Chemistry 136

Lab Report for the Determination of Unknown Compounds

Experiment number: _____

Name: _____ Drawer #: _____

Date: _____ **Unknown Number:** _____

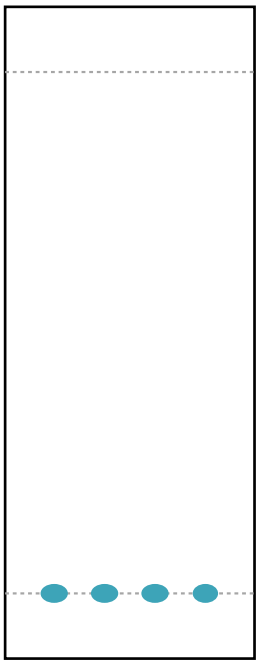
1. Physical appearance (color, form of the crystals, etc):

Unknown 1:

Unknown 2:

2. TLC Analysis (SiO_2, solvent?, 254 nm UV? or stain?)

Note: use the ChemBioDraw TLC tool if available to you and paste it here instead of the one provided. It allows you to get instant R_f values by moving the dots up to their relative observed positions. This will greatly facilitate your task.



Elution properties:

Unknown 1 (please label on the TLC plate) R_f: _____

Unknown 2 R_f: _____

Other observations:

3. Physical constants (mp or bp)

Unknown 1: mp / bp _____ ˚C

Unknown 2: mp / bp _____ ˚C

4. Molecular formula deduced from the NMR and IR data

Unknown 1: _____

Degree of unsaturation: _____

Unknown 2: _____

Degree of unsaturation: _____

Explain how you arrived at these molecular formulae:

5. Method(s) of separation or purification:

Characterization Data

6. **IR spectra**: (attach original spectra at the end of the report, or insert as JPEG file if available)

Please list only charasteristic (assignable) bands in IR:

IR DATA for UNKNOWN 1		
Absorption (cm^{-1})	Relative intensity	Assignment
e.g. 2895	e.g. m (or w, s, vs)	e.g. sp^3 C–H stretch

IR DATA for UNKNOWN 2		
Absorption (cm^{-1})	Relative intensity	Assignment
(e.g. 2895)	(e.g. m (or w, s, vs))	(e.g. sp^3 C–H stretch)

7. **^{1}H NMR spectra:** Show proposed structure below with assignment labels (e.g. H_a, H_b, H_c, etc):

^{1}H NMR DATA for UNKNOWN 1				
Chemical shift (ppm)	**Multiplicity**	**Integral**	**Coupling Constant (Hz)**	**Assignment**
(e.g. 4.04)	(e.g. ddt)	(e.g. 2H)	(e.g. J = 8.2, 4.5, 2.1 Hz)	(e.g. H_a)

^{1}H NMR DATA for UNKNOWN 2				
Chemical shift (ppm)	**Multiplicity**	**Integral**	**Coupling Constant (Hz)**	**Assignment**
(e.g. 4.04)	(e.g. ddt)	(e.g. 2H)	(e.g. J = 8.2, 4.5, 2.1 Hz)	(e.g. H_a)

8. **^{13}C NMR spectra:** Show proposed structure here with assignment labels (e.g. A, B, C, etc):

^{13}C NMR DATA for UNKNOWN 1	
Chemical shift (ppm)	**Assignment**
(e.g. 128.3)	(e.g. A)

^{13}C NMR DATA for UNKNOWN 1	
Chemical shift (ppm)	**Assignment**
(e.g. 128.3)	(e.g. A)

9. Other spectroscopy data if available (e.g. 2D NMR):

10. Relevant literature data supporting structure:

Unknown 1:

Unknown 2:

11. Logical reasoning used in deriving your structures:

(this should be less than one page in most cases. By citing specific data you have obtained, prove that your structure is what is shown above, eg. a C=O stretch in IR + corresponding C=O absorption in ^{13}C NMR to show that the compound is a ketone, etc)

Unknown 1:

Unknown 2: