

## Answers for Spectroscopy Problems

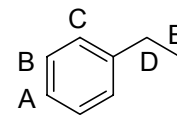
2) For the molecular formula and spectra provided, determine the correct structure. Assign all spectra the best that you can

a) MS  $M^+$  (106); M-15 (-CH<sub>3</sub>: 91)

IR CH<sub>arene</sub> (3040); CH<sub>alkane</sub> (2900); C=C<sub>arene</sub> (1500, 1600)

<sup>1</sup>H H<sub>A</sub>, H<sub>B</sub>, H<sub>C</sub> (7); H<sub>D</sub> (2.5); H<sub>E</sub> (1.2)

<sup>13</sup>C C<sub>aryl</sub> (125-145); C<sub>D</sub> (29); C<sub>E</sub> (16)

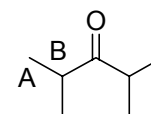


b) MS  $M^+$  (114); M-43 (-C(CH<sub>3</sub>)<sub>3</sub>: 71)

IR CH<sub>alkane</sub> (2900); C=O (1700)

<sup>1</sup>H H<sub>A</sub>, (1.1); H<sub>B</sub> (2.8)

<sup>13</sup>C C<sub>A</sub> (19); C<sub>B</sub> (39); C=O (>200)

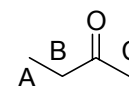


c) MS  $M^+$  (72); M-15 (-CH<sub>3</sub>: 57)

IR CH<sub>alkane</sub> (2900); C=O (1700)

<sup>1</sup>H H<sub>A</sub> (1.1); H<sub>B</sub> (2.5); H<sub>C</sub> (2.2)

<sup>13</sup>C C<sub>A</sub> (8); C<sub>B</sub> (29); C<sub>C</sub> (37); C=O (>200)

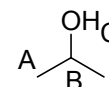


d) MS M-1 (-H: 59); M-15 (-CH<sub>3</sub>: 45)

IR OH (3300); CH<sub>alkane</sub> (2900); CO (1100)

<sup>1</sup>H H<sub>A</sub> (1.1); H<sub>B</sub> (3.8); H<sub>C</sub> (4.8)

<sup>13</sup>C C<sub>A</sub> (25); C<sub>B</sub> (64)

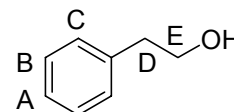


e) MS  $M^+$  (122); M-31 (-CH<sub>2</sub>OH: 91)

IR OH (3300); CH<sub>arene</sub> (3040); CH<sub>alkane</sub> (2900); C=C<sub>arene</sub> (1500, 1600)

<sup>1</sup>H H<sub>A</sub>, H<sub>B</sub>, H<sub>C</sub> (7); H<sub>D</sub> (2.6); H<sub>E</sub> (3.5); H<sub>OH</sub> (4.0)

<sup>13</sup>C C<sub>aryl</sub> (126-139); C<sub>D</sub> (39); C<sub>E</sub> (64)

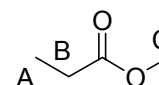


f) MS  $M^+$  (88); M-31 (-OCH<sub>3</sub>: 57)

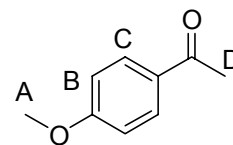
IR CH<sub>alkane</sub> (2900); C=O (1700); CO (1200)

<sup>1</sup>H H<sub>A</sub> (1.2); H<sub>B</sub> (2.4); H<sub>C</sub> (3.7)

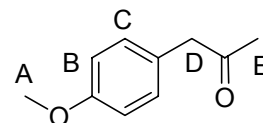
<sup>13</sup>C C<sub>A</sub> (9); C<sub>B</sub> (27); C<sub>C</sub> (51); C=O (175)



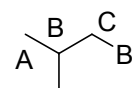
- g) MS  $M^+$  (150); M-15 (-CH<sub>3</sub>: 135)  
 IR CH<sub>alkane</sub> (2900); C=O (1700); C=C<sub>arene</sub> (1500, 1600); CO (1250)  
<sup>1</sup>H H<sub>A</sub> (3.9), H<sub>B</sub> (7), H<sub>C</sub> (8); H<sub>D</sub> (2.5)  
<sup>13</sup>C C<sub>aryl</sub> (121-148); C<sub>D</sub> (21); C<sub>E</sub> (21), C=O (170)



- h) MS  $M^+$  (164); M-43 (-COCH<sub>3</sub>: 121)  
 IR CH<sub>alkane</sub> (2900); C=O (1700); C=C<sub>arene</sub> (1500, 1600); CO (1250)  
<sup>1</sup>H H<sub>A</sub> (3.7), H<sub>B</sub> (6.7), H<sub>C</sub> (7.1); H<sub>D</sub> (3.6); H<sub>E</sub> (2.1)  
<sup>13</sup>C C<sub>aryl</sub> (114-159); C<sub>C</sub> (55); C<sub>D</sub> (50), C<sub>E</sub> (29); C=O (>200)

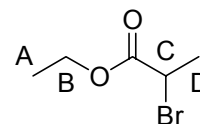


- i) MS  $M^+$  (136); M-79 (-Br: 57)  
 IR CH<sub>alkane</sub> (2900)  
<sup>1</sup>H H<sub>A</sub> (1), H<sub>B</sub> (2.1), H<sub>C</sub> (3.2)  
<sup>13</sup>C C<sub>A</sub> (21); C<sub>B</sub> (31), C<sub>C</sub> (42)

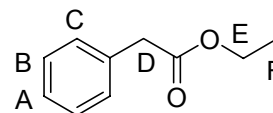


- j) CORRECT MOLECULAR FORMULA: C<sub>5</sub>H<sub>9</sub>BrO<sub>2</sub>

- MS  $M^+$  (180); M-45 (-OCH<sub>2</sub>CH<sub>3</sub>: 135)  
 IR CH<sub>alkane</sub> (2900); C=O (1700); CO (1150)  
<sup>1</sup>H H<sub>A</sub> (1.3); H<sub>B</sub> (3.4); H<sub>C</sub> (4.2); H<sub>D</sub> (1.8)  
<sup>13</sup>C C<sub>A</sub> (14); C<sub>B</sub> (58); C<sub>C</sub> (60); C<sub>D</sub> (20); C=O (172)



- k) MS  $M^+$  (164); M-73 (-CO<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>: 91)  
 IR CH<sub>arene</sub> (3040); CH<sub>alkane</sub> (2900); C=O (1700); C=C<sub>arene</sub> (1500, 1600); CO (1150)  
<sup>1</sup>H H<sub>A</sub>, H<sub>B</sub>, H<sub>C</sub> (7.2), H<sub>D</sub> (3.5), H<sub>E</sub> (4.1); H<sub>F</sub> (1.2)  
<sup>13</sup>C C<sub>aryl</sub> (127-134); C<sub>D</sub> (41); C<sub>E</sub> (61), C<sub>F</sub> (14); C=O (172)



- l) MS  $M^+$  (132); M-15 (-CH<sub>3</sub>: 117)  
 IR CH<sub>alkane</sub> (2900); C=O (1700); CO (1100)  
<sup>1</sup>H H<sub>A</sub> (3.3); H<sub>B</sub> (4.6); H<sub>C</sub> (2.6); H<sub>D</sub> (2.1)  
<sup>13</sup>C C<sub>A</sub> (54); C<sub>B</sub> (102); C<sub>C</sub> (47); C<sub>D</sub> (31); C=O (>200)

