Introduction to IR Spectroscopy

A Level

IR (infra-red) spectroscopy is a useful tool both for detecting previously studied substances in a sample, and for identifying the presence of functional groups in a compound.

Part A Compound detection

When detecting the presence of a particular compound, we compare the details of absorptions falling in the region below $1500\,\mathrm{cm}^{-1}$ to reference spectra. This part of the spectrum often contains a great number of absorptions corresponding to different vibrational modes of the molecule, and is called the ...

Part B Bond identification

Another way of using IR spectroscopy is to identify the presence of particular functional groups. While the absorptions seen correspond to vibrational modes of the whole molecule, we often instead think of the vibrations as occurring in isolated parts of the molecule. Absorptions that occur at wavenumbers above $1500\,\mathrm{cm}^{-1}$ can allow us to identify characteristic functional groups, as there is much less overlap between absorptions in this region of the spectrum, and it is only stretching modes that appear here. The stretching frequency of a bond depends both on the mass of the atoms and the strength of the bond in question.

We see absorptions due to the stretches of [ ] bonds to hydrogen above or around $3000\,\mathrm{cm}^{-1}$. This is because hydrogen is a very [ ] element, and the stretching frequency of its bonds is therefore much higher than that of other [ ] bonds, which usually appear below $1500\,\mathrm{cm}^{-1}$. We see [ ] bonds typical in organic chemistry (e.g. in alkenes or carbonyls) correspond to stretching frequencies between $1500\,\mathrm{cm}^{-1}$ and $2000\,\mathrm{cm}^{-1}$, while the even [ ] [ ] bonds typically have stretching frequencies between $2000\,\mathrm{cm}^{-1}$ and $2500\,\mathrm{cm}^{-1}$.

Items:

triple **stronger** **light** **single** **heavy** **weaker** **double** **hydrogen**

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IR Isomers

A Level

The two spectra **P** and **Q** below were obtained from compounds with the formula $C_4H_{10}O$.

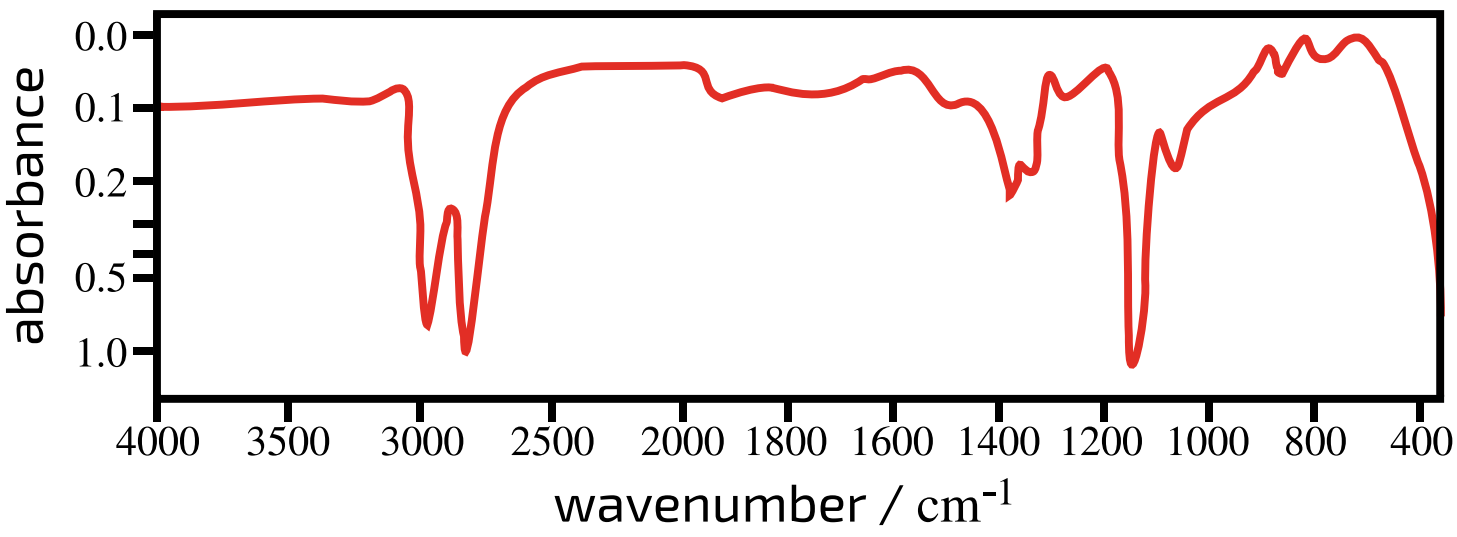

Figure 1: Infrared spectrum **P**

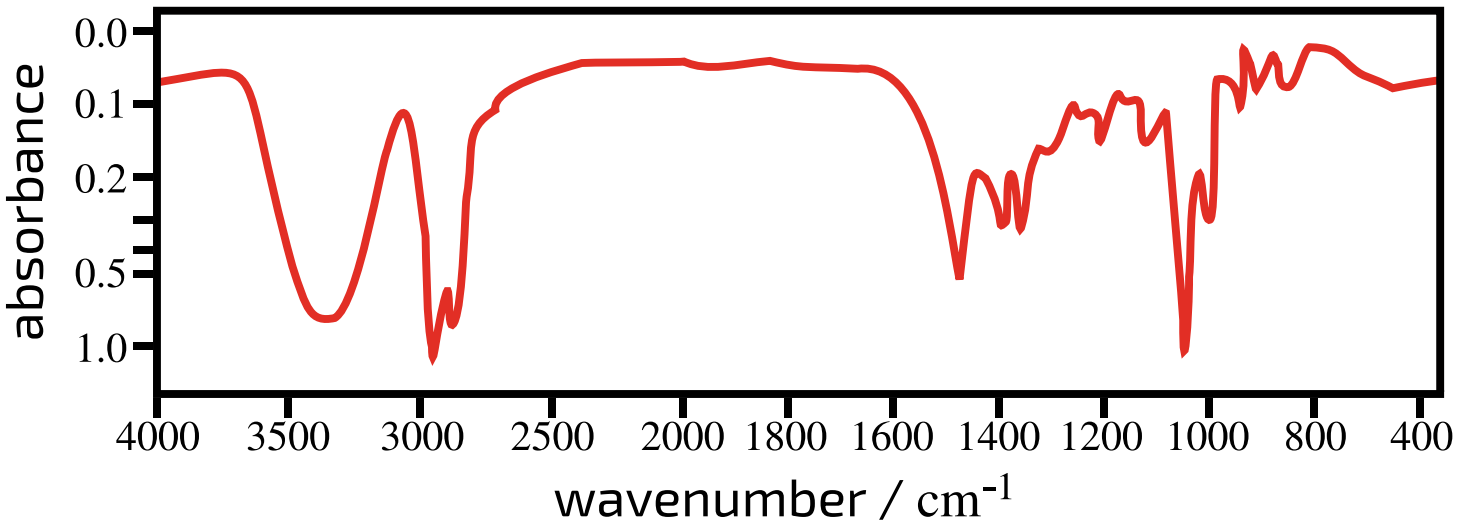

Figure 2: Infrared spectrum **Q**

Part A Molecular formula

Which of the following statement(s) is/are true for a compound with molecular formula $\mathrm{C_4H_{10}O}$?

- [ ] It cannot contain a double bond.
- [ ] It cannot contain a ring.
- [ ] It has to contain a double bond.
- [ ] It has to contain a ring.
- [ ] It has to contain either a double bond or a ring.
- [ ] It may contain a carbonyl group ($\mathrm{C{=}O}$).
- [ ] It may contain an alcohol group (OH).

Part B Spectrum P

Based on absorptions seen outside of the fingerprint region, suggest a possible structure with molecular formula $\mathrm{C_4H_{10}O}$ that would give spectrum **P**.

Enter your answer as a SMILES string.

Use the structure editor to draw the structural formula of the molecule. Click on the round, yellow smiley face to generate a SMILES string. Copy the SMILES string and paste it in the answer box. For more detailed help, visit our instructions for using the structure editor.

Part C Spectrum Q

Based on absorptions seen outside of the fingerprint region, suggest a possible structure with molecular formula $\mathrm{C_4H_{10}O}$ that would give spectrum **Q**.

Enter your answer as a SMILES string.

Use the structure editor to draw the structural formula of the molecule. Click on the round, yellow smiley face to generate a SMILES string. Copy the SMILES string and paste it in the answer box. For more detailed help, visit our instructions for using the structure editor.

Adapted with permission from UCLES, A Level Chemistry, June 1991, Paper 1, Question 1

Gameboard:

STEM SMART Chemistry Week 49

IR Oxidation

A Level

The following three infrared spectra were obtained at different stages of an oxidation reaction of an organic compound.

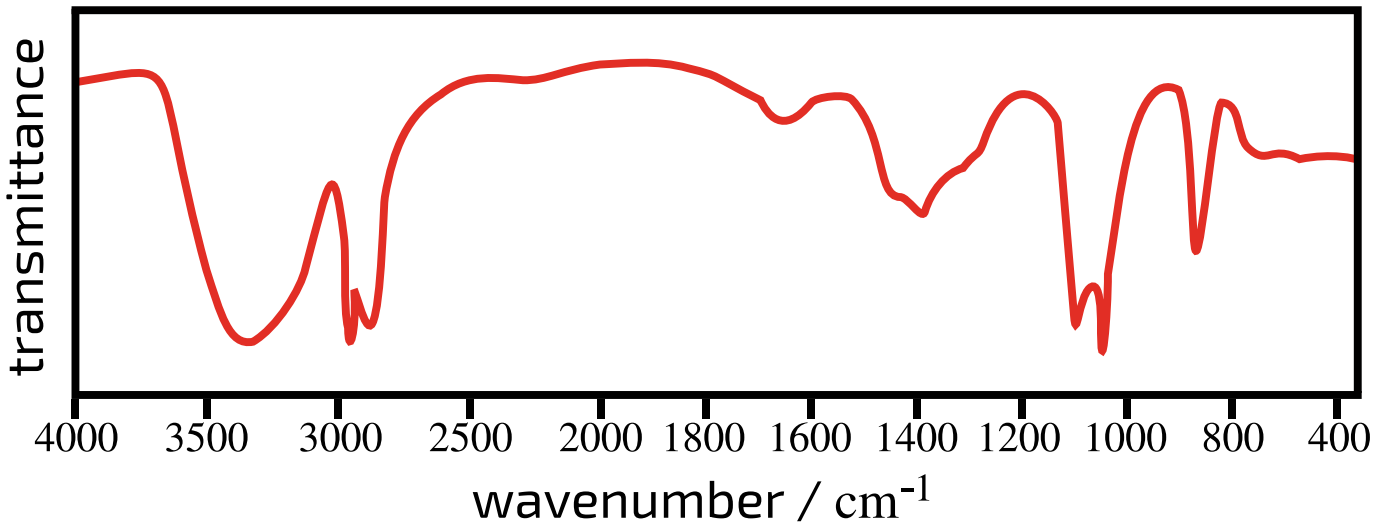

Figure 1: Spectrum for compound P

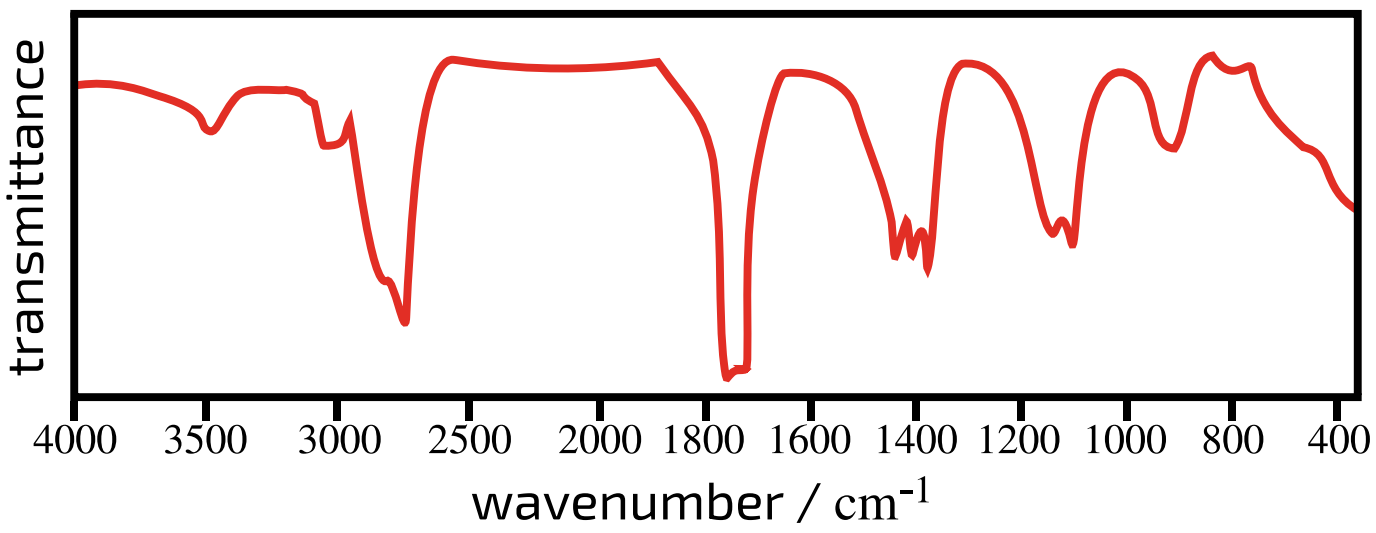

Figure 2: Spectrum for compound Q

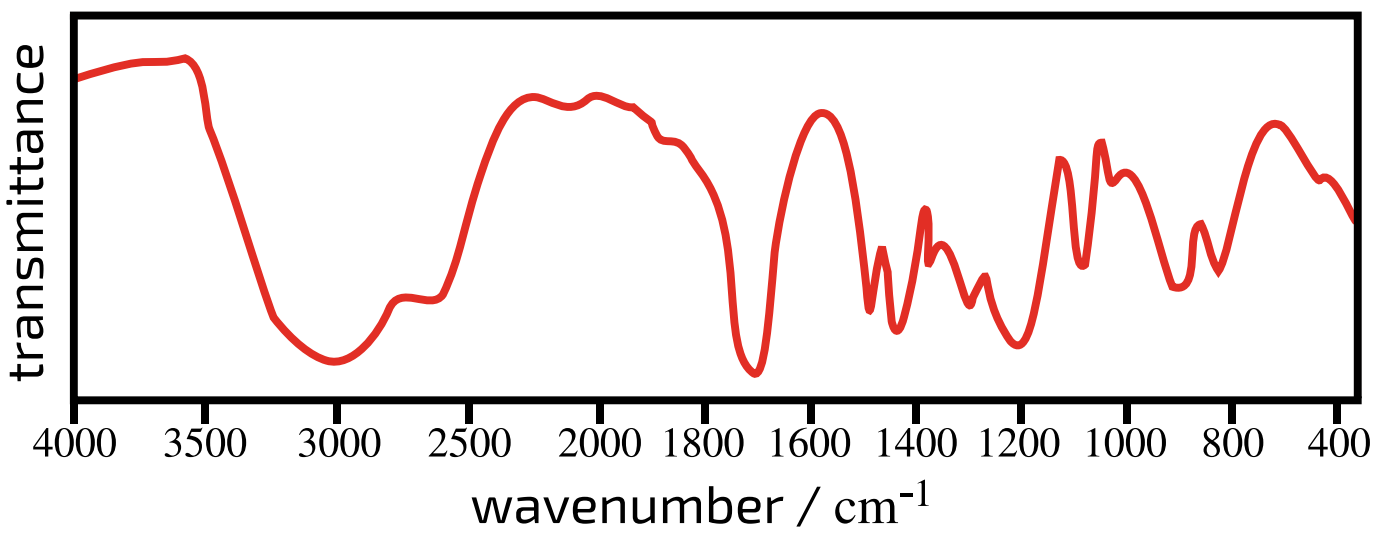

Figure 3: Spectrum for compound R

Part A Functional group in P

What is the functional group in P that gets oxidised over the course of the reaction?

Part B Spectrum of P

In which parts of the spectrum can we see characteristic absorptions based on the presence of the functional group from the previous part?

- [ ] $1600\ \mathrm{cm^{-1}}$ to $1800\ \mathrm{cm^{-1}}$
- [ ] $1800\ \mathrm{cm^{-1}}$ to $2000\ \mathrm{cm^{-1}}$
- [ ] $2000\ \mathrm{cm^{-1}}$ to $2500\ \mathrm{cm^{-1}}$
- [ ] $2500\ \mathrm{cm^{-1}}$ to $3000\ \mathrm{cm^{-1}}$
- [ ] $3000\ \mathrm{cm^{-1}}$ to $3500\ \mathrm{cm^{-1}}$

Part C Bond in Q

What characteristic bond appears during the oxidation, with a characteristic absorption in the spectra of Q and R?

A [ ] bond between [ ] and [ ] with a stretching frequency that falls in the [ ] $\mathrm{cm^{-1}}$ region.

Items:

single **double** **triple** **hydrogen** **carbon** **nitrogen** **oxygen** 1600-1800 1800-2000 2000-2500 2500-3000

Part D Functional group in R

What is the functional group formed in the oxidation and present in compound R?

Part E Spectrum of R

In which parts of the spectrum can we see characteristic absorptions based on the presence of the functional group from the previous part?

Around [ ], we see a broad absorption due to the vibration of a [ ] bond between [ ] and [ ]. The broadening is a result of [ ] bonding. Around [ ], we see a sharper absorption due to the vibration of a [ ] bond between [ ] and [ ].

Items:

$3000\ \mathrm{cm^{-1}}$	$1800\ \mathrm{cm^{-1}}$	**single**	**double**	**triple**	**hydrogen**	**carbon**	**nitrogen**	**oxygen**

Adapted with permission from UCLES, A Level Modular Sciences, March 1996, Methods of Analysis and Detection, Question 1

Gameboard:

STEM SMART Chemistry Week 49

Isomers of $C_2H_4O_2$

A Level

C C C

The isomers of $C_2H_4O_2$ can contain different functional groups. Draw the structures of **all** the isomers of $C_2H_4O_2$ which contain the following functional groups.

Use the structure editor to generate SMILES strings.

Enter their structures as SMILES strings in the format "**A**, **B**, ... etc." (space after commas).

Part A Carbonyl group

Part B Alkene group

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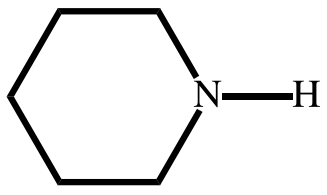
Black Pepper

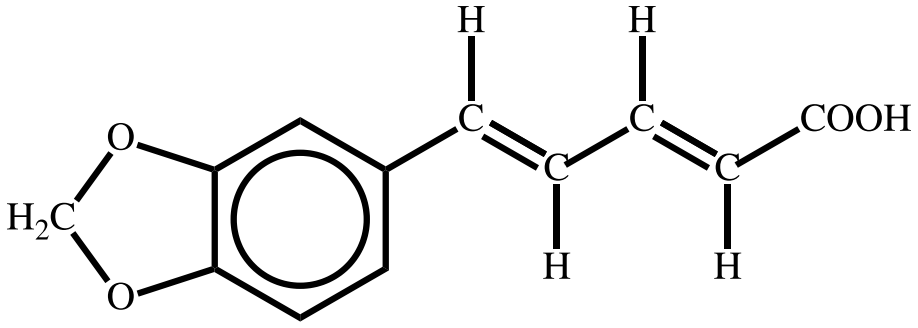
A Level

One of the constituents of black pepper is the neutral compound **N** with molecular formula $\mathrm{C_{17}H_{19}NO_3}$.

When heated with dilute acid under reflux, **N** produces two components: piperidine, **O** and an unsaturated carboxylic acid **P**, of formula $\mathrm{C_{12}H_{10}O_4}$. **P** adds two molecules of $\mathrm{Br_2}$ when treated with bromine in 1,1,1-trichloroethane to give compound **Q**.



O



P

Figure 1: Structures of **O** and **P**

Part A Compound N

Draw the compound **N**. Use the structure editor to generate a SMILES string.

In the editor, after drawing your structure, click on the round, yellow smiley face to generate a SMILES string. Copy the SMILES string and paste it in the answer box.

Using the structure editor

Part B Compound Q

Draw the compound **Q**. Use the structure editor to generate a SMILES string.

In the editor, after drawing your structure, click on the round, yellow smiley face to generate a SMILES string. Copy the SMILES string and paste it in the answer box.

Part C O with ethanoyl chloride

Suggest how piperidine **O** would react with ethanoyl chloride ($\mathrm{CH_3COCl}$). Draw the structure of the resulting compound formed.

Use the structure editor to generate a SMILES string as your answer.

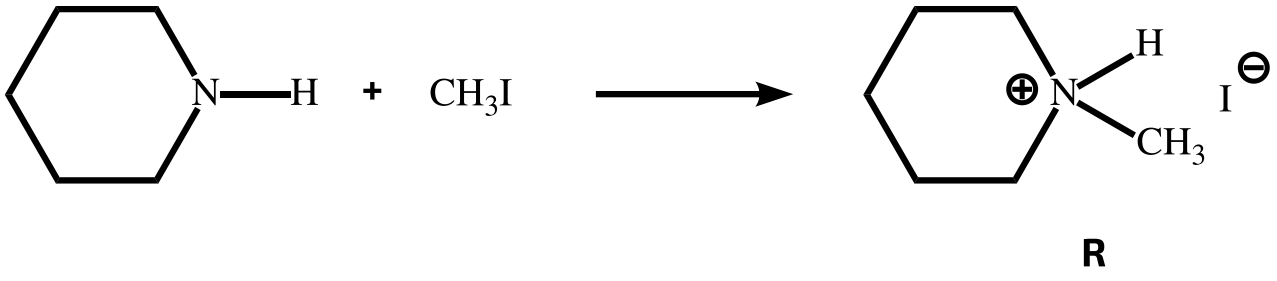
In the editor, after drawing your structure, click on the round, yellow smiley face to generate a SMILES string. Copy the SMILES string and paste it in the answer box.

Part D O with dilute HCl

Suggest how piperidine would react with dilute hydrochloric acid.

Part E Compound R

When piperidine is treated with one equivalent of iodomethane, compound **R** is formed.



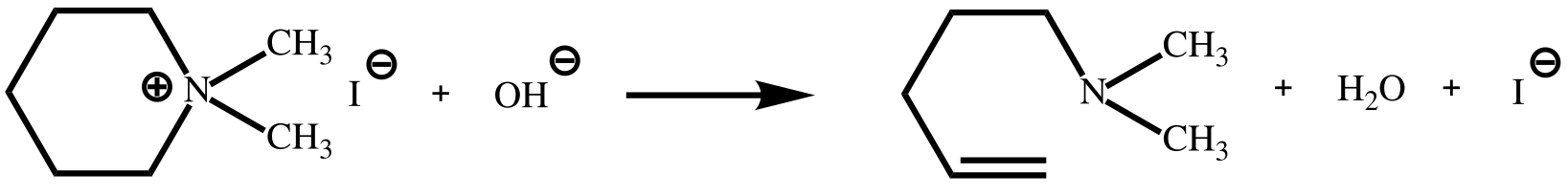
R

Figure 2: Compound **R**

Mechanistically, what type of reaction is occurring?

Part F Compound T

Further reaction of **R** with more iodomethane gives compound **S**, which on heating with alcoholic potassium hydroxide, reacts to form compound **T** in the following scheme.



S **T**

Figure 3: Compound **S** reacting to form compound **T**.

What type of reaction is occurring here?

Part G T with iodomethane

What might be formed if compound **T** were treated with more iodomethane, followed by alcoholic potassium hydroxide?

Use the structure editor to generate a SMILES string as your answer.

In the editor, after drawing your structure, click on the round, yellow smiley face to generate a SMILES string. Copy the SMILES string and paste it in the answer box.

Adapted with permission from UCLES, A-Level Chemistry, November 1990, Special Paper, Question 8.