CHM 4380
Final Examination

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Name: _____

Student number:_____

Time allowed: 3 hours
Basic non-alphanumeric calculator permitted

This exam has 6 pages.

Instructions: Circle the single most appropriate response for each of the 25 questions. All questions are valued equally.

1. A nucleus having spin quantum number, $I = 1$:
   a) will have 1 energy transition but only when in an external magnetic field.
   b) has 3 Zeeman energy levels in the absence of an external magnetic field.
   c) has spin quantum numbers, $m = ½, 0, – ½$.
   d) is quadrupolar
   e) is not NMR active.

2. A NOESY pulse sequence:
   a) is a 2D experiment used to measure J coupling correlations between two unlike isotopes.
   b) uses pulsed field gradients to distinguish between molecules with different diffusion constants.
   c) can show correlations between protons close to one another in space and also between protons exchanging with one another.
   d) is one of the simplest imaging sequences.
   e) requires a triple resonance NMR probe.

3. A variable evolution delay:
   a) is used when all resonances have very long T_1 relaxation times.
   b) must always be used between short high power (sin x)/x pulses.
   c) is used in all 2D pulse sequences.
   d) is less important for running liquids NMR rather than solids NMR.
   e) is used to get around the receiver dead time problem.

4. The J modulated spin echo experiment:
   a) is used to measure ^{1}H - ^{1}H coupling constants.
   b) uses a fixed delay equal to $1/(^{1}J_{C-H})$ to phase encode ^{13}C resonances based on the number of attached protons.
   c) is most often run as a 2D experiment except Fourier transformations in the indirect domain are not calculated.
   d) requires the use of the proton decoupler for the entire duration of the pulse sequence.
   e) is used to make relaxation time measurements for J coupled spins.

5. A technique which can significantly improve rolling baseline problems in a spectrum is:
   a) backward linear prediction.
   b) exponential line broadening.
   c) resolution enhancement by using a Gaussian weighting function on the FID.
   d) zero filling
   e) quadrature detection.

6. The splitting in a ^{1}H NMR spectrum between the 3 lines of a J coupled triplet is 12 Hz when measured on a 300 MHz spectrometer. The spiltting:
   a) would be 24 Hz if measured on a 600 MHz spectrometer.
   b) would be 0.04 ppm if measured on a 600 MHz spectrometer.
   c) would be 0.02 ppm if measured on a 600 MHz spectrometer.
   d) would be 0.08 ppm if measured on a 600 MHz spectrometer.
   e) would not be equal to any of the above on a 600 MHz spectrometer.

7. The signal-to-noise ratio in an NMR spectrum was much lower than expected. What was the problem?
   a) The relaxation delay was too long.
   b) The pulse used was much less than 90°.
   c) There was a problem with the zero filling.
   d) The excitation profile of the pulse was too wide.
   e) The resources of the computer running the spectrometer were being shared by a web browser.

8. All of the lines in a particular NMR spectrum have a distortion which broadens the lines symmetrically at the base. What would explain the problem?
   a) There was a significant receiver dead time after the pulse.
   b) The Z^2 and Z^4 shims were set poorly.
   c) The Z^3 and Z^5 shims were set poorly.
   d) The excitation profile of the pulse was too narrow.
   e) The acquisition time was not long enough.

9. The literature value for the ^{29}Si chemical shift of tetramethylsilane (TMS) is 0.00 ppm. A proton decoupled ^{29}Si NMR spectrum of TMS was acquired without the use of digital filters. The carrier frequency was set at -50 ppm and the spectral width set at 90 ppm. Which statement best describes the spectrum?

a) A signal at 0.00 ppm.
b) No signal.
c) A signal at -55 ppm.
d) A signal at -180 ppm.
e) A signal at -90 ppm.

10. The inversion transfer experiment can be used to:

a) measure T_2*.
b) measure T_1.
c) distinguish between the components of a mixture based on their diffusion coefficients.
d) detect chemical exchange.
e) help determine how many protons are attached to a carbon.

11. How many lines are in the ^{19}F NMR spectrum of the isotopomer $^{13}CDF_3$? (The spin quantum numbers for ^{2}H, ^{19}F and ^{13}C are $I = 1$, $I = ½$ and $I = ½$, respectively.

a) 6
b) 16
c) 4
d) 3
e) 2

12. A ^{1}H NMR spectrum of $H_2{}^{77}Se$ consists of a 1:1 doublet. The $^{1}J_{Se\text{-}H}$ coupling constant is 64.8 Hz. The plot has the peaks labelled in ppm as -0.1843 and -0.3139 ppm. Which spectrometer was used to run the spectrum?

a) Nicolet 360
b) Varian XL-300
c) Bruker AVANCE 400
d) JEOL ECLIPSE 930
e) Bruker ARX 500

13. The rotating frame of reference:
    a) is a mathematical concept used to help explain why some gyromagnetic ratios are negative.
    b) always rotates at the proton Larmor frequency.
    c) is a concept which helps simplify the description of magnetization vectors in the presence of a magnetic field under the influence of radio frequency pulses.
    d) is a mathematical concept where the YZ plane of a Cartesian axis system rotates about the X axis.
    e) is not described accurately by any of the above.

14. The free induction decay:
    a) follows the decay of magnetization on the z axis.
    b) is a frequency domain function.
    c) always decays according to the T_1 relaxation time constant.
    d) can change its appearance depending on the position of the carrier frequency.
    e) all of the above are true.

15. Superconducting magnets require an external source of power:
    a) to slow down the evaporation of liquid helium.
    b) to cool the solenoid coil of the magnet to 77 K.
    c) to keep the magnet shims cold so they will not generate noise.
    d) to keep the NMR probe cool.
    e) only when being brought up to their specified field strength.

16. A technique which can be used to eliminate Nyquist fold-backs and increase the signal-to-noise ratio in an NMR spectrum is:
    a) digital filtering.
    b) backward linerar prediction.
    c) forward linear prediction.
    d) apodization of the FID with a Gaussian function.
    e) zero filling.

17. The following pulse sequence:
    $(90_{-y}) - (180_x) - (90_y) - (180_x)$
would leave an equilibrium magnetization along the:
    a) x axis.
    b) y axis.
    c) -z axis.
    d) -x axis.
    e) -y axis.

18. Exponential line broadening:
    a) is a processing technique used to improve digital spectral resolution.
    b) has the effect of artificially expanding the spectra width.
    c) can be used to recover information lost in the spectrometer dead time.
    d) can improve the signal-to-noise ratio in a spectrum at the expense of resolution.
    e) eliminates Nyquist fold-backs.

19. A properly recorded NMR spectrum acquired with 16 scans had a signal-to-noise ratio of 2. How many scans would be needed to get a signal to noise ratio of 20?
    a) 160
    b) 320
    c) 1,600
    d) 3,200
    e) 16,000

20. The spectrometer amplifier power:
    a) affects the spectral width.
    b) is an important parameter to ensure that the receiver dead time is kept to a minimum.
    c) can affect the resolution in an NMR spectrum.
    d) affects T_2* but not T_1 or T_2.
    e) affects the duration of 90º pulses.

21. The observed line width at half height of an NMR signal, $\Delta\nu_{1/2}$, for a liquid:
    a) depends on the relaxation delay allowed in the pulse program.
    b) tends to be larger for nuclei with larger gyromagnetic ratios.
    c) is inversely proportional to T_1.
    d) depends on T_2*.
    e) depends critically on the receiver dead time.

22. Solenoid r.f. coils are generally not used in NMR probes designed to collect NMR data for liquid samples because:
    a) they make sample handling cumbersome.
    b) they are less efficient at transmitting r.f. power to the sample than Helmholtz coils.
    c) they are not superconducting.
    d) they are much more expensive to incorporate into an NMR probe.
    e) they make an NMR probe difficult to tune and match.

23. 1-Dimensional TOCSY NMR data:
    a) requires the use of a variable delay.
    b) requires the use of a shaped pulse.
    c) can be used to determine whether nuclei are quadrupolar.
    d) can be used to determine whether or not two protons are close to one another in space.
    e) is described accurately by all of the above.

24. Gated proton decoupling:
    a) would be used in conjunction with long recycle delays to acquire a quantitative ^{13}C NMR spectrum.
    b) would be used to observe a fully coupled ^{13}C spectrum with a nuclear Overhauser enhancement.
    c) can be used to determine T_1.
    d) is a simple alternative to the COSY experiment.
    e) can only be applied during the dwell time between sampling points of the FID.

25. The intermediate frequency of an NMR spectrometer:
    a) is the frequency of the rotating frame of reference.
    b) is equal to the Larmor frequency.
    c) is the frequency difference between a resonance line and the center of the spectrum.
    d) is the intermediate frequency between that of ^{1}H and ^{13}C.
    e) is not described well by any of the above.