

## Week 8 Worksheet

1. In Mass Spectrometry a sample molecule is ionized forming cations by the loss of an electrons.
2. A magnetic field focuses the ion beam to the detector.
3.  $m/z$  is short for Mass (molar mass) to charge ratio.
4. Use the given mass spectrometry data to determine the molecular formula.

Peak	$m/z$	Relative Intensity
M	59	100%
M+1	60	3.85%
M+2	61	0.0127%

**Step 1:** Check to see if the relative intensity of the M peak is 100%. If not, you would have to rescale the values.

**Step 2:** Is the  $m/z$  value for the M peak even or odd? The M peak equals the molecular mass of the compound, which in this case is 59 amu. This is an odd number, so according to the Nitrogen Rule, there must be an odd number of nitrogen atoms in the compound. The minimum number of nitrogen atoms is one.

**Step 3:** Use the relative intensity of the M+1 peak to find the number of carbon atoms. Here,  $3.85\%/1.1\% = 3.5$ . This means that there are three or four carbons in the compound.

**Step 4:** Look at the M+2 peak to check for the presence of S, Cl, or Br. Since the intensity of the M+2 peak is less than 4% (approximate relative abundance of S), there are no S, Cl, or Br atoms in this molecule.

**Step 5:** Subtract the isotopic masses of the known atoms from the mass of the entire compound ( $m/z$  of M peak). The remaining value represents the amu left over for the other atoms. So,

$M - C_3 - N \quad \longleftarrow$  We must have at least 3 C and 1 N

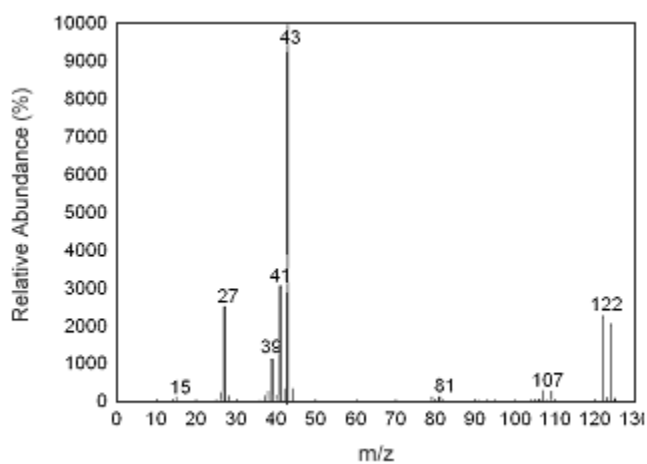
$59 - (3(12) + 14) = 9$  amu left over for O, H, more N atoms (must be odd), or another C atom.

**Step 6:** Evaluate all possibilities for the molecular formula, and assess whether they are reasonable.

In this instance, there is no need to construct a chart for the number of each type of atom. 9 amu are not enough for oxygen (16 amu), nitrogen (14 amu each), or another carbon (12 amu). Thus, the 9 amu must come from nine hydrogen atoms.

In conclusion, the only possible molecular formula is  $C_3H_9N$

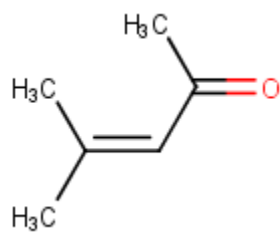
5. Is the following Spectrum of a Alkyl Bromide or Chloride?



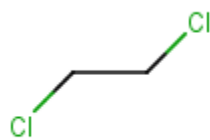
6. What technique would you use to differentiate between the following two compounds  $C_3H_8$  and  $CH_3CHO$  and why?

High Res mass spec

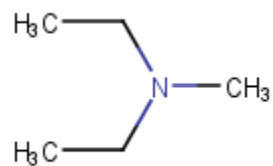
7. Match the following compounds with their respective Mass spectrum.



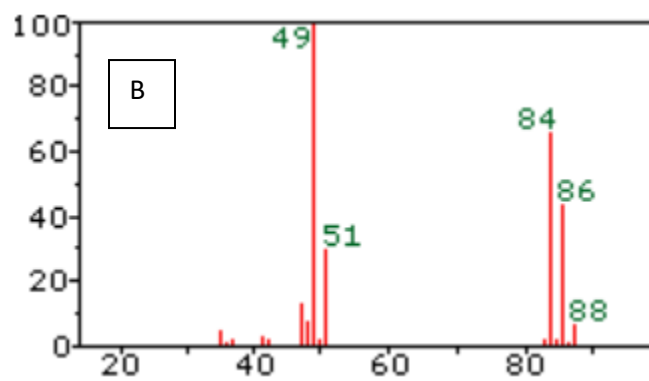
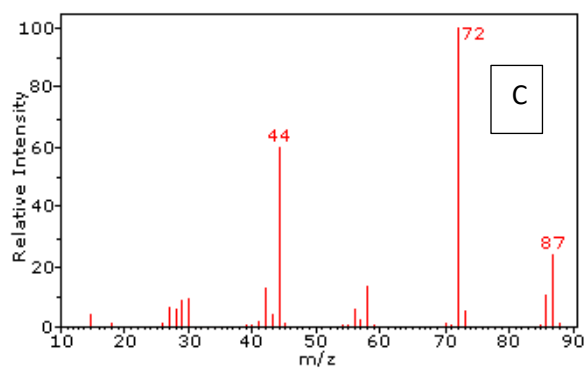
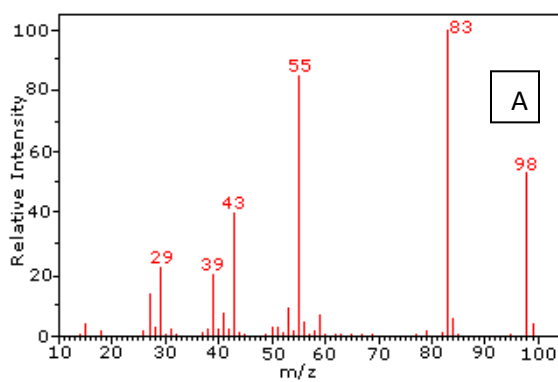
A



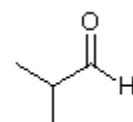
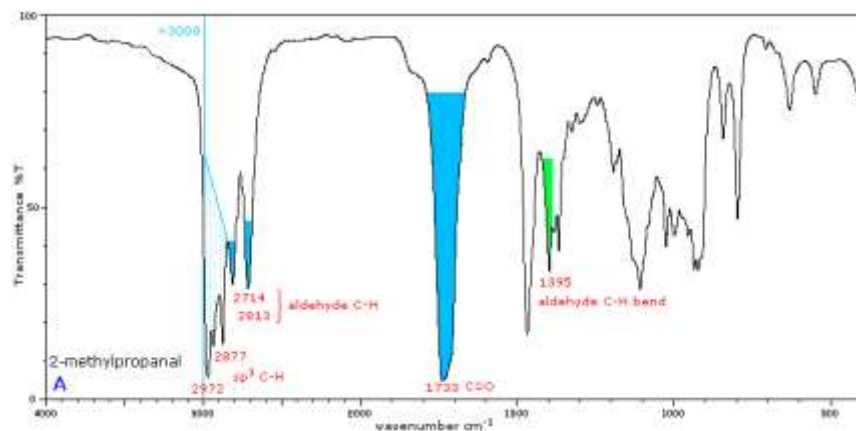
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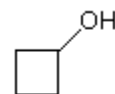
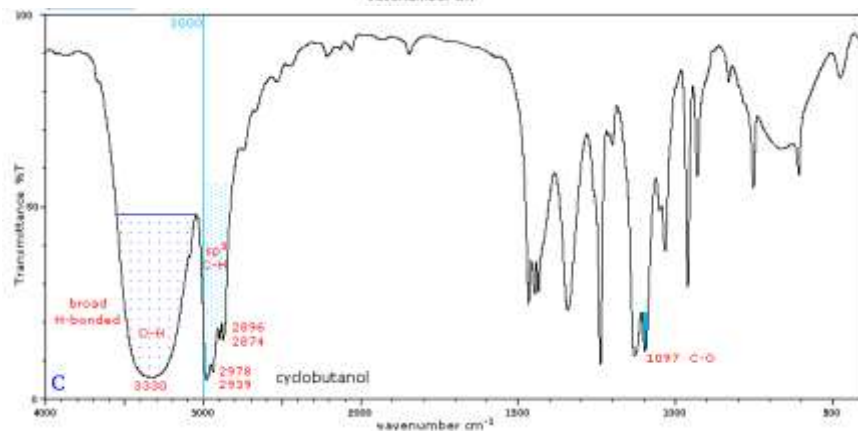
C



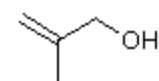
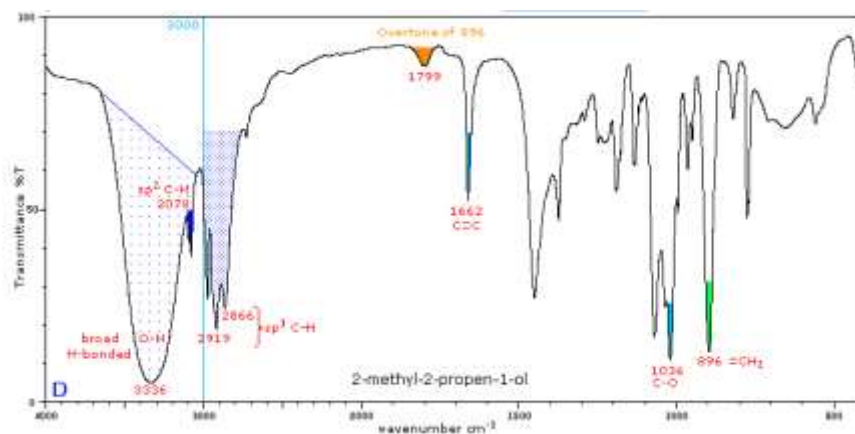
8. Match the following molecules with their respective IR spectrum



2-methylpropanal



cyclobutanol



2-methyl-2-propen-1-ol