CHEM202 REPORT

STRUCTURAL PROBLEMS A & B

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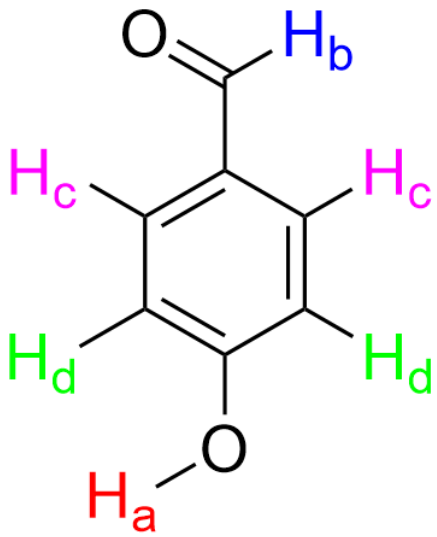
Unknown ID Numbers: **25A, 33B** **Date:** 20-03-25

Structural Elucidation of Unknown 25A

Abstract

ADD AN ABSTRACT HERE.



Derivation of the structure

Microanalysis shows the following percentage composition by mass:

C: 71.98 %; H: 6.71 %; O: 21.31 %

The empirical formula of the product can be calculated as follows:

$$\text{Moles of Carbon} = \frac{71.98\ g}{12\ g/mol} = 5.998\ mol$$

$$\text{Moles of Hydrogen} = \frac{6.71\ g}{1\ g/mol} = 6.71\ mol$$

$$\text{Moles of Oxygen} = \frac{21.31\ g}{16\ g/mol} = 1.332\ mol$$

$$\text{C ratio} = \frac{5.998\ mol}{1.332\ mol} \approx 4.5 \qquad \text{H ratio} = \frac{6.71\ mol}{1.332\ mol} \approx 5 \qquad \text{O Ratio} = \frac{1.332\ mol}{1.332\ mol} = 1$$

$$\text{Number of atoms C: } 4.5 \times 2 = 9;\ \text{H: } 5 \times 2 = 10;\ \text{O: } 1 \times 2 = 2$$

M_r = 150 g

IR spectrum of unknown.

v / cm^{-1}	**intensity**	**appearance**	**assignment**	**inference**
2965	m	sh	C-H stretch	Alkyl CH
1669	s	sh	C=O stretch	Ketone conjugated with aromatic ring
1606	s	sh	C=C stretch	Aromatic skeletal stretch
1360	s	sh	C-H bend	Methyl C-H bending
~1300-1050	s	sh	C-O stretch	Ether C-O stretch
834	s	sh	C-H deformation	1,4-distubstituted benzene derivative

^{1}H NMR (frequency, solvent)

d/ppm	**Relative # of hydrogens**	**multiplicity**	**coupling constant(s)/Hz**	**assignment**
7.9	1	d	9	H_c
6.9	1	d	9	H_d
3.87	1.69	s	~	H_a
2.56	1.61	s	~	H_b

Discussion of structure solving

To find the structure of the unknown molecules various spectroscopic and elemental data was analysed. Looking at the elemental microanalysis data, it revealed an empirical formula of $C_9H_{10}O_2$ and a molecular weight of 150 g/mol. Spectroscopic data from IR and ^{1}H NMR provided further information on the functional group present and structure of their arrangement.

Looking at the IR data showed several prominent absorption bands. A strong and sharp peak can be observed at 1669 cm^{-1} suggesting the presence of a conjugated carbonyl (C=O) which is a characteristic of a aromatic ketone. Further down the absorption band a strong, sharp peak at 1606 cm^{-1} is typical of C=C stretching in aromatic rings, consistent with our other observations. Looking at the 1300-1050 cm^{-1} region strong, sharp absorption bands provide evidence for C-O single bond,

suggesting the presence of ether function group, additionally the presence of a distinct absorption at 830 cm^{-1} indicates the 1,4-disubstituted derivative of the aromatic ring.

The ^{1}H NMR data further supports the observation made from the IR spectra. The aromatic region presented itself as 2 doublets at chemical shifts of 7.9 ppm and 6.9 ppm. The splitting pattern of 2 doublets provides additionally evidence of a para-disubstituted benzene ring structure. The peaks 3.87 ppm and 2.56 ppm indicate the presence of a methoxy substituent ($-OCH_3$) and an acetyl substituent ($-COCH_3$)

Appendix 1

Unknown ID No.: 33B