

## Problems related to spectroscopy

1. A compound of MF  $C_5H_{12}O$  gave following spectral data: IR:  $3400\text{ cm}^{-1}$ ;  $^1\text{H-NMR}$ : 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),  $1725\text{ cm}^{-1}$ ;  $^1\text{H NMR}$ : 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:  $1690\text{ cm}^{-1}$ ;  $^1\text{H-NMR}$ : 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,  $J = 8\text{Hz}$ , 2H), 7.81 (d,  $J = 8\text{Hz}$ , 2H);  $^{13}\text{C NMR}$ : 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:  $1725\text{ cm}^{-1}$ ;  $^1\text{H NMR}$ : 1.34 (s, 9H), 2.27 (s, 6H), 2.82 (t, 2H), 4.35 (t, 2H), 7.29 (t, 1H), 7.50 (d,  $J = 8\text{Hz}$ , 1H), 7.77 (d,  $J = 8\text{Hz}$ , 1H), 8.00 (s, 1H);  $^{13}\text{C NMR}$ : 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  $2250\text{ cm}^{-1}$  and  $1720\text{ cm}^{-1}$ . The compound shows only two singlets in the ratio of 3:2 in  $^1\text{H NMR}$  spectrum. Identify the compound.

9. A compound of MF  $C_{10}H_{13}NO_2$  gave following spectral data: IR:  $3300$ ,  $1660\text{ cm}^{-1}$ ;  $^1\text{H NMR}$ : 1.32 (t, 3H), 2.10 (s, 3H), 4.02 (q,  $J = 6\text{Hz}$ , 2H), 6.8 (d,  $J = 8\text{Hz}$ , 2H), 7.4 (d,  $J = 8\text{Hz}$ , 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:  $1725\text{ cm}^{-1}$ ;  $^1\text{H}$ NMR: 1.24 (t, 3H), 2.05 (d, 3H), 4.13 (q, 2H), 5.83 (d,  $J = 12\text{Hz}$ , 1H), 6.88 (m, 1H);  $^{13}\text{C}$  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:  $^1\text{H}$  NMR ( $\delta, \text{CDCl}_3$ ): 1.25 (t, 3H); 2.2 (s, 3H), 2.55 (t, 2H), 2.7 (t, 2H), 4.15 (q, 2H);  $^{13}\text{C}$  NMR: 10, 28, 31, 38, 61, 172, 208; IR( $\text{cm}^{-1}$ ): 1710, 1750. Find out structure of the compound.

12. A compound having molecular formula  $C_9H_{11}\text{BrO}$  shows the following spectral data:  $^1\text{H}$  NMR ( $\delta, \text{CDCl}_3$ ): 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:  $^1\text{H}$  NMR ( $\delta, \text{CDCl}_3$ ): 2.0 (brs, 1H, exchangeable with  $\text{D}_2\text{O}$ ), 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  $^1\text{H}$  NMR in the intensity ratio of 1:2:2 and strong absorption in IR at  $2250\text{ cm}^{-1}$ . Propose suitable structure to the compound.

15. An organic compound having molecular formula  $C_{14}H_{21}\text{NO}_2$  shows the following spectral data:  $^1\text{H}$  NMR ( $\delta, \text{CDCl}_3$ ): 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:  $^1\text{H}$  NMR ( $\delta, \text{CDCl}_3$ ): 2.1 (pentet, 2H), 2.9 (t, 4H), 7.25 (s, 4H);  $^{13}\text{C}$  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:  $^1\text{H}$  NMR ( $\delta, \text{CDCl}_3$ ): 3.9 (s, 3H), 7.0 (d,  $J = 9\text{Hz}$ , 2H), 7.9 (d,  $J = 9\text{Hz}$ , 2H), 9.9 (s, 1H);  $^{13}\text{C}$  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.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR of two compounds  $C_5H_8O$  (A) and  $C_5H_{10}O$  (B) are given below  
Compound A:  $^1\text{H}$  NMR ( $\delta, \text{CDCl}_3$ ): 1.2 (s, 6H), 2.6 (s, 1H), 3.2 (s, 1H);  $^{13}\text{C}$  NMR: 45, 68, 72, 85.  
Compound B:  $^1\text{H}$  NMR ( $\delta, \text{CDCl}_3$ ): 1.25 (s, 6H), 3.3 (s, 1H), 4.8-5.1 (m, 2H), 5.7-6.0 (m, 1H);  $^{13}\text{C}$  NMR: 44, 72, 110.7, 146.5. Resonance at  $\delta$  3.2 and 3.3 disappears on shaking with  $\text{D}_2\text{O}$ . 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:  $^1\text{H}$  NMR ( $\delta, \text{CDCl}_3$ ): 1.5 (s, 9H), 3.75 (s, 3H), 4.25 (s, 2H), 6.85 (d,  $J = 8\text{Hz}$ , 2H), 7.15 (d,  $J = 8\text{Hz}$ , 2H);  $^{13}\text{C}$  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. MS of an unknown organic compound shows M<sup>+</sup> 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 <sup>1</sup>H NMR. <sup>13</sup>C 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<sub>10</sub>H<sub>14</sub>O shows the following spectral data: <sup>1</sup>H NMR (δ, CDCl<sub>3</sub>): 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<sub>4</sub>H<sub>8</sub>O<sub>2</sub> shows the following spectral data: <sup>1</sup>H NMR (δ, CDCl<sub>3</sub>): 1.2 (t, 3H), 1.97(s, 3H), 4.1(q, 2H). Identify the compound.

23. An organic compound having molecular formula C<sub>7</sub>H<sub>14</sub>O shows the following spectral data: <sup>1</sup>H NMR (δ, CDCl<sub>3</sub>): 1.01(d, 12H), 2.45 (sept, 2H). IR (cm<sup>-1</sup>): 1710. Find out structure of the compound.

24. An organic compound having molecular formula C<sub>10</sub>H<sub>12</sub>O<sub>2</sub> shows the following spectral data: <sup>1</sup>H NMR (δ, CDCl<sub>3</sub>): 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<sup>-1</sup>): 1685, 1220. Identify the compound.

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

26. An organic compound shows strong absorption at 1720 cm<sup>-1</sup> and MS shows peaks at 135 (100%), 136 (6.75%), 137 (33%). The <sup>1</sup>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<sub>11</sub>H<sub>16</sub>N<sub>2</sub>O shows the following spectral data: IR (cm<sup>-1</sup>): 3442, 3360 and 1690. <sup>1</sup>H NMR (δ, CDCl<sub>3</sub>): 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); <sup>13</sup>C NMR (δ, CDCl<sub>3</sub>): 31(-), 33(-), 35(+), 38(+), 112(+), 114(+), 117(+), 129(+), 141 (Cquart), 146 (Cquart), 174 (Cquart). MS (m/z): 192(M<sup>+</sup>), 162, 175, 148. Identify the compound.

28. An organic compound having molecular formula C<sub>11</sub>H<sub>16</sub>N<sub>2</sub>O shows the following spectral data: IR (cm<sup>-1</sup>): 3450, 3430, 1680. <sup>1</sup>H NMR (δ, CDCl<sub>3</sub>): 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); <sup>13</sup>C NMR (δ, CDCl<sub>3</sub>): 35(+), 36(+), 39(-), 44(-), 124(+), 126(+), 128(+), 129(+), 134 (Cquart), 140 (Cquart), 166 (Cquart). MS (m/z): 192(M<sup>+</sup>), 162, 175, 148. Identify the compound.

29. An organic compound with MF C<sub>10</sub>H<sub>12</sub>O shows following spectral data: <sup>1</sup>H NMR (δ, CDCl<sub>3</sub>): 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). <sup>13</sup>C NMR (CDCl<sub>3</sub>): 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:  $^1H$  NMR ( $\delta, CDCl_3$ ): 1.71 (d, 3H), 3.71 (s, 3H), 6.06 (m, 1H), 6.41 (d,  $J = 13\text{Hz}$ , 1H), 6.65 (dd,  $J = 8, 1.5\text{Hz}$ , 1H), 6.81 (t,  $J = 1.5\text{Hz}$ , 1H), 6.86 (dd,  $J = 8, 1.5\text{Hz}$ , 1H), 7.10 t,  $J = 8\text{Hz}$ , 1H).  $^{13}C$  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:  $^1H$  NMR ( $\delta, CDCl_3$ ): 2.27 (s, 6H), 3.52 (s, 2H), 3.71 (s, 2H), 5.0 (brs, 1H,  $D_2O$  exchangeable), 6.48 (t,  $J = 1.5\text{ Hz}$ , 1H), 6.54 (dd,  $J = 8, 1.5\text{ Hz}$ , 1H), 6.62 (dd,  $J = 8, 1.5\text{ Hz}$ , 1H), 6.97 (t,  $J = 8\text{Hz}$ , 1H);  $^{13}C$  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:  $^1H$  NMR ( $\delta, CDCl_3$ ): 2.0 (brs, 1H,  $D_2O$  exchangeable), 2.85 (s, 6H), 3.71 (s, 2H), 4.69 (s, 2H), 6.35 (dd,  $J = 8, 1.5\text{ Hz}$ , 1H), 6.40 (dd,  $J = 8, 1.5\text{ Hz}$ , 1H), 6.45 (t,  $J = 1.5\text{Hz}$ , 1H), 6.96 (t,  $J = 8\text{Hz}$ , 1H);  $^{13}C$  NMR ( $CDCl_3$ ): 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,  $J = 5.5, 2.5\text{ Hz}$ ), 3.09 (dd, 1H,  $J = 5.5, 4.1\text{ Hz}$ ), 3.81 (dd, 1H,  $J = 4.1, 2.5\text{ Hz}$ ), 7.42 (t,  $J = 8\text{Hz}$ , 1H), 7.90 (d,  $J = 8\text{Hz}$ , 1H), 8.55 (d,  $J = 8\text{Hz}$ , 1H), 8.70 (s, 1H);  $^{13}C$  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:  $^1H$  NMR: 4.23 (d,  $J = 5\text{Hz}$ , 1H), 4.86 (d,  $J = 5\text{Hz}$ , 1H), 7.42 (t,  $J = 8\text{Hz}$ , 1H), 7.90 (d,  $J = 8\text{Hz}$ , 1H), 8.55 (d,  $J = 8\text{Hz}$ , 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  $1680\text{ cm}^{-1}$  and MS shows peaks at 135 (100%), 136 (6.75%), 137 (33%). The  $^1H$  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  $^1H$  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.