

## Z17 SOLUTION

### IR

Signal (cm <sup>-1</sup> )	Interpretation
~ 3000	CH <sub>st</sub>
1800-2000 (weak)	Aromatic overtones?
1700 (strong)	C=O
1600, 1580	C=C of aromatic ring

Summary:

Hints of carbonyl and aromatic;

No indication of -OH or -NH or X≡Y; X=Y=Z

## MS

### Hypothesis 1

m/z	$\Delta m/z$	Interpretation
163		$M^+??$ ; If yes, N contained; no signs of Cl, Br, S
147	-16	Base peak; $^{13}C \sim 11\% \Rightarrow \sim 10C$ loss of $CH_4$ ; O; $NH_2$
119	-28	loss of CO; $C_2H_4$ ; $N_2$
51;77;91		Suggestive of aromatic ring

### Hypothesis 2

m/z	$\Delta m/z$	Interpretation
162		$M^+??$ ; If yes, even-numbered N; no signs of Cl, Br, S
147	-15	Base peak; $^{13}C \sim 11\% \Rightarrow \sim 10C$ loss of $CH_3$ ;
119	-28	loss of CO; $C_2H_4$ ; $N_2$
51;77;91		Suggestive of aromatic ring

### <sup>13</sup>C-NMR

$\delta$ (ppm)	DEPT	Interpretation
192	CH	C=O
158.5	C	Aromatic region: 4-different carbons (2x quaternary and 2xCH)
134	C	
129.7	CH	
126	CH	
35.4	C	
31.1	CH <sub>3</sub>	CH <sub>3</sub>

$$\Sigma_C \geq 7; \Sigma_H \geq 6$$

### <sup>1</sup>H-NMR

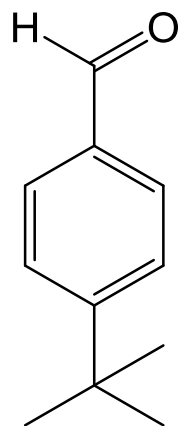
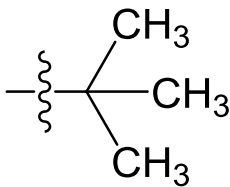
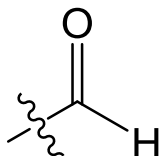
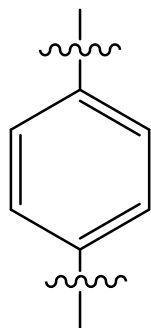
$\delta$ (ppm)	integral	Signal	Interpretation
9.97	1	S	CHO
7.82	2	high order	Aromatic (para-disubstituted ring; AA'BB')
7.55	2	high order	
1.35	9	s	3x CH <sub>3</sub> (isolated; no coupling)

$$\Sigma_H = 14 \text{ (4 aromatic + 3xCH}_3 \text{ + CHO)}$$

=> 2 x CH from <sup>13</sup>C-NMR @ 126-130 ppm & 3 x CH<sub>3</sub> from <sup>13</sup>C-NMR @ 31.1 ppm

- ⇒ Chemical Formula: C<sub>11</sub>H<sub>14</sub>O
- ⇒ Molecular Weight: 162
- ⇒ DBE= 5 (4 from aromatic ring + 1 aldehyde)

## Fragments



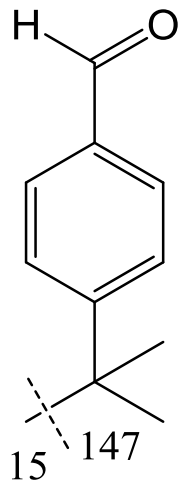
4-(*tert*-butyl)benzaldehyde  
Chemical Formula:  $C_{11}H_{14}O$   
Molecular Weight: 162.23

## Confirmation

### IR

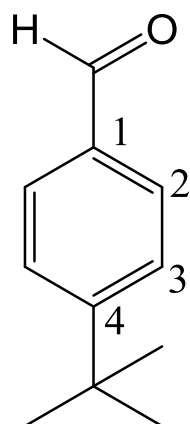
Signal (cm <sup>-1</sup> )	Interpretation
~ 3000	CH <sub>st</sub>
1800-2000 (weak)	Aromatic overtones
1700 (strong)	C=O (aromatic )
1600, 1580	C=C of aromatic ring

### MS



m/z 163 Contamination of carboxylic acid -CH<sub>3</sub>?

### <sup>13</sup>C-NMR



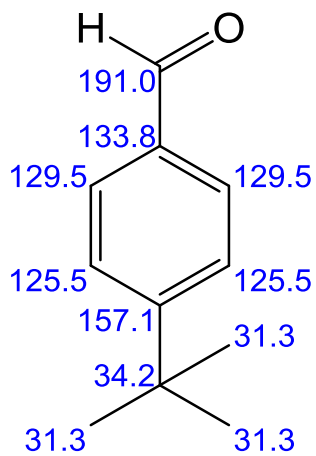
$$\delta_1 = 128.5 + 8.2 - 3.1 = 133.6 \text{ (exp. } \sim 134)$$

$$\delta_2 = 128.5 + 1.2 - 0.4 = 129.3 \text{ (exp. } \sim 130)$$

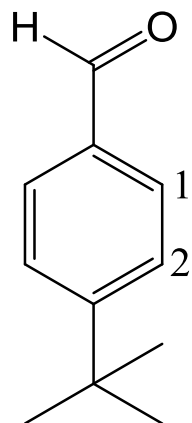
$$\delta_3 = 128.5 + 0.5 - 3.3 = 125.7 \text{ (exp. } \sim 126)$$

$$\delta_4 = 128.5 + 5.8 + 18.6 = 152.9 \text{ (exp. } \sim 158)$$

### ChemNMR <sup>13</sup>C Estimation



## <sup>1</sup>H-NMR



$$\delta_1 = 7.34 - 0.04 + 0.54 = 7.84 \text{ (exp. } \sim 7.82)$$

$$\delta_2 = 7.34 + 0.05 + 0.19 = 7.58 \text{ (exp. } \sim 7.55)$$

## ChemNMR <sup>1</sup>H Estimation

