Chloro Compound

A Level

A compound **A**, $C_3H_5O_2Cl$, after boiling for half an hour with aqueous acid, yielded compounds **B**, $C_2H_3O_2Cl$, and **C**, CH_4O. Boiling **A** for half an hour with aqueous sodium hydroxide, yielded compounds **D**, $C_2H_3O_3Na$, and **C**.

When compound **B** was boiled with aqueous sodium hydroxide, and the mixture acidified, it gave **E**, $HOCH_2CO_2H$. Treatment of **E** with aqueous sodium carbonate resulted in a vigorous effervescence as **E** was converted into **D**.

Deduce the structures of compounds **A** to **D** inclusive.

Use the structure editor to generate SMILES strings as your answers.

Part A Compound A

Compound **A** is:

Part B Compound B

Compound **B** is:

Part C Compound C

Compound **C** is:

Part D Compound D

The *anion* of compound **D** is:

Part E E and C reaction

What product would be obtained when compounds **E** and **C** react together?

Adapted with permission from OCSEB A Level Structured Science Scheme, January 1997, Unit C3: Essential Organic Chemistry, Question 3.

Fruit Alcohols

A Level

Alcohol **A** has esters which are responsible for the flavours of various fruits and has the molecular formula $C_5H_{12}O$. Reaction of **A** with acidified potassium dichromate(VI) produces a compound **B**, $C_5H_{10}O_2$. Heating **A** over Al_2O_3 produces **C**, C_5H_{10}. Reaction of **C** with hydrogen bromide forms 3-bromo-2-methylbutane as one of the products.

Suggest structures for **A**, **B** and **C**.

Use the structure editor to generate a SMILES string.

Part A Alcohol A

Suggest a structure for alcohol **A**.

Use the structure editor to generate a SMILES string.

Part B Compound B

Suggest a structure for compound **B**.

Use the structure editor to generate a SMILES string.

Part C Compound C

Suggest a structure for compound **C**.

Use the structure editor to generate a SMILES string.

Adapted with permission from UCLES, A-Level Chemistry, November 1994, Paper 1, Question 10.

Geraniol

A Level

Geraniol, $C_{10}H_{18}O$, has a rose-like odour and is present in many plants including *Pelargonium odorantissimum*; it has a melting point of $77^{\circ}C$ and a boiling point of $230^{\circ}C$.

It is easily oxidised by acidified potassium dichromate(VI), first to **citral** $C_{10}H_{16}O$, then to **geranic acid**, $C_{10}H_{16}O_2$. Prolonged oxidation of geraniol yields a variety of products, the principal ones being **propanone**, **ethanedioic acid** and **4-oxopentanoic acid**, $CH_3COCH_2CH_2CO_2H$.

One mole of geraniol absorbs two moles of hydrogen when reduced in the presence of a platinum catalyst to give **3,7-dimethyloctanol**; under milder conditions only one mole of hydrogen is absorbed to give **citronellol**, which occurs naturally as an optically active compound but is optically inactive when prepared by reduction of geraniol.

Part A 3,7-dimethyloctanol

Draw the structure of 3,7-dimethyloctanol.

Use the structure editor to generate a SMILES string.

Part B Gernaniol

Suggest a likely structure of geraniol.

Use the structure editor to generate a SMILES string.

Part C Citral

Give the structure of citral.

Use the structure editor to generate a SMILES string.

Part D Geranic acid

Give the structure of geranic acid.

Use the structure editor to generate a SMILES string.

Part E Citronellol

Give the structure of citronellol.

Use the structure editor to generate a SMILES string.

Adapted with permission from UCLES, A-Level Chemistry, November 1989, Special Paper, Question 9.

Gameboard:

STEM SMART Chemistry Week 48 (extension)

Perfumery

A Level

The esters of alcohol **J** are used in the perfumery industry. The alcohol exhibits optical isomerism. When treated with hot concentrated sulfuric acid, each optical isomer of **J** produces three substances **K**, **L** and **M**, which are isomers of each other. Only a small quantity of **M** is produced. Both **K** and **L** react with bromine to give 1,2-dibromo-1-phenylpropane, whereas **M** with the same reagent gives 2,3-dibromo-1-phenylpropane.

Part A Compound J

Suggest a structure for alcohol **J**.

Draw the structure using the structure editor and give your answer as a SMILES string.

Part B Compounds K and L

Suggest structures for compounds **K** and **L**.

Draw the structures using the structure editor and give your answer as SMILES strings in the format A, B (space after comma).

Part C Compound M

Suggest a structure for compound **M**.

Draw the structure using the structure editor and give your answer as a SMILES string.

Part D Isomerism K and L

What type of isomerism do compounds **K** and **L** show with respect to each other?

- Structural Isomerism - Chain
- Stereoisomerism - Geometric
- Structural Isomerism - Position
- Structural Isomerism - Functional
- Stereoisomerism - Optical

Part E Isomerism M and L

What type of isomerism do compounds **M** and **L** show with respect to each other?

- Stereoisomerism - Optical
- Structural Isomerism - Chain
- Structural Isomerism - Position
- Structural Isomerism - Functional
- Stereoisomerism - Geometric

Part F J $\longrightarrow$ K, L, M reaction

What type of reaction does alcohol **J** undergo to produce compounds **K**, **L** and **M**?

Adapted with permission from UCLES, A-Level Chemistry, November 1994, Paper 1, Question 11.