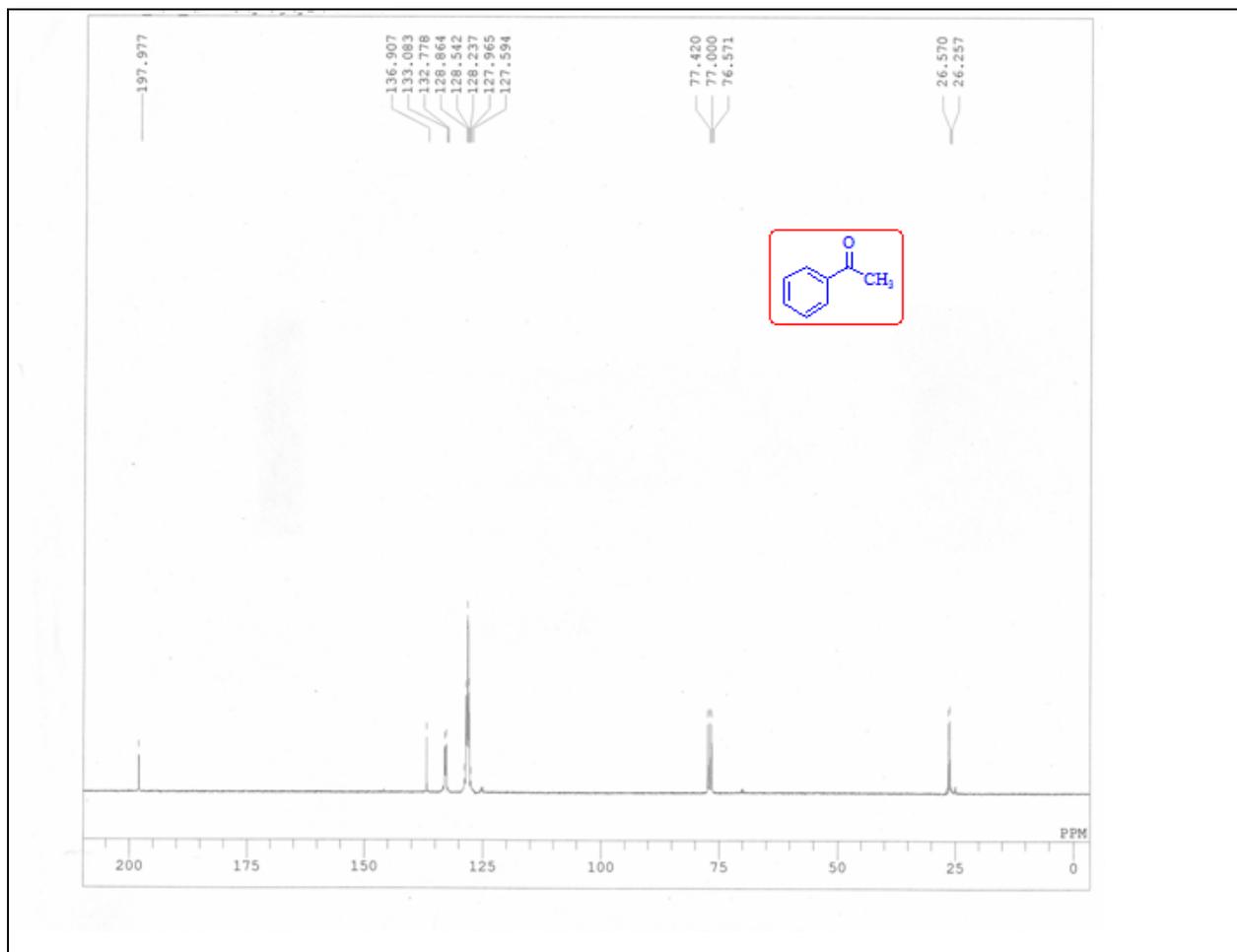


Figure 15. ^{13}C NMR Spectra of acetophenone

16. 4-chloro acetophenone (2i)

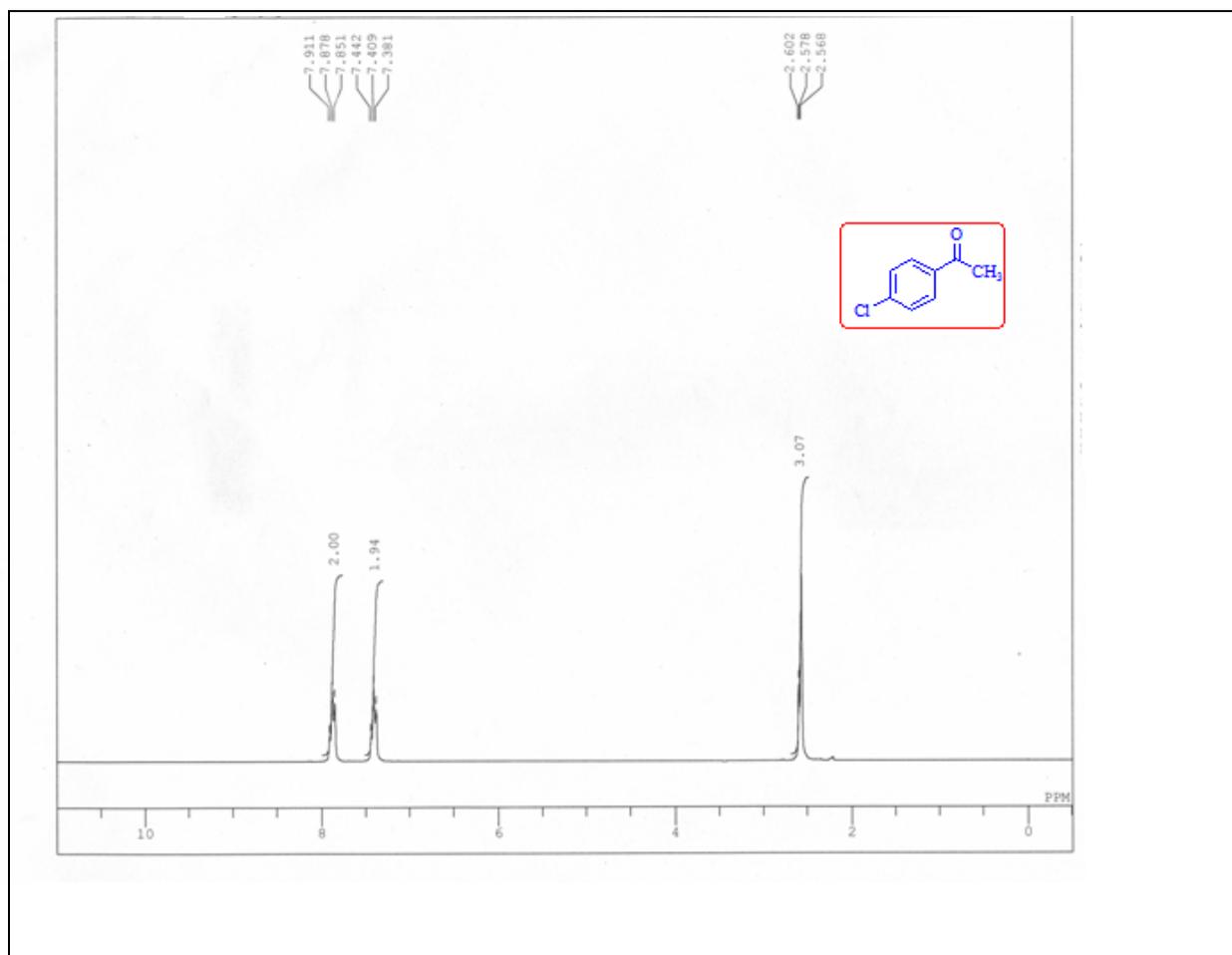


Figure 16. ¹H NMR Spectra of 4-chloro acetophenone

17. 4-chloro acetophenone (2i)

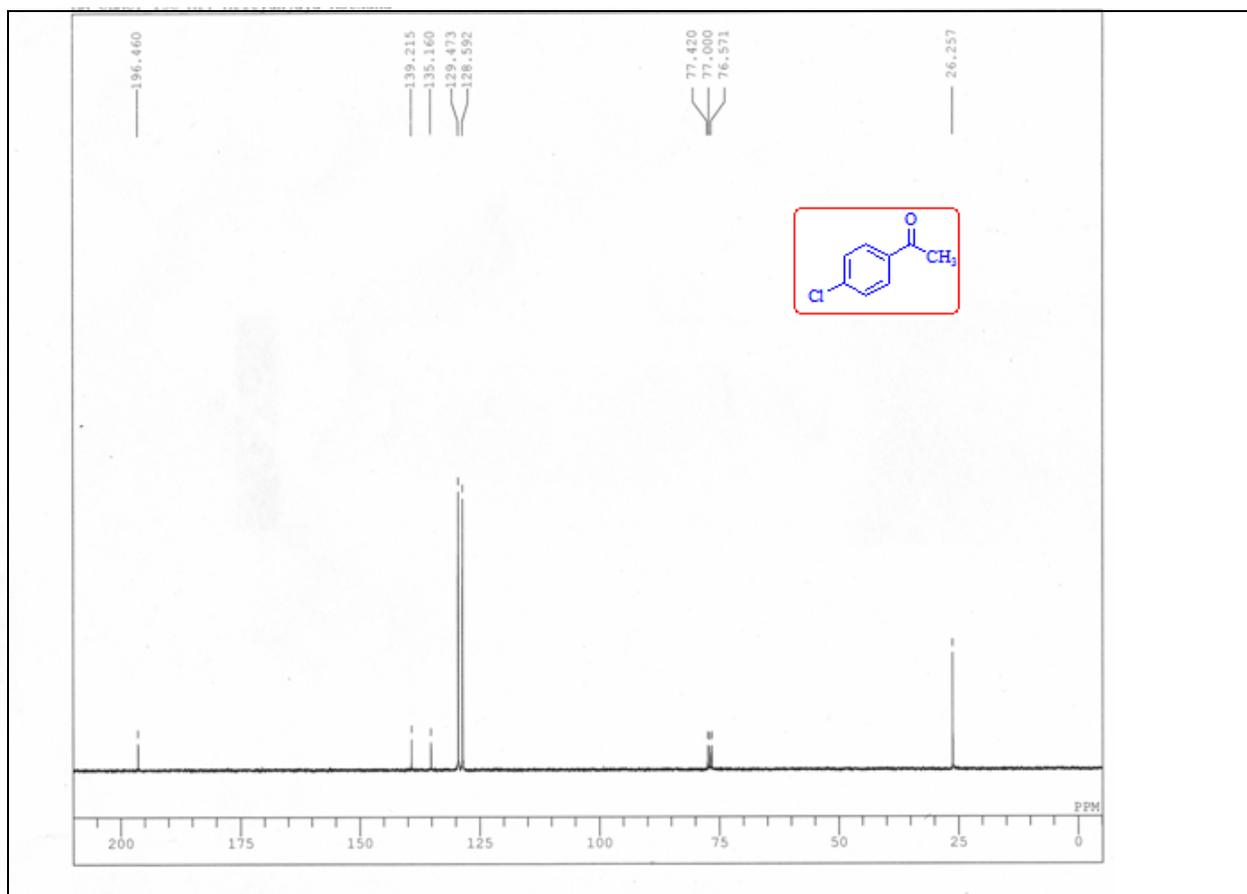


Figure 17. ^{13}C NMR Spectra of 4-chloro acetophenone

18. 4-methyl acetophenone(2j)

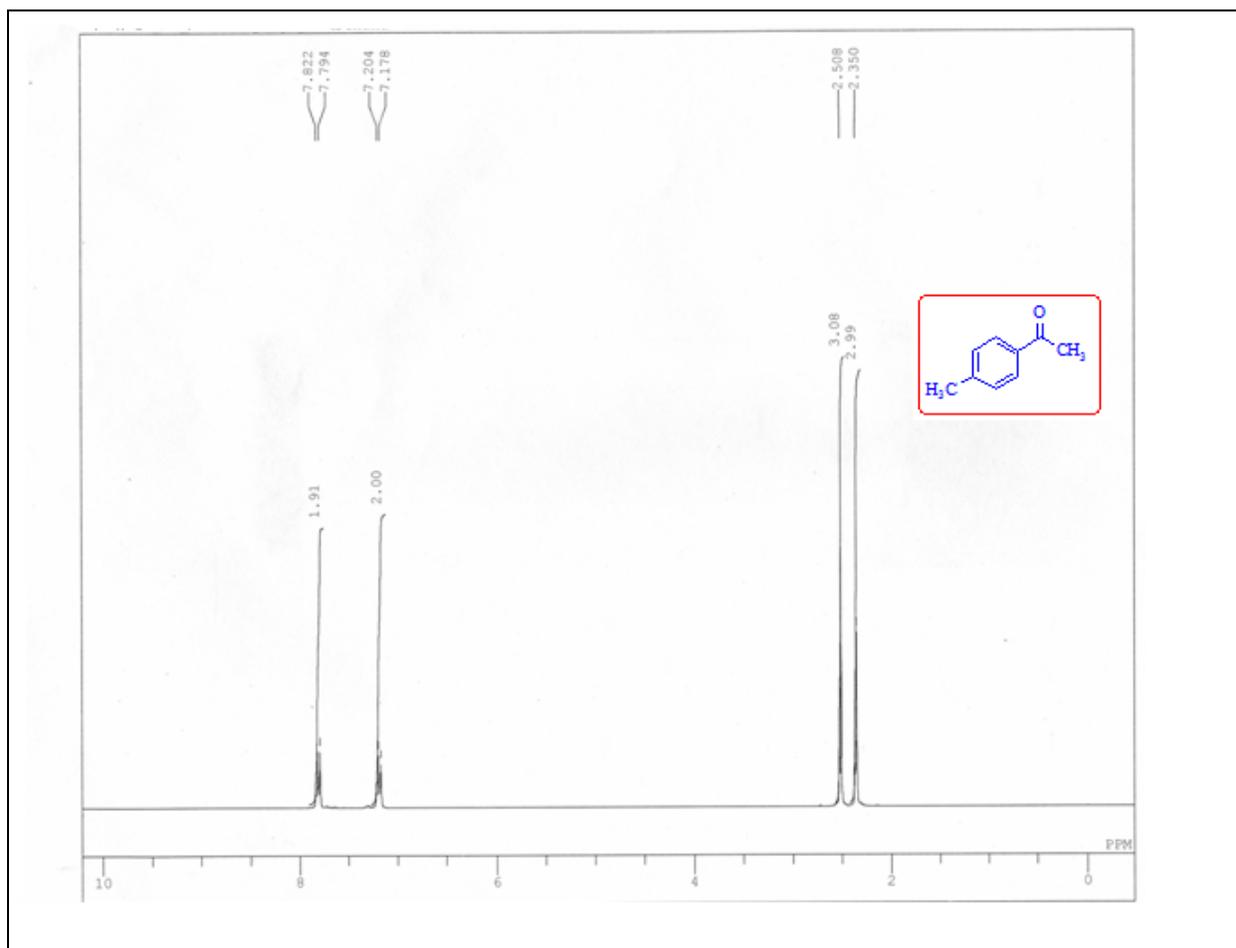


Figure 18. ¹H NMR Spectra of 4-methyl acetophenone

19. 4-methyl acetophenone(2j)

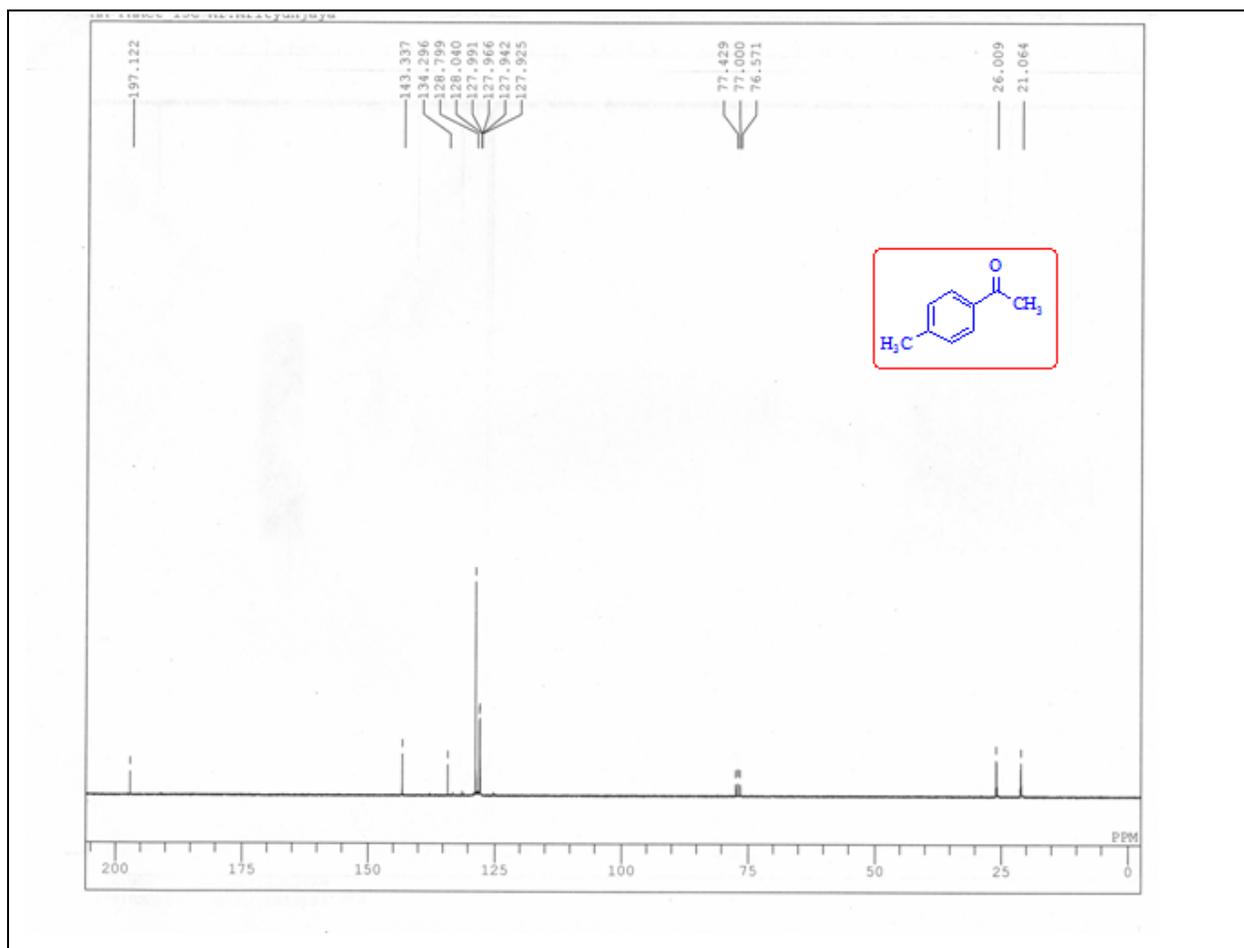


Figure 19. ^{13}C NMR Spectra of 4-methyl acetophenone