Problems related to spectroscopy

1. A compound of MF $C_5H_{12}O$ gave following spectral data: IR: 3400 (cm^{-1}); ^{1}H-NMR: 0.95 (d, 6H), 1.8-1.9 (m, 3H), 2.70 (s, 1H), 3.9 (t, 2H). Peak at 2.70 disappears on shacking with D_2O. Find out structure of the compound.

2. A compound of MF $C_{13}H_{20}O_2N_2$ gave following spectral data: IR: 3442, 3360 (IR of aniline), 1725 cm^{-1}; ^{1}H NMR: 1.15 (t, 6H), 2.4-2.8 (m, 6H), 3.70 (brs, 2H), 4.10 (t, 2H), 6.8 (d, J = 8Hz, 2H), 7.8 (d, J = 8Hz, 2H); ^{13}C NMR: 13.7 (+), 46.4(-), 53.2 (-), 66.2 (-), 115 (+), 120.5 (Cquart), 130.4 (+), 151.2 (Cquart), 167.2 (Cquart); MS (m/z): 236 (M+), 235, 207, 164, 150, 121. Find out structure of the compound, and assign all the peaks.

3. A compound of MF C_7H_7N gave following spectral data: ^{1}H NMR: 5.35 (dd, J =8, 2Hz, 1H), 5.85 (dd, J = 14, 2Hz, 1H), 6.66 (dd, J = 14, 8Hz, 1H), 7.2 (d, J = 8Hz, 2H), 8.5 (d, J = 8Hz, 2H); ^{13}C NMR: 118.9 (-), 120.7 (+), 135.5 (+), 144.3 (Cquart), 150.4 (+). Find out structure of the compound.

4. A compound of MF C_7H_7NO gave following spectral data: ^{1}H NMR: 2.76 (dd, 1H, J = 5.5, 2.5 Hz), 3.09 (dd, 1H, J = 5.5, 4.1 Hz), 3.81 (dd, 1H, J = 4.1, 2.5 Hz), 7.52 (d, J = 8Hz, 2H), 8.66 (d, J = 8Hz, 2H); ^{13}C NMR: 48.8 (-) 57.3 (+), 123.2 (+), 149.7 (+), 152.7 (Cquart); MS (m/z): 121 (M+). Find out structure of the compound, and assign all the peaks.

5. A compound of MF C_9H_{12} gave following spectral data: 1H NMR: 1.2 (d, J = 6Hz, 6H), 2.87 (sept, 1H), 7.23 (s, 5H). Find out structure of the compound.

6. A compound of MF $C_{16}H_{25}ON$ gave following spectral data: IR: 1690 (cm-1); ^{1}H-NMR: 1.11 (t, 6H), 1.29 (d, 6H), 2.40 (q, 4H), 2.55 (t, 2H), 2.65 (t, 2H), 3.12 (septet, 1H), 7.21 (d, J = 8Hz, 2H), 7.81 (d, J = 8Hz, 2H); ^{13}C NMR: 13.7 (+), 24.2 (+), 31. 2 (+), 38.8 (-), 46.2 (-), 47.5 (-), 126.3 (+), 128.5 (+), 134.1 (Cquart), 152.5 (Cquart), 196.2 (Cquart); MS (m/z): 247 (M+), 232, 218, 175, 161, 147. Find out structure of the compound, and assign all the peaks.

7. A compound of MF $C_{15}H_{23}NO_2$ gave following spectral data: IR: 1725 (cm^{-1}); ^{1}H NMR: 1.34 (s, 9H), 2.27 (s, 6H), 2.82 (t, 2H), 4.35 (t, 2H), 7.29 (t, 1H), 7.50 (d, J = 8Hz, 1H), 7.77 (d, J = 8Hz, 1H), 8.00 (s, 1H); ^{13}C NMR: 31 (+), 35 (Cquart), 41 (+), 58 (-), 65 (-), 126 (+), 127 (+), 128 (+), 129 (+), 130 (Cquart), 147 (Cquart), 167 (Cquart). Find out structure of the compound,and assign all the peaks.

8. An unknown organic compound with MF C_4H_5NO displays strong intensity band at 2250 cm^{-1} and 1720 cm^{-1}. The compound shows only two singlets in the ratio of 3:2 in ^{1}H NMR spectrum. Identify the compound.

9. A compound of MF $C_{10}H_{13}NO_2$ gave following spectral data: IR: 3300, 1660 cm^{-1}; ^{1}H NMR: 1.32 (t, 3H), 2.10 (s, 3H), 4.02 (q, J = 6Hz, 2H), 6.8 (d, J = 8Hz, 2H), 7.4 (d, J = 8Hz, 2H), 7.9 (brs, 1H); MS (m/z): 179 (M+), 164, 136, 134. Find out structure of the compound, and assign all the peaks.

10. A compound of MF $C_6H_{10}O_2$ gave following spectral data: IR: 1725 cm^{-1}; ^{1}HNMR: 1.24 (t, 3H), 2.05 (d, 3H), 4.13 (q, 2H), 5.83 (d, J = 12Hz, 1H), 6.88 (m, 1H); ^{13}C NMR: 16 (+), 23 (+), 60 (-), 121.2 (+), 140.2 (+), 165.5 (Cquart). In the NOE experiment, intensity of the signal at 5.83 ppm increases on double irradiation of the peak at 2.05 ppm. Identify structure of the compound.

11. A compound having molecular formula $C_7H_{12}O_3$shows the following spectral data: ^{1}H NMR (δ,$CDCl_3$): 1.25 (t, 3H); 2.2 (s, 3H), 2.55 (t, 2H), 2.7 (t, 2H), 4.15 (q, 2H); ^{13}C NMR: 10, 28, 31, 38, 61, 172, 208; IR(cm^{-1}): 1710, 1750. Find out structure of the compound.

12. A compound having molecular formula $C_9H_{11}BrO$ shows the following spectral data: ^{1}H NMR (δ,$CDCl_3$): 7.15 (m, 2H), 6.82 (m,1H), 6.77 (m, 2H), 4.17 (t, 2H), 3.5 (t, 2H), 2.2 (pentate, 2H). Find out structure of the compound.

13. An organic compound having molecular formula $C_8H_{10}O_2$shows the following spectral data: ^{1}H NMR (δ, $CDCl_3$): 2.0 (brs, 1H, exchangeable with D_2O), 3.73 (s, 3H), 4.79 (s, 2H), 6.70 (m, 2H), 7.08 (m, 2H). Find out structure of the compound.

14. The MS of an unknown organic compound shows M+ peak at 87 (100%) and M+2 peak at m/z 89 (4.9%). It shows three signals in the 1H NMR in the intensity ratio of 1:2:2 and strong absorption in IR at 2250 cm^{-1}. Propose suitable structure to the compound.

15. An organic compound having molecular formula $C_{14}H_{21}NO_2$shows the following spectral data: 1H NMR (δ, $CDCl_3$): 1.1 (t, 6H), 2.22 (s, 3H), 2.5-2.9 (m, 6H), 4.1 (t, 2H), 6.9 (d, J= 8Hz, 2H), 7.8(d, J = 8Hz, 2H). Find out structure of the compound.

16. An organic compound having molecular formula C_9H_{10}shows the following spectral data: ^{1}H NMR (δ, $CDCl_3$): 2.1 (pentet, 2H), 2.9(t, 4H), 7.25(s, 4H); ^{13}C NMR: 25.3(t), 32.8(t), 124.2(d), 125.9(d), 143.9(s). Find out structure of the compound.

17. An organic compound having molecular formula $C_8H_8O_2$ shows the following spectral data: 1H NMR (δ,CDCl3): 3.9 (s, 3H), 7.0(d, J=9Hz, 2H), 7.9(d, J=9Hz, 2H), 9.9 (s, 1H); 13C NMR: 55.5(q), 114.5(d), 130.2(d), 132.2(d), 164.9(s), 191.0 (d). Find out structure of the compound.

18. ^{1}H NMR and ^{13}C NMR of two compounds C_5H_8O (A) and $C_5H_{10}O$ (B) are given below Compound A: ^{1}H NMR (δ,$CDCl_3$): 1.2 (s, 6H), 2.6 (s, 1H), 3.2 (s, 1H); ^{13}C NMR: 45, 68, 72, 85. Compound B 1H NMR (δ, $CDCl_3$): 1.25 (s, 6H), 3.3 (s, 1H), 4.8-5.1(m, 2H), 5.7-6.0 (m, 1H); ^{13}C NMR: 44, 72, 110.7, 146.5. Resonance at δ 3.2 and 3.3 disappears on shaking with D_2O. Find the structures of compound A and B.

19. An organic compound having molecular formula $C_{13}H_{18}O_3$shows the following spectral data: 1H NMR (δ,$CDCl_3$): 1.5 (s, 9H), 3.75(s, 3H), 4.25 (s, 2H), 6.85(d, J=8Hz, 2H), 7.15(d, J=8Hz, 2H); 13C NMR : 28.0(q), 61.6(q), 120.5(d), 132(s), 41.6(t), 78.5(s), 129.5(d), 150.5(s), 170.6(s). Find out structure of the compound.

20. MS of an unknown organic compound shows M+ peak at 166 (100%), M+2 at 168 (130%) and M+4 peak at 170 (30%). It shows two singlets of equal intensity in the 1H NMR. 13C NMR of this compound shows four signals at 22, 30, 77 and 78 ppm. Propose suitable structure of the compound.

21. An organic compound having molecular formula $C_{10}H_{14}O$ shows the following spectral data: 1H NMR (δ,$CDCl_3$): 1.25 (d, 6H), 2.7 (sept, 1H), 3.6 (s, 3H), 6.7 (d, J=9Hz, 2H), 7.2 (d, J= 9Hz, 2H). Find out structure of the compound.

22. An organic compound having molecular formula $C_4H_8O_2$shows the following spectral data: ^{1}H NMR (δ, $CDCl_3$): 1.2 (t, 3H), 1.97(s, 3H), 4.1(q, 2H). Identify the compound.

23. An organic compound having molecular formula $C_7H_{14}O$ shows the following spectral data: 1H NMR (δ, $CDCl_3$): 1.01(d, 12H), 2.45 (sept, 2H). IR (cm^{-1}): 1710. Find out structure of the compound.

24. An organic compound having molecular formula $C_{10}H_{12}O_2$shows the following spectral data: 1H NMR (δ, $CDCl_3$): 1.3(t, 3H), 2.92 (q, 2H), 3.7(s, 3H), 6.9 (d, J = 9Hz, 2H), 7.42 (d, J = 9Hz, 2H). IR (cm^{-1}): 1685, 1220. Identify the compound.

25. A compound shows M+ peak at 142 (100%), and M+2 at 144 (131%), M+4, at 146 (30%). It shows two signals in the 1H NMR at 3.2, and 2.9 ppm of equal intensity. Identify the compound.

26. An organic compound shows strong absorption at 1720 $cm^{-1}$and MS shows peaks at 135 (100%), 136 (6.75%), 137 (33%). The ^{1}H NMR of the compound shows three singlets in the ratio of 2:2:6. Identify the compound.

27. An organic compound having molecular formula $C_{11}H_{16}N_2O$ shows the following spectral data: IR (cm^{-1}): 3442, 3360 and 1690. ^{1}H NMR (δ,$CDCl_3$): 2.51 (t, 2H), 2.80 (s, 3H), 2.85 (t, 2H), 2.9 (s, 3H), 4.0 (brs, 2H), 6.30 (s, 1H), 6.38 (d, J = 8Hz, 1H), 6.48 (d, J = 8Hz, 1H), 6.96 (t, J = 8Hz, 1H); ^{13}C NMR (δ,$CDCl_3$): 31(-), 33(-), 35(+), 38(+), 112(+), 114(+), 117(+), 129(+), 141 (Cquart), 146 (Cquart), 174 (Cquart). MS (m/z): 192(M+), 162, 175, 148, Identify the compound.

28. An organic compound having molecular formula $C_{11}H_{16}N_2O$ shows the following spectral data: IR (cm^{-1}): 3450, 3430, 1680. ^{1}H NMR (δ,$CDCl_3$): 2.0 (brs, 2H), 2.81 (t, 2H), 2.85 (s, 3H), 2.9 (s, 3H), 2.98 (t, 2H), 7.37 (d, J = 8Hz,1H), 7.42 (t, J = 8Hz, 1H), 7.77 (d, J = 8Hz, 1H), 7.84 (s, 1H); 13C NMR (δ,$CDCl_3$): 35(+), 36(+), 39(-), 44(-), 124(+), 126(+), 128(+), 129(+), 134 (Cquart), 140 (Cquart), 166 (Cquart). MS (m/z): 192(M+), 162, 175, 148, Identify the compound.

29. An organic compound with MF $C_{10}H_{12}O$ shows following spectral data: 1H NMR (δ,$CDCl_3$): 1.8 (d, 3H), 3.8 (s, 3H), 6.1-6.2 (m, 1H), 6.4 (d, J = 13Hz, 1H), 6.8 (d, J = 8Hz, 2H), 7.2 (d, J = 8Hz, 2H). 13C NMR ($CDCl_3$): 16(+), 56(+), 114(+), 121(+), 126(+),127.5(Cquart), 128.5(+), 161(Cquart). Propose the structure of the compound.

30. An organic compound with MF $C_{10}H_{12}O$ shows following spectral data: ^{1}H NMR (δ,$CDCl_3$): 1.71 (d, 3H), 3.71 (s, 3H), 6.06 (m, 1H), 6.41 (d, J = 13Hz, 1H), 6.65 (dd, J = 8, 1.5Hz, 1H), 6.81 (t, J = 1.5Hz, 1H), 6.86 (dd, J = 8, 1.5Hz, 1H), 7.10 t, J = 8Hz, 1H). 13C NMR ($CDCl_3$): 16(+), 56(+), 111(+), 113(+), 118(+), 121(+), 128(+), 129(+), 134(Cquart), 162 (Cquart). Propose the structure of the compound.

31. An organic compound with MF $C_{11}H_{15}NO_2$ shows following spectral data: ^{1}H NMR (δ,$CDCl_3$): 2.27 (s, 6H), 3.52 (s, 2H), 3.71 (s, 2H), 5.0 (brs, 1H, D_2O exchangeable), 6.48 (t, J = 1.5 Hz, 1H), 6.54 (dd, J = 8, 1.5 Hz, 1H), 6.62 (dd, J = 8, 1.5 Hz, 1H), 6.97 (t, J = 8Hz, 1H); 13C NMR ($CDCl_3$): 41(+), 44(-), 69(-), 114(+), 116(+), 122(+), 130(+), 135(Cquart, 157(Cquart), 206(Cquart). Propose the structure of the compound.

32. An organic compound with MF $C_{11}H_{15}NO_2$ shows following spectral data: ^{1}H NMR (δ,$CDCl_3$): 2.0 (brs, 1H, D_2O exchangeable), 2.85 (s, 6H), 3.71 (s, 2H), 4.69 (s, 2H), 6.35 (dd, J = 8, 1.5 Hz, 1H), 6.40 (dd, J = 8, 1.5 Hz, 1H), 6.45 (t, J =1.5Hz, 1H), 6.96 (t, J = 8Hz, 1H); ^{13}C NMR (CDCl3): 42(-), 43(+), 72(-), 111(+), 113(+), 118(+), 129(+), 130(+), 135(Cquart, 144(Cquart), 206(Cquart). Propose the structure of the compound.

33. An organic compound C_7H_8 undergoes catalytic hydrogenation to give tetrahydro product C_7H_{12}. The broad band proton-decoupled ^{13}C NMR spectrum of the parent compound shows three signals at 50 (CH), 68 (CH_2), 142 (CH) ppm. Identify the structure of the parent compound.

34. A compound of MF C_7H_7NO gave following spectral data: 1H NMR: 2.76 (dd, 1H, J = 5.5, 2.5 Hz), 3.09 (dd, 1H, J = 5.5, 4.1 Hz), 3.81 (dd, 1H, J = 4.1, 2.5 Hz),, 7.42 (t, J = 8Hz, 1H), 7.90 (d, J = 8Hz, 1H), 8.55 (d, J = 8Hz, 1H), 8.70 (s, 1H),; 13C NMR: 48.8 (-) 57.3 (+), 123.2 (+), 135 (+), 139 (Cquart), 147(+), 149(+); MS (m/z): 121 (M+). Find out structure of the compound, and assign all the peaks.

35. A compound of MF C_7H_6BrNO gave following spectral data: ^{1}H NMR: 4.23 (d, J = 5Hz, 1H), 4.86 (d, J = 5Hz, 1H), 7.42 (t, J = 8Hz, 1H), 7.90 (d, J = 8Hz, 1H), 8.55 (d, J = 8Hz, 1H), 8.7 (s, 1H); ^{13}C NMR: 63(+), 68(+), 123(+), 135(+), 139(Cquart) 147(+), 149(+); MS (m/z): 199(M+), 201(+2). Find out structure of the compound, and assign all the peaks.

36. An organic compound shows strong absorption at 1680 $cm^{-1}$and MS shows peaks at 135 (100%), 136 (6.75%), 137 (33%). The ^{1}H NMR of the compound shows two triplets and two singlets in the ratio of 2:2:3:3. Identify the compound.

38. MS of an unknown organic compound shows M+ peak at 166 (100%), M+2 at 168 (130%) and M+4 peak at 170 (30%). It shows two singlets of equal intensity in the ^{1}H NMR. ^{13}C NMR of this compound shows two quaternary carbons 77 and 78 ppm. Propose suitable structure of the compound.

39. An organic compound shows M^+ peak at 125 (75%), M^++1 at 126 (5.0%) and M^++2 peak at 127 (3.5%). Calculate the molecular formula of the compound.