

Problems related to spectroscopy

1. A compound of MF $C_5H_{12}O$ gave following spectral data: IR: $3400\text{ (cm}^{-1}\text{)}$; $^1\text{H-NMR}$: 0.95 (d, 6H), 1.8-1.9 (m, 3H), 2.70 (s, 1H), 3.9 (t, 2H). Peak at 2.70 disappears on shaking 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 (PSK, cm^{-1}); $^1\text{H NMR}$: 1.15 (t, 6H), 2.4-2.8 (m, 6H), 3.70 (brs, 2H), 4.10 (t, 2H), 6.8 (d, $J = 8\text{Hz}$, 2H), 7.8 (d, $J = 8\text{Hz}$, 2H); $^{13}\text{C NMR}$: 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: $^1\text{H NMR}$: 5.35 (dd, $J = 8$, 2Hz, 1H), 5.85 (dd, $J = 14$, 2Hz, 1H), 6.66 (dd, $J = 14$, 8Hz, 1H), 7.2 (d, $J = 8\text{Hz}$, 2H), 8.5 (d, $J = 8\text{Hz}$, 2H); $^{13}\text{C NMR}$: 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: $^1\text{H NMR}$: 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, $J = 8\text{Hz}$, 2H), 8.66 (d, $J = 8\text{Hz}$, 2H); $^{13}\text{C NMR}$: 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: $^1\text{H NMR}$: 1.2 (d, $J = 6\text{Hz}$, 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}); 1H -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}); 1H 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 1H 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} ; 1H 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} ; 1H NMR: 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: 1H NMR ($\delta, CDCl_3$): 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: 1H NMR ($\delta, CDCl_3$): 7.15 (m, 2H), 6.82 (m, 1H), 6.77 (m, 2H), 4.17 (t, 2H), 3.5 (t, 2H), 2.2 (pentet, 2H). Find out structure of the compound.

13. An organic compound having molecular formula $C_8H_{10}O_2$ shows the following spectral data: 1H NMR ($\delta, CDCl_3$): 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.

$M+2$ peak at m/z 89 (4.9%) indicate that S atom is present.

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

16. An organic compound having molecular formula C_9H_{10} shows the following spectral data: 1H NMR ($\delta, CDCl_3$): 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 ($\delta, CDCl_3$): 3.9 (s, 3H), 7.0(d, $J=9Hz$, 2H), 7.9(d, $J=9Hz$, 2H), 9.9 (s, 1H); ^{13}C 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. 1H NMR and ^{13}C NMR of two compounds C_5H_8O (A) and $C_5H_{10}O$ (B) are given below
Compound A: 1H NMR ($\delta, CDCl_3$): 1.2 (s, 6H), 2.6 (s, 1H), 3.2 (s, 1H); ^{13}C NMR: 45, 68, 72, 85.
Compound B 1H NMR ($\delta, CDCl_3$): 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 ($\delta, CDCl_3$): 1.5 (s, 9H), 3.75 (s, 3H), 4.25 (s, 2H), 6.85 (d, $J = 8Hz$, 2H), 7.15(d, $J = 8Hz$, 2H); ^{13}C 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. An organic compound having molecular formula $C_{10}H_{14}O$ shows the following spectral data: 1H NMR ($\delta, CDCl_3$): 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.