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## CHEMISTRY INORGANIC CHEMISTRY II

Level & Board	AQA (A-LEVEL)
TOPIC:	NMR SPECTROSCOPY
PAPER TYPE:	QUESTION PAPER - 4
TOTAL QUESTIONS	10
TOTAL MARKS	36

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## NMR Spectroscopy - 4

**1.** There are several isomers with the molecular formula  $C_6H_{16}N_2$ 

One isomer is shown.

 $H_{3}C - CH_{2}$  $H_{3}C - CH_{2}$  N  $- CH_{2}$   $- CH_{2} - NH_{2}$ 

(a) Give the number of peaks in the <sup>13</sup>C NMR spectrum of this isomer.

State and explain the splitting pattern of the peak for the hydrogens labelled a in its <sup>1</sup>H NMR spectrum.

(b)Draw the structure of the isomer of C<sub>6</sub>H<sub>16</sub>N<sub>2</sub> that contains two primary amine groups and has only two peaks in its <sup>13</sup>C NMR spectrum.

(c)Draw the structure of the isomer of C<sub>6</sub>H<sub>16</sub>N<sub>2</sub> that contains two tertiary amine groups and has only two peaks in its <sup>13</sup>C NMR spectrum.

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(1)

**2.** Figure shows the <sup>1</sup>H NMR spectrum of Q,  $C_3H_7CIO$ 



The table below shows the chemical shifts ( $\delta$  values) and integration values for each peak.

δ value / ppm	3.95	3.65	3.35
Integration value	0.6	0.6	0.9

Deduce the structure of Q.

Explain your answer.

(5)

- **3.** Two isomers of CH<sub>3</sub>CHClCOCH(CH<sub>3</sub>)<sub>2</sub> each have two singlet peaks only in their <sup>1</sup>H NMR spectra.
- Deduce the structures of these two isomers.

**4.** Deduce the splitting pattern for each of the peaks given by the H atoms labelled x, y and z in the <sup>1</sup>H NMR spectrum of the compound shown.

у x CH<sub>3</sub>CHClCOCH(CH<sub>3</sub>)<sub>2</sub>

(3)

5. The structural formula of the compound propenal is shown below



Explain why propenal has three peaks in its low-resolution n.m.r. spectrum.

Suggest the relative areas under the peaks.

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6. When the molecular formula of a compound is known, spectroscopic and other analytical techniques can be used to distinguish between possible structural isomers.

Draw one possible structure for each of the compounds.

(a)K and L are cyclic compounds with the molecular formula  $C_6H_{10}O$ .

Both have four peaks in their <sup>13</sup>C n.m.r. spectra. K is a ketone and L is an aldehyde.

(b)Compounds M and N have the molecular formula  $C_6H_{15}N$ .

M is a tertiary amine with only two peaks in its 1H n.m.r. spectrum. N is a secondary amine with only three peaks in its 1H n.m.r. spectrum.

(2)

**7.** N.m.r. spectroscopy can be used to study the structures of organic compounds.

Compound K was studied using <sup>13</sup>C n.m.r. spectroscopy.

$$CH_3 - CH_2 - CH_2 - CH_2 - CH_3 = 0$$

(a) Give the number of peaks in the <sup>13</sup>C n.m.r. spectrum of K.

(b)Suggest a  $\delta$  value of the peak for the carbon labelled b.

(c) Give the IUPAC name of K.

(1)

(1)

(1)

**8.** The structure of N-phenylethanamide is Use this structure to determine the number of peaks in the <sup>13</sup>C n.m.r. spectrum of N-phenylethanamide.



(1)

**9.** The structure of compound G is shown below.



Sketch the <sup>1</sup> H n.m.r. spectrum of compound G and label the relative peak areas.

Label any peaks that would be lost from the spectrum on shaking with  $D_2O$ .



(4)

**10.** This question is about NMR spectroscopy.

A compound is usually mixed with  $Si(CH_3)_4$  and either  $CCI_4$  or  $CDCI_3$  before recording the compound's 1H NMR spectrum.

State why Si(CH<sub>3</sub>)<sub>4</sub>, CCl<sub>4</sub> and CDCl<sub>3</sub> are used in <sup>1</sup>H NMR spectroscopy.

Explain how their properties make them suitable for use in <sup>1</sup>H NMR spectroscopy.



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