Chem 2312 Lab Report Grading Guidelines

Product purity

- Based on GC trace and NMR spectrum

Product yield

- Evidence of product isolated from/produced by the reaction 7 points
- Remaining points based on percent yield: 10-39%, +1 pt; 40-79%, + 2 pts; 80-100%, + 3 pts

Spectral quality

- All spectra should be clearly labeled to indicate which product they correspond to
- IR
    - Appropriate concentration (aiming for y-axis scale to start around 100% transmittance and the most intense peaks >10% transmittance
    - Peak maxima picked by the software – can some be added manually on the computer?) appropriately
    - specify if the sample has been deposited onto the salt plate as a DCM solution
- GCMS
    - Concentration in the chromatogram: targeting a TIC of between 10,000–1,000,000 for the tallest (i.e., most intense) peak. Bottom line: a concentration of <5 mg per 100 mL of solvent is near the sweet spot
    - MS spectrum printed for the product peak
- NMR
    - Referenced to TMS (annotate the reference peak on MNova so we can see that it is referenced correctly)
    - Appropriate concentration – typically too dilute early in the semester (aim for at least 5 mg of sample in 500 uL of $CDCl_3$)
    - Peaks manually picked, no auto peak-picking
    - Show the integrations on the spectrum; what you report in the line listing is <u>what you observe</u> (to the nearest whole integer), <u>not what should be</u> in the spectrum
    - Appropriate chemical shift width for the x-axis, generally (ca. 9 ppm to -1 ppm)

Spectral interpretation

- IR
    - Appropriate peaks reported (just those for which a specific bond stretch can be associated) and to the nearest whole wavenumber (i.e., cm^{-1})
    - Wavenumbers that are reported are assigned to functional groups present in the molecule
    - Correct description of the nature of the sample (thin film, solid from DCM, etc.)
- GCMS
    - Specify the GC column <u>and the method</u> used to collect the data
    - Indicate the retention time
    - Report key, identifiable MS fragment positive ions along with their relative intensities [% relative to that of the base peak (i.e., the 100%)]
- NMR
    - Protons clearly assigned (reader can tell which proton is responsible for each resonance from reading only at the line listing)
    - Splitting patterns (e.g., s, dd, dt, ddd, etc.) assigned and reported with all *J* values
    - Shifts (δs) reported to 2 decimal places, *J* values reported to 1 decimal place
    - Magnet strength and sample solvent

Lab report

- Independently-produced figures with compound numbering starting at 1
- Grammar and spelling
- Scientific writing formatting (spaces between numbers and units, amounts in parentheses, etc.)
- Indicate quantities (mass and volume) to 2 or 3 significant figures
- Provide yields to 2 significant figures
- Quality of writing (concise, procedure reported correctly, etc.)

Questions

- ca. 1 point per answer to the questions