Name: _____ Set: _____

NMR Spectroscopy

1 **(a)** An aromatic compound **D**, of M_r 122, is a possible sex attractant for insects. It has the following composition by mass: C, 78.7%; H, 8.2%; O, 13.1%.

What is the molecular formula of **D**? Calculate and choose the correct answer from the option given below.

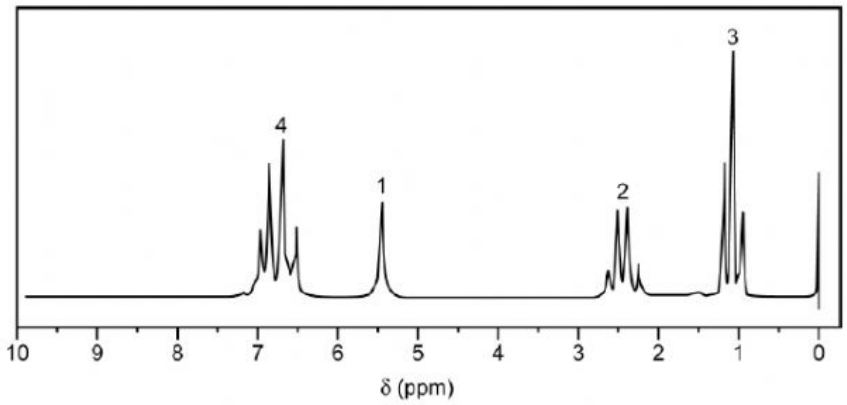
A. $C_8H_{10}O$

B. $C_{10}H_8O$

C. $C_6H_{10}O$

D. $C_{10}H_6O$

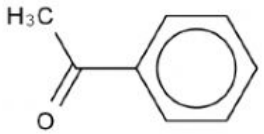
(b) The NMR spectrum of **D** is shown below.

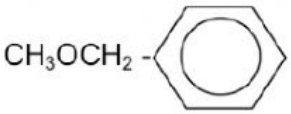


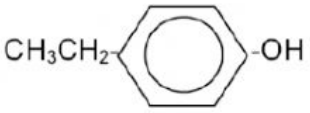
Use the spectrum and explanation below to deduce the structure for D. Choose the correct answer from the option given below.

Triplet at δ1 is due to CH_3 next to a CH_2.
Quartet at δ2.5 is due to CH_2 next to a CH_3.
Peak at δ6.8 is due to 4 aryl hydrogen.
Singlet at δ5.5 is due to OH group of phenol.

The structure of D is _____.







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(c) Explain what effect you would expect the addition of a small amount of D_2O to have on the NMR spectrum of **D**.

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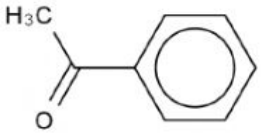
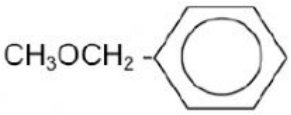
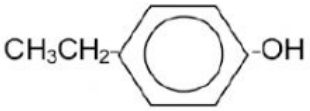
(d) An isomer of **D** shows no effect on the NMR spectrum on adding D_2O.

Choose the structure of the isomer from the list given and suggest how its NMR spectrum would differ from that of D.







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2 The NMR spectrum of cysteine, $H_2NCH(CH_2SH)CO_2H$, shows five absorptions.

After shaking a solution of cysteine with a few drops of D_2O, the NMR spectrum shows **only two** absorptions, **E** and **F**, shown below.

E **F**

(i) Identify the **two** types of protons responsible for the absorptions **E** and **F**.

E .....

F .....

(ii) State and explain the splitting patterns of the absorptions **E** and **F**.

E .....

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F .....

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