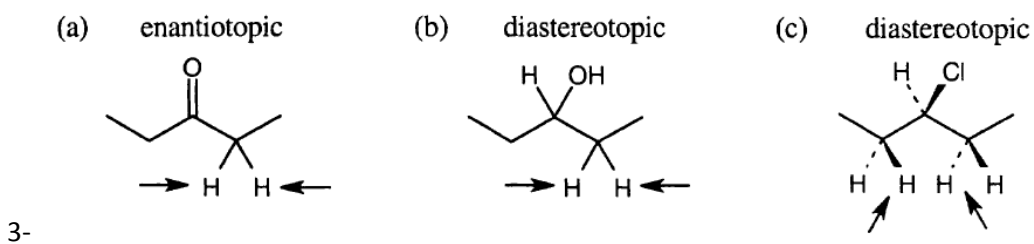
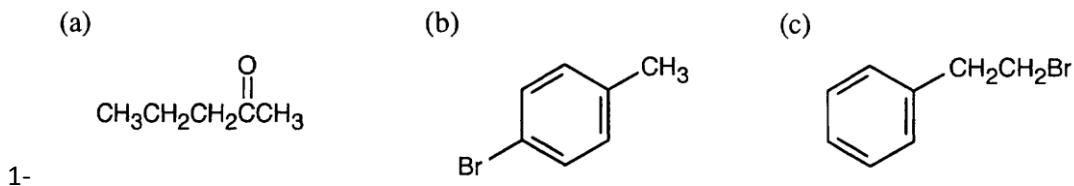
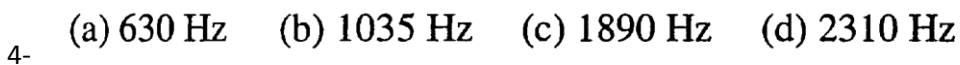


2017 Solution:



$$\delta \times 300 \text{ MHz} = \text{Observed chemical shift (in Hz)}$$



5-

(a) Since the symbol " δ " indicates ppm downfield from TMS, chloroform absorbs at 7.3 ppm.

(b)

$$\delta = \frac{\text{Observed chemical shift (in Hz)}}{\text{Spectrometer frequency in MHz}}$$

$$7.3 \text{ ppm} = \frac{\text{chemical shift}}{360 \text{ MHz}}; \quad 7.3 \text{ ppm} \times 360 \text{ MHz} = \text{chemical shift}$$

$$2600 \text{ Hz} = \text{chemical shift}$$

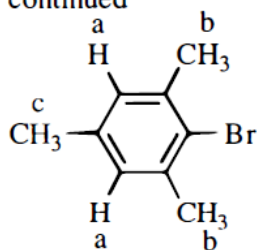
(c) The value of δ is still 7.3 because the chemical shift measured in δ is independent of the operating frequency of the spectrometer.

The formula $C_9H_{11}Br$ indicates four elements of unsaturation, just enough for a benzene ring.

Here is the most accurate method for determining the number of protons per signal from integration values *when the total number of protons is known*. Add the integration heights: $4.4 \text{ cm} + 13.0 \text{ cm} + 6.7 \text{ cm} = 24.1 \text{ cm}$. Divide by the total number of hydrogens: $24.1 \text{ cm} \div 11H = 2.2 \text{ cm/H}$. Each 2.2 cm of integration height = 1H, so the ratio of hydrogens is 2 : 6 : 3.

The 2H singlet at δ 7.1 means that only two hydrogens remain on the benzene ring, that is, it has 4 substituents. The 6H singlet at δ 2.3 must be two CH_3 's on the benzene ring in identical environments. The 3H singlet at δ 2.2 is another CH_3 in a slightly different environment from the first two. Substitution of the three CH_3 's and the Br in the most symmetric way leads to the structures on the next page.

continued



a = δ 7.1 (singlet, 2H)
 b = δ 2.3 (singlet, 6H)
 c = δ 2.2 (singlet, 3H)

a second structure is also possible although it is less likely because the Br would probably deshield the Hs labeled "a" to about 7.3-7.4

