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Introduction to Spectroscopy | (5th Edition)

Chapter 6, Problem 24P

(2 Bookmarks)

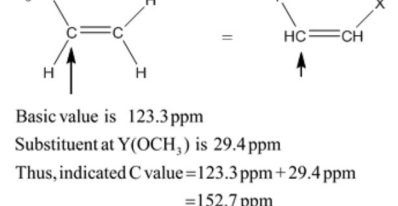
Show all steps: ☒ ON

Step-by-step solution

Step 1 of 78

(a)

The basic value of ethylene is 123.3 ppm. Use the values for alkene listed in the table 8.4 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

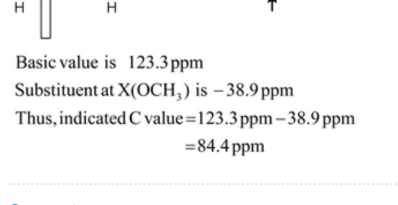


Basic value is 123.3 ppm
Substituent at Y(OCH₃) is 29.4 ppm
Thus, indicated C value = 123.3 ppm + 29.4 ppm
= 152.7 ppm

Comment

Step 2 of 78

The basic value of ethylene is 123.3 ppm. Use the values for alkene listed in the table 8.4 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:



Basic value is 123.3 ppm
Substituent at X(OC(=O)CH₃) is -38.9 ppm
Thus, indicated C value = 123.3 ppm - 38.9 ppm
= 84.4 ppm

Comment

Step 3 of 78

Therefore, expected C-13 chemical shift values for the indicated carbon atoms in the structure are as follows:



Comment

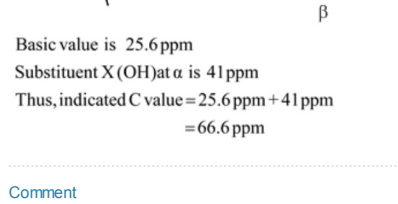
Step 4 of 78

Comment

Step 5 of 78

(b)

The basic value of cyclopentane is 25.6 ppm. Use the values for cycloalkane listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

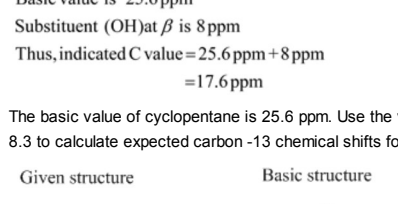


Basic value is 25.6 ppm
Substituent X(OH) at α is 41 ppm
Thus, indicated C value = 25.6 ppm + 41 ppm
= 66.6 ppm

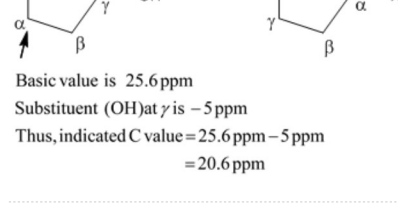
Comment

Step 6 of 78

The basic value of cyclopentane is 25.6 ppm. Use the values for cycloalkane listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:



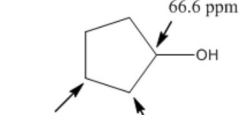
The basic value of cyclopentane is 25.6 ppm. Use the values for cycloalkane listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:



Comments (1)

Step 7 of 78

Thus, expected C-13 chemical shift values for the indicated carbon atoms in the structure is as follows:

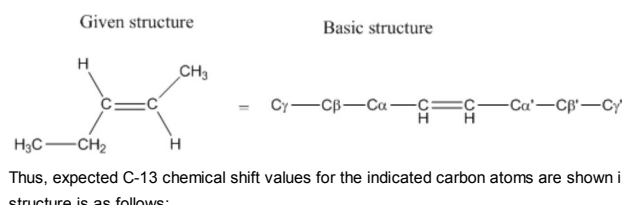


Comment

Step 8 of 78

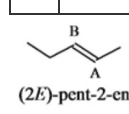
(c)

The basic value of cyclopentane is 123.3 ppm. Use the values for alkene listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:



Thus, expected C-13 chemical shift values for the indicated carbon atoms in the structure is as follows:

Peak	Calculated Shift	
A	123.3+10.6-7.9-1.8	124.2
B	123.3+10.6+7.2-7.9	132.2

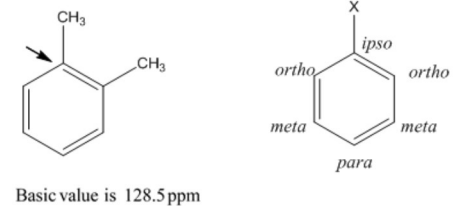


Comment

Step 9 of 78

(d)

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

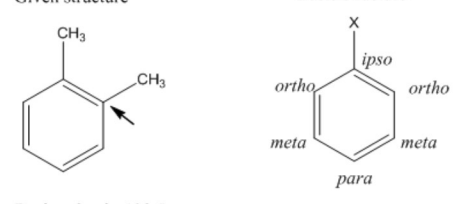


Basic value is 128.5 ppm
Substituent (CH₃) at ipso is 9.3 ppm
Substituent (CH₃) at ortho is 0.7 ppm
Thus, indicated C value = 128.5 ppm + 9.3 ppm + 0.7 ppm
= 138.5 ppm

Comment

Step 10 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

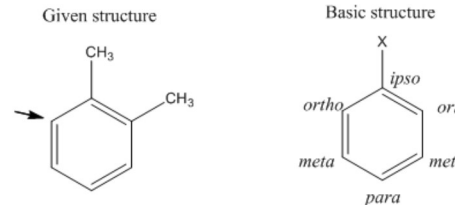


Basic value is 128.5 ppm
Substituent (CH₃) at ipso is 9.3 ppm
Substituent (CH₃) at ortho is 0.7 ppm
Thus, indicated C value = 128.5 ppm + 9.3 ppm + 0.7 ppm
= 138.5 ppm

Comment

Step 11 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

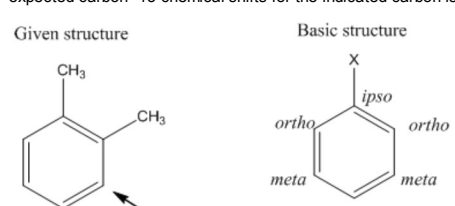


Basic value is 128.5 ppm
Substituent (CH₃) at ipso is 0.7 ppm
Substituent (CH₃) at meta is -0.1 ppm
Thus, indicated C value = 128.5 ppm + 0.7 ppm - 0.1 ppm
= 129.1 ppm

Comment

Step 12 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

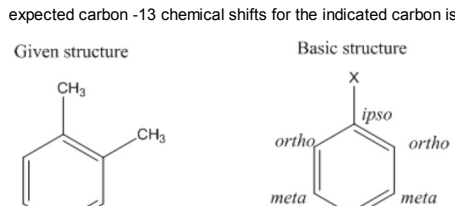


Basic value is 128.5 ppm
Substituent (CH₃) at ipso is 0.7 ppm
Substituent (CH₃) at meta is -0.1 ppm
Thus, indicated C value = 128.5 ppm + 0.7 ppm - 0.1 ppm
= 129.1 ppm

Comment

Step 13 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

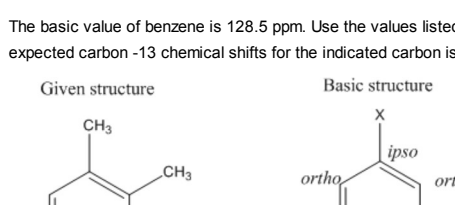


Basic value is 128.5 ppm
Substituent (CH₃) at meta is -0.1 ppm
Substituent (CH₃) at para is -2.9 ppm
Thus, indicated C value = 128.5 ppm - 0.1 ppm - 2.9 ppm
= 125.5 ppm

Comment

Step 14 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

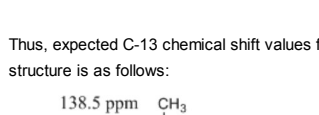


Basic value is 128.5 ppm
Substituent (CH₃) at meta is -0.1 ppm
Substituent (CH₃) at para is -2.9 ppm
Thus, indicated C value = 128.5 ppm - 0.1 ppm - 2.9 ppm
= 125.5 ppm

Comment

Step 15 of 78

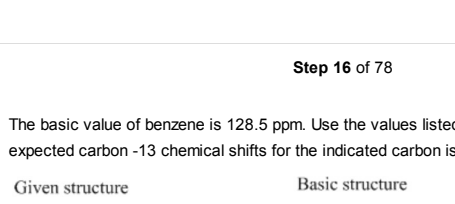
Thus, expected C-13 chemical shift values for the indicated carbon atoms are shown in the structure is as follows:



Comment

Step 16 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

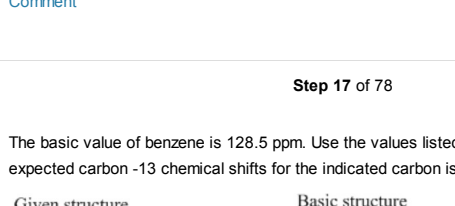


Basic value is 128.5 ppm
Substituent (CH₃) at ipso is 9.3 ppm
Substituent (CH₃) at meta is -0.1 ppm
Thus, indicated C value = 128.5 ppm + 9.3 ppm - 0.1 ppm
= 137.7 ppm

Comment

Step 17 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

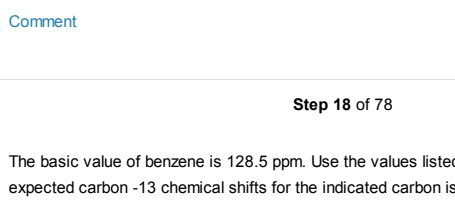


Basic value is 128.5 ppm
Substituent (CH₃) at ipso is 9.3 ppm
Substituent (CH₃) at meta is -0.1 ppm
Thus, indicated C value = 128.5 ppm + 9.3 ppm - 0.1 ppm
= 137.7 ppm

Comment

Step 18 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

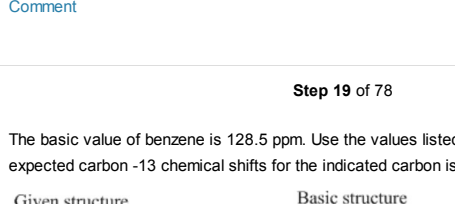


Basic value is 128.5 ppm
Two Substituents (CH₃) at ortho is 1.4 ppm (2 × 0.7 ppm)
Thus, indicated C value = 128.5 ppm + 1.4 ppm
= 129.9 ppm

Comment

Step 19 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:



Basic value is 128.5 ppm
Substituent (CH₃) at ortho is 0.7 ppm
Substituent (CH₃) at para is -2.9 ppm
Thus, indicated C value = 128.5 ppm + 0.7 ppm - 2.9 ppm
= 126.3 ppm

Comment

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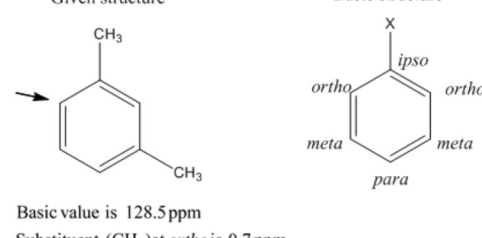
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Step 20 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

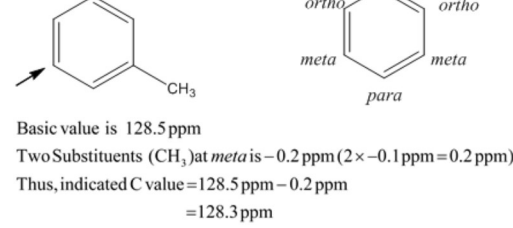


Basic value is 128.5 ppm
Substituent (CH₃) at *ortho* is 0.7 ppm
Substituent (CH₃) at *para* is -2.9 ppm
Thus, indicated C value = 128.5 ppm + 0.7 ppm - 2.9 ppm
= 126.3 ppm

[Comment](#)

Step 21 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

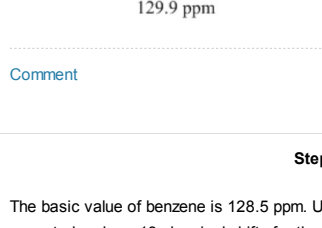


Basic value is 128.5 ppm
Two Substituents (CH₃) at *meta* is -0.2 ppm (2 × -0.1 ppm = 0.2 ppm)
Thus, indicated C value = 128.5 ppm + 0.2 ppm
= 128.3 ppm

[Comment](#)

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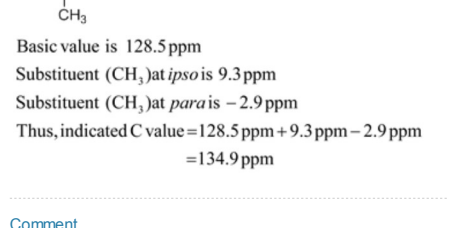
Thus, expected C-13 chemical shift values for the indicated carbon atoms are shown in the structure is as follows:



[Comment](#)

Step 23 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

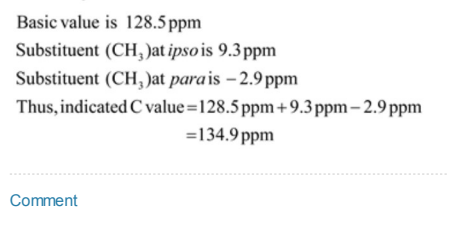


Basic value is 128.5 ppm
Substituent (CH₃) at *ipso* is 9.3 ppm
Substituent (CH₃) at *para* is -2.9 ppm
Thus, indicated C value = 128.5 ppm + 9.3 ppm - 2.9 ppm
= 134.9 ppm

[Comment](#)

Step 24 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

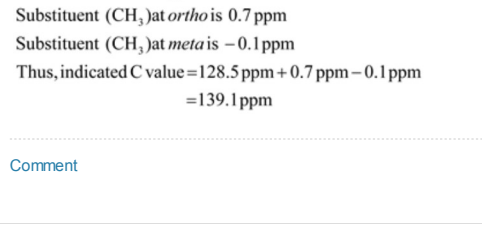


Basic value is 128.5 ppm
Substituent (CH₃) at *ipso* is 9.3 ppm
Substituent (CH₃) at *para* is -2.9 ppm
Thus, indicated C value = 128.5 ppm + 9.3 ppm - 2.9 ppm
= 134.9 ppm

[Comment](#)

Step 25 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

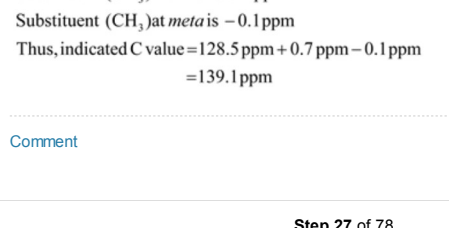


Basic value is 128.5 ppm
Substituent (CH₃) at *ortho* is 0.7 ppm
Substituent (CH₃) at *meta* is -0.1 ppm
Thus, indicated C value = 128.5 ppm + 0.7 ppm - 0.1 ppm
= 129.1 ppm

[Comment](#)

Step 26 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

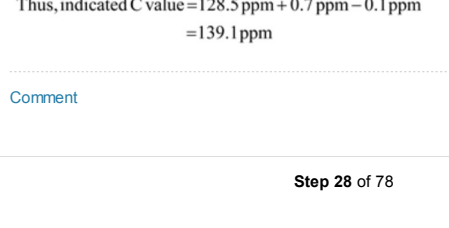


Basic value is 128.5 ppm
Substituent (CH₃) at *ortho* is 0.7 ppm
Substituent (CH₃) at *meta* is -0.1 ppm
Thus, indicated C value = 128.5 ppm + 0.7 ppm - 0.1 ppm
= 129.1 ppm

[Comment](#)

Step 27 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

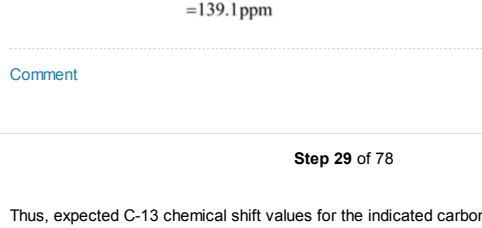


Basic value is 128.5 ppm
Substituent (CH₃) at *ortho* is 0.7 ppm
Substituent (CH₃) at *meta* is -0.1 ppm
Thus, indicated C value = 128.5 ppm + 0.7 ppm - 0.1 ppm
= 129.1 ppm

[Comment](#)

Step 28 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

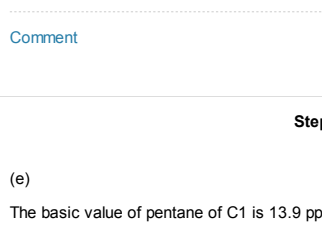


Basic value is 128.5 ppm
Substituent (CH₃) at *ortho* is 0.7 ppm
Substituent (CH₃) at *meta* is -0.1 ppm
Thus, indicated C value = 128.5 ppm + 0.7 ppm - 0.1 ppm
= 129.1 ppm

[Comment](#)

Step 29 of 78

Thus, expected C-13 chemical shift values for the indicated carbon atoms are shown in the structure is as follows:



[Comment](#)

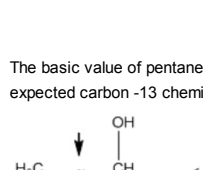
Step 30 of 78

[Comment](#)

Step 31 of 78

(e)

The basic value of pentane of C1 is 13.9 ppm. Use the values listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

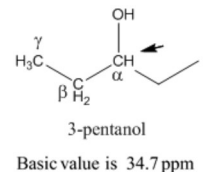


Basic value is 13.9 ppm
Substituent (OH) at α is -5 ppm
Thus, indicated C value = 13.9 ppm - 5 ppm
= 8.9 ppm

[Comment](#)

Step 32 of 78

The basic value of pentane of C2 is 22.8 ppm. Use the values listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

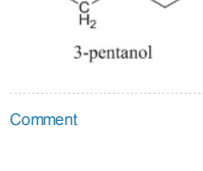


Basic value is 22.8 ppm
Substituent (OH) at β is 8 ppm
Thus, indicated C value = 22.8 ppm + 8 ppm
= 30.8 ppm

[Comment](#)

Step 33 of 78

The basic value of pentane of C3 is 34.7 ppm. Use the values listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

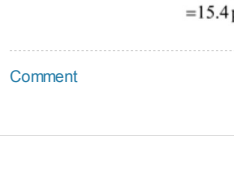


Basic value is 34.7 ppm
Substituent (OH) at α is 41 ppm
Thus, indicated C value = 34.7 ppm + 41 ppm
= 75.1 ppm

[Comment](#)

Step 34 of 78

Thus, expected C-13 chemical shift values for the indicated carbon atoms are shown in the structure is as follows:

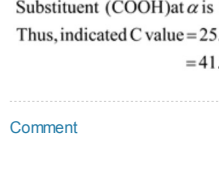


[Comment](#)

Step 35 of 78

(f)

The basic value of butane of C1 is 13.4 ppm. Use the values listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

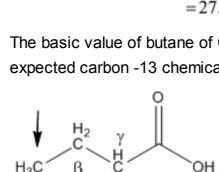


Basic value is 13.4 ppm
Substituent (COOH) at β is 2 ppm
Thus, indicated C value = 13.4 ppm + 2 ppm
= 15.4 ppm

[Comment](#)

Step 36 of 78

The basic value of butane of C2 is 25.2 ppm. Use the values listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

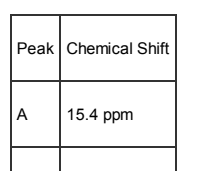


Basic value is 25.2 ppm
Substituent (COOH) at β is 2 ppm
Thus, indicated C value = 25.2 ppm + 2 ppm
= 27.2 ppm

[Comment](#)

Step 37 of 78

The basic value of butane of C3 is 25.2 ppm. Use the values listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:



Basic value is 25.2 ppm
Substituent (COOH) at β is 2 ppm
Thus, indicated C value = 25.2 ppm + 2 ppm
= 27.2 ppm

[Comment](#)

Step 38 of 78

Thus, expected C-13 chemical shift values for the indicated carbon atoms are shown in the structure is as follows:

Peak	Chemical Shift
A	15.4 ppm
B	41.2 ppm
C	27.2 ppm
D	11.4 ppm



[Comment](#)

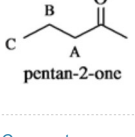
Step 39 of 78

(g)

The basic value of ethylene is 123.3 ppm. Use the values for alkene listed in the table 8.4 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

B 16.3+1 17.3

C 15.8-2 13.8

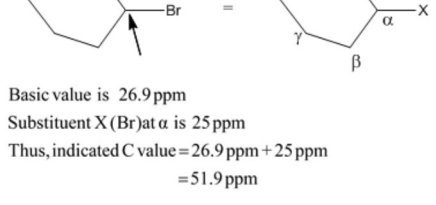


[Comment](#)

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(o)

The basic value of cyclohexane is 26.9 ppm. Use the values for cycloalkane listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

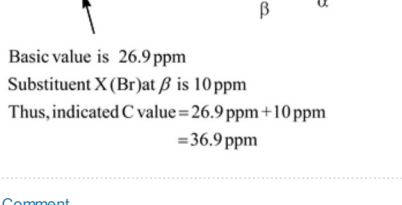


Basic value is 26.9 ppm
Substituent X (Br) at α is 25 ppm
Thus, indicated C value = 26.9 ppm + 25 ppm
= 51.9 ppm

[Comment](#)

Step 59 of 78

The basic value of cyclohexane is 26.9 ppm. Use the values for cycloalkane listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

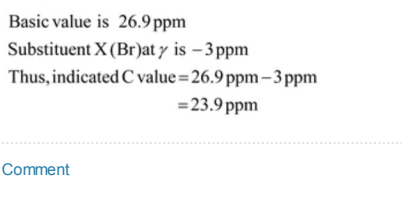


Basic value is 26.9 ppm
Substituent X (Br) at β is 10 ppm
Thus, indicated C value = 26.9 ppm + 10 ppm
= 36.9 ppm

[Comment](#)

Step 60 of 78

The basic value of cyclohexane is 26.9 ppm. Use the values for cycloalkane listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

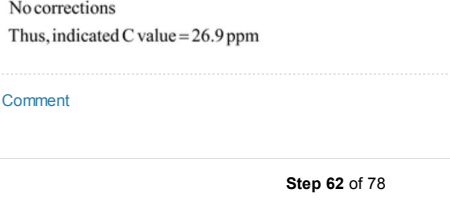


Basic value is 26.9 ppm
Substituent X (Br) at γ is -3 ppm
Thus, indicated C value = 26.9 ppm - 3 ppm
= 23.9 ppm

[Comment](#)

Step 61 of 78

The basic value of cyclohexane is 26.9 ppm. Use the values for cycloalkane listed in the table 8.3 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:



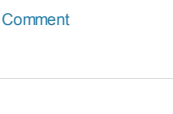
Basic value is 26.9 ppm
No corrections
Thus, indicated C value = 26.9 ppm

[Comment](#)

Step 62 of 78

Thus, expected C-13 chemical shift values for the indicated carbon atoms are shown in the structure is as follows:

Peak	Chemical Shift
A	51.9 ppm
B	36.9 ppm
C	23.9 ppm
D	26.9 ppm


bromocyclohexane

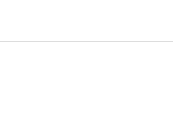
[Comment](#)

Step 63 of 78

(p)

Use the values listed in the table 8.3 for propane to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

Peak	Calculated Shift	
A	15.8+2	17.8
B	16.3+16	32.3

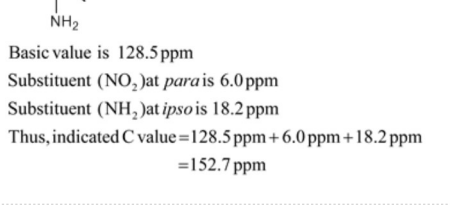

2-methylpropanoic acid

[Comment](#)

Step 64 of 78

(q)

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

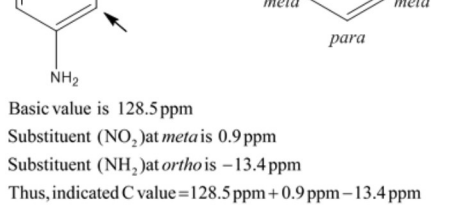


Basic value is 128.5 ppm
Substituent (NO₂) at *para* is 6.0 ppm
Substituent (NH₂) at *ipso* is 18.2 ppm
Thus, indicated C value = 128.5 ppm + 6.0 ppm + 18.2 ppm
= 152.7 ppm

[Comment](#)

Step 65 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

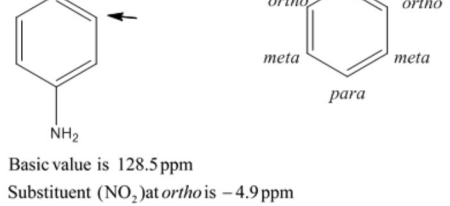


Basic value is 128.5 ppm
Substituent (NO₂) at *meta* is 0.9 ppm
Substituent (NH₂) at *ortho* is -13.4 ppm
Thus, indicated C value = 128.5 ppm + 0.9 ppm - 13.4 ppm
= 116 ppm

[Comment](#)

Step 66 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

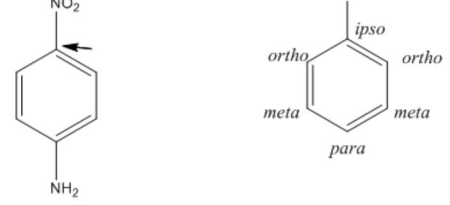


Basic value is 128.5 ppm
Substituent (NO₂) at *ortho* is -4.9 ppm
Substituent (NH₂) at *meta* is 0.8 ppm
Thus, indicated C value = 128.5 ppm - 4.9 ppm + 0.8 ppm
= 124.4 ppm

[Comment](#)

Step 67 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:



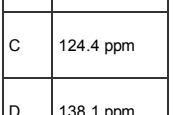
Basic value is 128.5 ppm
Substituent (NO₂) at *ipso* is 19.6 ppm
Substituent (NH₂) at *para* is -10.0 ppm
Thus, indicated C value = 128.5 ppm + 19.6 ppm - 10.0 ppm
= 138.1 ppm

[Comment](#)

Step 68 of 78

Thus, expected C-13 chemical shift values for the indicated carbon atoms are shown in the structure is as follows:

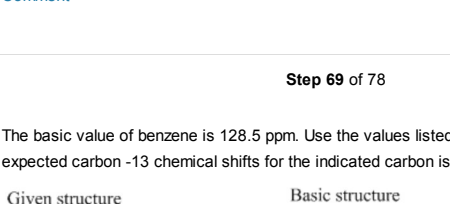
Peak	Chemical Shift
A	152.7 ppm
B	116 ppm
C	124.4 ppm
D	138.1 ppm


4-nitroaniline

[Comment](#)

Step 69 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

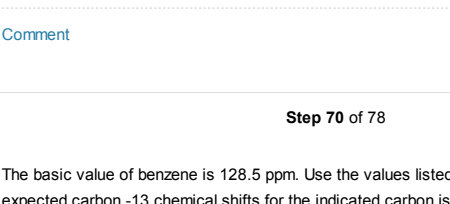


Basic value is 128.5 ppm
Substituent (NO₂) at *para* is 6.0 ppm
Substituent (NH₂) at *ortho* is 0.8 ppm
Thus, indicated C value = 128.5 ppm + 6.0 ppm + 0.8 ppm
= 135.3 ppm

[Comment](#)

Step 70 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

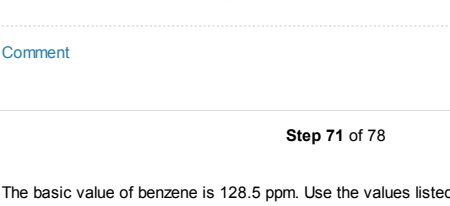


Basic value is 128.5 ppm
Substituent (NO₂) at *meta* is 0.9 ppm
Substituent (NH₂) at *ortho* is -13.4 ppm
Thus, indicated C value = 128.5 ppm + 0.9 ppm - 13.4 ppm
= 116 ppm

[Comment](#)

Step 71 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

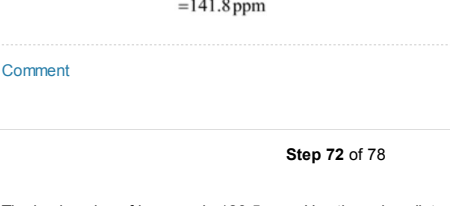


Basic value is 128.5 ppm
Substituent (NO₂) at *ortho* is -4.9 ppm
Substituent (NH₂) at *ipso* is 18.2 ppm
Thus, indicated C value = 128.5 ppm - 4.9 ppm + 18.2 ppm
= 141.8 ppm

[Comment](#)

Step 72 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

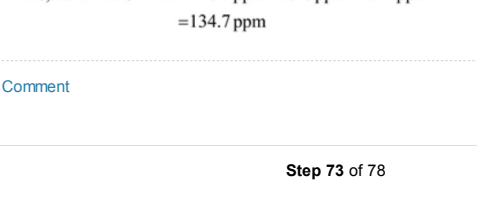


Basic value is 128.5 ppm
Substituent (NO₂) at *ortho* is 19.6 ppm
Substituent (NH₂) at *ortho* is -13.4 ppm
Thus, indicated C value = 128.5 ppm + 19.6 ppm - 13.4 ppm
= 134.7 ppm

[Comment](#)

Step 73 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

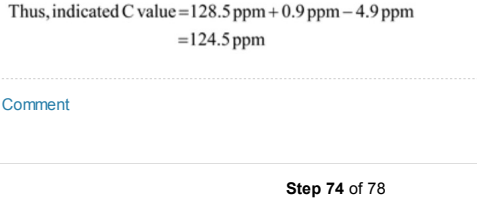


Basic value is 128.5 ppm
Substituent (NO₂) at *ortho* is -4.9 ppm
Substituent (NH₂) at *meta* is 0.9 ppm
Thus, indicated C value = 128.5 ppm + 0.9 ppm - 4.9 ppm
= 124.5 ppm

[Comment](#)

Step 74 of 78

The basic value of benzene is 128.5 ppm. Use the values listed in the table 8.7 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:



Basic value is 128.5 ppm
Substituent (NO₂) at *meta* is 0.9 ppm
Substituent (NH₂) at *para* is -10.0 ppm
Thus, indicated C value = 128.5 ppm + 0.9 ppm - 10.0 ppm
= 119.4 ppm

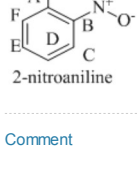
[Comment](#)

Step 75 of 78

Thus, expected C-13 chemical shift values for the indicated carbon atoms are shown in the structure is as follows:

Peak	Chemical Shift
A	141.8 ppm
B	134.7 ppm

D 119.4 ppm
E 135.3 ppm
F 116.0 ppm



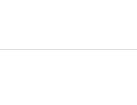
[Comment](#)

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(f)

Use the values listed in the table 8.4 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

Peak	Calculated Shift	
A	123.3+13.6-7.4	129.5
B	123.3+12.9-7	129.2



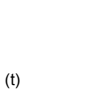
[Comment](#)

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(g)

Use the values listed in the table 8.4 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:

Peak	Calculated Shift	
A	123.3+(10.6+7.2-1.5)-(7.9+1.8-1.5)+(-1.1)	130.3



[Comment](#)

Step 78 of 78

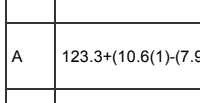
(t)

The basic value of ethylene is 123.3 ppm. Use the values for alkene listed in the table 8.5 to calculate expected carbon -13 chemical shifts for the indicated carbon is as follows:



$$\delta_{C_1} = 123.3 + [10.6\alpha + 7.2\beta - 1.5\gamma] - [7.9\alpha' + 1.8\beta' - 1.5\gamma'] + \Sigma(\text{steric corrections})$$

Given the following structure:



Thus, expected C-13 chemical shift values for the indicated carbon atoms are shown in the structure is as follows:

Peak	Calculated Shift	
A	123.3+(10.6(1)-(7.9(1)+1.8(2)))	122.4
B	123.3+(10.6(1)+7.2(2)-(7.9(1))+2.3	142.7

[Comment](#)

Was this solution helpful? ☐ 1 ☐ 0

Recommended solutions for you to review

