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Welcome to

WebSpectra - This site was established to provide chemistry students with a library of spectroscopy problems.

Interpretation of spectra is a technique that requires practice - this site provides 1

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¹H NMR and ¹³C NMR, DEPT, COSY and IR spectra of various compounds for students to interpret. Hopefully, these problems will provide a useful resource to better understand spectroscopy.

H Nmr
Spectroscopy

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Model 3: ^{13}C NMR
Spectroscopy –
Number of Signals

1. The molecule on the left has 5 types of C atom and the molecule on the right has 7 types of C atom *. 2. The molecule on the left will give 5 signals and the molecule on

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the right will give 7
signals. 3. See
below. CH₃ CH₂ B
r a b CH₃ CH₃ CH
3 O CH₃ CH₃ CH₂
CH₃ CH₂ C CH₃
CH₃

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The infra-red
spectra of H, I and J

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are given below, but it does indicate which is - which. Identify the three compounds H, I and J, using the infra-red spectra below, and decide which spectrum belongs to which compound.

(iii) Compound E, which is a branched chain haloalkane, was found to have

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the composition by
mass of 39.8% C,
7.3% H, 2)

Chemsheets AS
029

(Thermodynamics
) ANS 2

Example 2 25.0
cm³ of 1.00 mol
dm⁻³ hydrochloric
acid was added to
25.0 cm³ of 1.00
mol dm⁻³ sodium

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hydroxide solution.

The temperature
rose by 6.7 C.

Calculate the
enthalpy of
neutralisation for
this reaction.

Assume that the
density of the
solution is 1.00 g
cm⁻³, the specific
heat capacity of the
solution is 4.18 J
g⁻¹ K⁻¹.

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moles CH_3COCH_3

$= \text{mass} / M_r =$

$0.55 / 58.0 =$

$0.00948 \quad H = q /$

$\text{moles} = -15.82 /$

$0.00948 = -1669$

kJ mol^{-1} 8) $q = mc$

$T = 50 \times 4.18 \times$

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$$(33.9 - 20.2) =$$
$$2863 \text{ J} = 2.863 \text{ kJ}$$

moles KOH = conc
x vol (dm³) = 2.0
x 25/1000 =

$$0.0500 \text{ moles HNO}$$
$$3 = \text{conc} \times \text{vol (dm}$$
$$3) = 2.0 \times 25/1000$$
$$= 0.0500$$

IR TASK 1 -

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(Spectroscopy) -
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students in the age
range 11-18. All
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with model answers

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and have been tried
and tested with
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0 ...

8 25 cm³ of 2.0
mol dm⁻³ nitric acid
was reacted with 25
cm³ of 2.0 mol
dm⁻³ potassium
hydroxide in an
insulated cup. The
temperature rose
from 20.2 °C to
33.9 °C. Calculate

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H for the reaction
given the specific
heat capacity of
water is $4.18 \text{ J mol}^{-1} \text{ K}^{-1}$.

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A20
3017Jul12 Light is
one form of
electromagnetic
radiation. Light is
only a very small

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3 90-150 (CH₂),
90-150 (C₅ H₄ H₃
2) propene 3)
90-150 (CH₂), 90
-150 (C₅ H₄ H₃
2-chloropropane),
2 5-40 (CH₃ 10-70
(CHCl) propanone
, 2 20-50 (CH₃
190-220 (CO)
methylamine 1
25-60 (CH₃) ethyl
propanoate 3 5 2
5-40 (CH₂ CH₂

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CO), 20-50 (CH
CO), 160-185 (CO),
50-90 (OCH 2),
5-40 (OCH 2 CH 3)

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TASK 1 – Bronsted-
Lowry acids &
bases

Infrared (IR)
Spectroscopy -
Three Steps for
Solving IR ...

We also
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relative intensity =
0.3 : 0.15 : 0.3 : 0.6
= 2 : 1 : 2 : 6

TASK 2 – Finding
the relative
intensity of signals
from a spectrum

For each of the
NMR spectra below,

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calculate the
relative number of
H atoms associated
with each signal. 8
7 6 5 4 3 2 1 0
chemical shift δ

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1070 Page 1 TASK

2 – Finding the
relative intensity of
signals from a

spectrum Spectrum

A: Spectrum nmr-b
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(Acids & bases)

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1070 Page 3 TASK
1 – Predicting ^1H
NMR spectra

Compound

Structure Number

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of signals
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Organic
Nomenclature 3
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- The frequencies at which they vibrate are in the infra-red region of the electromagnetic spectrum.
- If infra-red light is passed through the

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compound, it will absorb some or all of the light at the frequencies at which its bonds vibrate.

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