Lab Report 1 - Rubric

General Guidelines

- The lab report will be in lab notebook format, no journal-style formatting is required. However, readability is important, so we expect you to format it accordingly. You may think as if this lab notebook will be read by a new graduate student to repeat the experiments after you leave.
- Plots and fits are to be done in Python, Matlab, Mathematica, or Origin. We will not accept screenshots of data and plots.
- For every experiment, provide the pulse program in the report. Please only include the code you wrote within templates. Please explain what the pulse sequence does.
- For every experiment, please provide all the parameters you used to run the experiment. Please include your reasoning for the parameters used.
- Below, some important points for each experiment are provided to help you. Your report should include information about these points, but it may not be limited to this. We expect you to provide reasoning and understanding for the conduct and result of the experiments. Please explain what went wrong if your results were suboptimal.

Lab 1

Experiment 1: Free Induction Decay (Water) - 1H

- What is the measured chemical shift of the 1H spin of water in ppm and in Hz?
- What does the FID signal look like on resonance and off resonance?
- What happens when you pulse outside the bandwidth of the acquisition window?
- How the observable signal change with different pulse lengths? What is the approximate pulse length for 180 degree rotation? Is the 180-degree pulse at the expected value compared to 90-degree pulse?
- What does repetition time mean? How do you determine the repetition time?
- Please calculate your T2* time from your FID decay.
- What is the dwell time and number of points you used? How do signal amplitude, noise, and Fourier-transformed lineshape change with these parameters? Please examine your FID time signal according to your Fourier transform parameters and Nyquist theorem. Consider cases where dwell time and number of points changed while the acquisition time is kept constant.
- What is the phase correction parameter that you used?

Experiment 2 : Proton pulse length calibration

- Please provide all the parameters used in this experiment and all the experiments alongside the pulse program.
- Provide the integrated signal vs pulse length plot and apply an appropriate fit to determine pi/2 pulse length. Comment on the results and possible error sources.

Experiment 3: T1 relaxation measurement with inversion recovery

- Please define T1 time, the underlying decay mechanism, and the pulse sequence you used for the measurement.

- Please include the mathematical expression for T1 decay you used to fit your measurement data.
- What is the repetition time you used during the sweep? How did you determine this repetition time?

Experiment 4: T1 relaxation measurement with saturation recovery

- Please research and add your understanding of how saturation recovery works and how it can be used to determine T1 time.
- What is the purpose of using a delay as long as T2* between pulses?

Experiment 5: Hahn echo experiment

- Describe what is the meaning of T2 and T2* times and their difference.
- What is the linewidth of the FID signal and T2* time after spoiling the shim values?
- Identify the FID signal and the echo signal in your measurement.
- How does echo amplitude change in time signal with different echo times? Explain the underlying reason.

Experiment 6: Pulse amplitude calibration

- Please compare the results of pulse length and pulse amplitude calibration and comment if there is any discrepancy between the pi/2 pulse you used in previous experiments and obtained in this experiment. You may need to repeat your experiment if there is a phase error due to imperfections.

Lab 2

Please comment on the specs of the sample you used in this experiment. What are the sources of NMR signal in this sample?

Experiment 1: 1H- Free Induction Decay

- Please identify the origins of each signal line with appropriate coupling strengths and identify the particular spin states for each transition.
- Please provide T2* time you measured during the experiment.
- What are the sources of other spurious lines in the experiment? Is it possible for you to identify the ratio of 12-C compared to 13-C atoms in the solution through the experiment?
- How did you select the center frequency? How does changing center frequency affect the measurement?

Experiment 2: T1 measurement (1H)

- Compare the T1 time of 1H in water and in chloroform samples.

Experiment 3: 13-C Free Induction Decay

- Please identify each peak in the spectrum
- What is the J-coupling strength? How is the value you calculated compared to 1H spectrum?
- What are the contributing factors for the low SNR of the FID signal from 13-C?

- How can we improve the SNR of 13-C FID signal? Please think about possible experimental and post-processing-related precautions.

Experiment 4: 13-C Pulse length calibration

- Report and comment on the pi/2 pulse you determined in this experiment.

Experiment 5: Polarization transfer and decoupling

- Research and explain how polarization transfer increases the SNR of 13-C signal by taking nuclear Overhauser effect (NOE) into account and provide your results.
- How does the decoupling work for 13-C and 1-H?
- Review and comment on how the provided pulse sequence work.
- How much improvement is obtained in signal compared to standard FID experiment?

Experiment 6: T1 measurement (13C)

- Report T1 time in default mode as given in the lab manual.
- Does coupling to 1H affect the 13C T1 time?
- Compare T1 measurements done with and without turning on the decoupling sequence. Discuss the value of T1 observed in both cases.

Experiment 7: CPMG experiment

- Please explain what the provided pulse sequence does.
- How long is the T2 time obtained after the CPMG experiment? Comment on how CPMG affects the qubit and changes the T2 time?