California State Polytechnic University, Pomona

CHM 3140 Organic Chemistry I, Dr. Laurie S. Starkey

Chapter 15 Summary (Klein 4th ed. textbook): **NMR Spectroscopy**

I. Introduction to NMR Spectroscopy (15.1-15.3)
   A) Analysis of molecular structure
   B) Radiowave energy causes nuclear spin to flip
   C) ^{1}H and ^{13}C nuclei can be observed

II. Number of NMR Signals (15.4) **SkillBuilders 5.1, 5.2**
   A) Indicate the number of unique types of protons (or carbon atoms)
   B) Determine relationship of protons by using "swap test" (replace with Cl atom)
      i) Homotopic protons are equivalent in NMR
      ii) Enantiotopic protons are equivalent in NMR
      iii) Diastereotopic protons are NOT equivalent in NMR

III. Peak Integration (5.6) **SkillBuilder 5.4**
   A) Indicates the number of protons giving rise to a signal
   B) Values given as #H (1H, 2H, 3H, etc.), or integral trails or values beneath each peak

IV. Chemical Shift (δ value) (15.5) **SkillBuilder 15.3**
   A) Values given in ppm
   B) Chemical shift tables are provided, and can also be calculated
   C) Higher ppm (downfield) indicates more electron-rich environment
      i) Tetramethylsilane (TMS) is a common reference at 0 ppm
   D) Lower ppm (upfield) indicates more electron-deficient environment
      i) Electronegative groups cause downfield shift (*e.g.* MeO ~3.8 ppm)
      ii) Pi bonds cause downfield shift (*e.g.* aromatic ~7 ppm, alkenyl ~5 ppm)
   E) Protons on oxygen or nitrogen have variable δ values (typically broad singlets)

V. Shape of Signal: Multiplicity/Splitting Patterns (15.7) **SkillBuilder 15.5**
   A) Indicates the number of nonequivalent *neighboring* protons
   B) *n*+1 Rule = *n* neighboring protons results in *n*+1 peaks
      i) no neighboring protons → singlet (s)
      ii) 1 proton neighbor → doublet (d)
      iii) 2 proton neighbors → triplet (t)
      iv) 3 proton neighbors → quartet (q), and so on…

VI. Putting it all together
   A) Predicting a ^{1}H "Proton" NMR Spectrum (15.8) **SkillBuilder 15.6**
   B) Using ^{1}H NMR data to distinguish between compounds (15.9) **SkillBuilder 15.7**

VII. ^{13}C NMR Spectroscopy (15.11, 15.12) **SkillBuilder 15.9**

========== Stop Here for Exam II ==========

VIII. Interpreting a ^{1}H NMR Spectrum (15.10) **SkillBuilder 15.8**

Skip DEPT ^{13}C NMR *(Section 15.13 and SkillBuilder 5.10)*