CHEM 4616: Exam #3

Name: _____ **ID#:** _____

Some potentially useful information:

- $h = 6.6261 \times 10^{-34}$ J s (Planck's constant)
- $\hbar = h/2\pi = 1.0546 \times 10^{-34}$ J s
- Speed of light in a vacuum, $c = 2.9979 \times 10^{8}$ m s $^{-1}$
- Mass of an electron, $m_e = 9.1094 \times 10^{-31}$ kg
- 1 amu (u) $= 1.6605 \times 10^{-27}$ kg
- 1 eV $= 1.6022 \times 10^{-19}$ J
- 1 J = 1 N m = 1 kg m^2 s^{-2}
- 1 Å $= 1.0 \times 10^{-10}$ m

Multiple Choice Questions (5 points each):

(1) Which of the following molecules is **not** chiral?

(a) CHFClBr

(b) H_2O_2

(c) $CH_3CHClCH_2CH_3$

(d) 1,3-dichloroallene

(e) None of the above.

(2) Which region of the electromagnetic spectrum gives rise to the transitions appearing in NMR spectra?

(a) Radio

(b) Infrared

(c) Visible

(d) Ultraviolet

(e) X-ray

(3) Which of the following is a typical electronic transition in organic molecules?

(a) $d \rightarrow d$

(b) $\pi \rightarrow \pi^*$

(c) MLCT

(d) LMCT

(e) None of the above

(4) Optical rotation of a chiral compound relates to which physical phenomenon:

(a) The Franck-Condon principle

(b) Absorption

(c) Heisenberg uncertainty

(d) Refraction

(e) Phosphorescence

(5) Which of the following statements about NMR spectroscopy is **incorrect**?

(a) Nuclear spin transitions are caused by radiofrequency radiation.

(b) Fine structure is caused by spin-spin coupling.

(c) The chemical shift (δ) of a proton is greater in a 500 MHz spectrometer than a 250 MHz spectrometer.

(d) The local magnetic field felt by a given nucleus is dependent on its surrounding environment.

(e) The reference compound for proton NMR is TMS.

(1) (35 points) Identify all of the symmetry elements in the following molecules:

(a) 1,3-dichlorobenzene

(b) ethylene

(c) ammonia

(2) (35 points) In diethyl ether, the chemical shift (δ) of the CH_3 protons is 1.16 and that of the CH_2 protons is 3.36. The spin-spin coupling parameter (J) is 6.97 Hz. Sketch the NMR spectrum (incuding fine structure and relative peak heights) of diethyl ether as it would be measured by (a) a 200 MHz spectrometer and (b) a 400 MHz spectrometer.

(3) (35 points) The specific rotation of the sugar α-D-mannose is $[\alpha]_D^{20} = +29.3$ deg/[dm (g/mL)].

(a) What is the total rotation (at the sodium D-line at 20°C) of a 0.300 g/mL sample of α-D-mannose in a polarimeter with a 20.0 cm path length at 20°C?

(b) When α-D-mannose is dissolved in water, part of the sugar is converted into β-D-mannose until an equilibrium is formed. Given that the specific rotation of β-D-mannose is $[\alpha]_D^{20} =$ -17.0 deg/[dm (g/mL)] and the specific rotation at equilbrium is $[\alpha]_D^{20} = +14.2$ deg/[dm (g/mL)], calculate the percentages of α- and β-D-mannose in the solution at equilibrium.

(4) (35 points) A 0.10 mol/L solution of a dye transmits 80% of the light at 435.6 nm in a glass cell 1.0 cm thick.

(a) What percent of light will be **absorbed** by a solution containing 2.0 mol/L in a cell 1.0 cm thick?

(b) What percent of the light will be **transmitted** by a solution of the dye containing 0.10 mol/L in a cell 5.0 cm thick?

(5) (35 points) What is the resonance (Larmor) frequency of a free ^{13}C nucleus ($I = 1/2$) in a 10.0 T magnetic field, given that its magnetogyric ratio (γ) is 6.7272 $\times 10^7$ T^{-1} s^{-1}? Show your work and express your answer in MHz.