

TWQ 3 (25points)

Name _____

1-5) Mass Spectrometry involves many abbreviated terms. What do these five abbreviations stand for?

GC-MS

EI

ESI

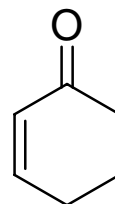
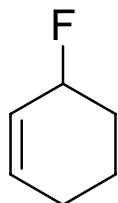
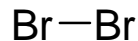
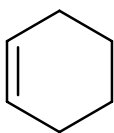
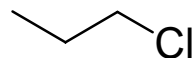
HRMS

HPLC

6) Mass spectrometers do not truly measure the *mass* of an ionized species. What quantity do they measure?

7) Besides a **Quadrupole**, name one other type of Mass Analyzer.

8-16) Indicate which electron is most easily removed from the following compounds under EI conditions.



17-20) Draw the products of the following **thermal fragmentation** and **hydrogen abstraction** reactions.

Draw arrows for each reaction mechanism.

Briefly explain why the two reactions generate different radicals.



21-25) Bearing in mind $C = 12$ and $H = 1$, draw an accurate predicted EI positive ion mass spectrum for butane (include the molecular ion and major fragments) for n-BUTANE.



1-5) Mass Spectrometry involves many abbreviated terms. What do these five abbreviations stand for?

GC-MS Gas Chromatography Mass Spectrometry

EI Electron Ionization

ESI Electro spray Ionization

HRMS High Resolution Mass Spectrometry

HPLC High Performance Liquid Chromatography

6) Mass spectrometers do not truly measure the *mass* of an ionized species. What quantity do they measure?

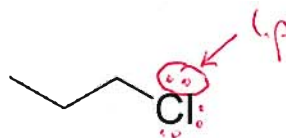
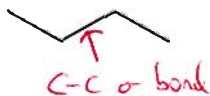
m/z , or Mass to Charge Ratio

7) Besides a **Quadrupole**, name one other type of Mass Analyzer.

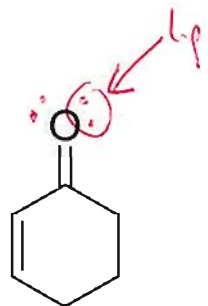
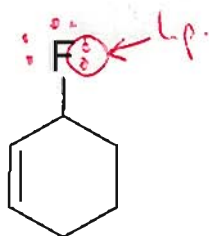
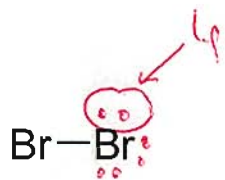
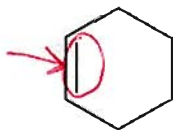
Magnetic Sector, Ion trap, triple quad, Time of flight, ...

8-16) Indicate which electron is most easily removed from the following compounds under EI conditions.

ONE ELECTRON FROM ...



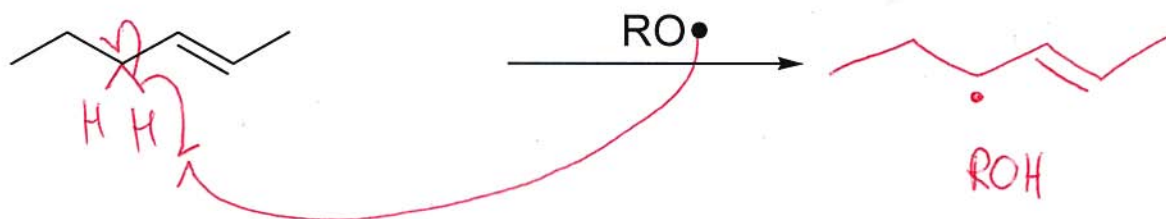
↑
 π bond



17-20) Draw the products of the following **thermal fragmentation** and **hydrogen abstraction** reactions.

Draw arrows for each reaction mechanism.

Briefly explain why the two reactions generate different radicals.

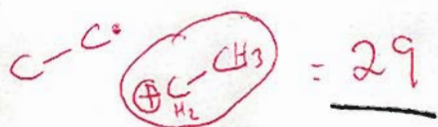
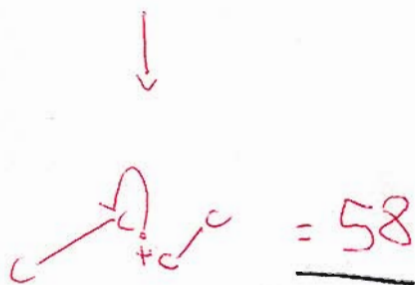
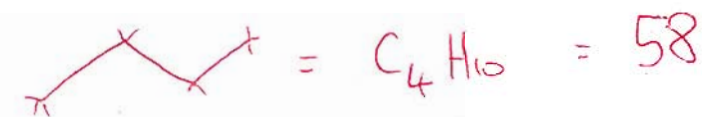
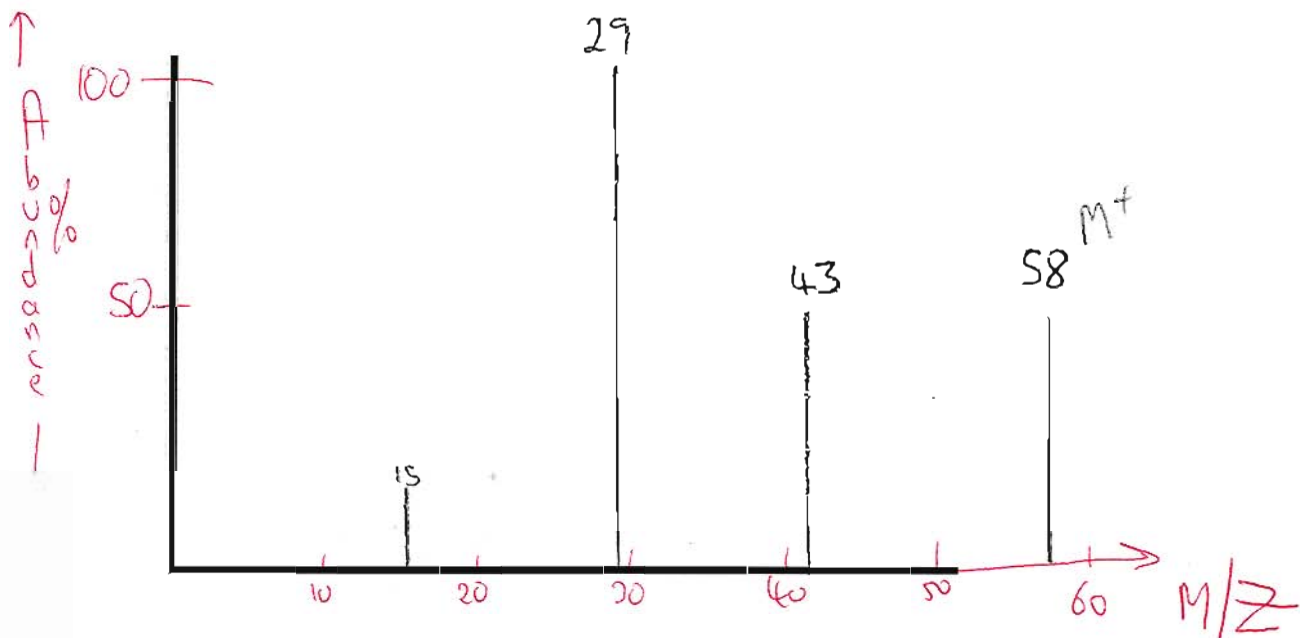


Both of these reactions generate RESONANCE stabilized radicals.

The weakest bond in the starting material is the C-C bond and when heated, this is the bond that breaks.

However when another reagent is present, the reaction is different because we must now consider the energy change in forming a very stable RO-H bond.

21-25) Bearing in mind $C = 12$ and $H = 1$, draw an accurate predicted EI positive ion mass spectrum for butane (include the molecular ion and major fragments) for n-BUTANE.



Best Fragment

