## CEM 251, Problem Set 6: Spectroscopy

1. Match the following compounds with the IR spectra given.





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2. For the following molecular formulas calculate the number of RDBs (rings or double bonds, degrees of unsaturation).
\#RDBs

| $\mathrm{C}_{8} \mathrm{H}_{7} \mathrm{~N}$ |  |
| :--- | :--- |
| $\mathrm{C}_{7} \mathrm{H}_{11} \mathrm{BrO}$ |  |
| $\mathrm{C}_{8} \mathrm{H}_{15} \mathrm{NO}$ |  |
| $\mathrm{C}_{10} \mathrm{H}_{14}$ |  |
| $\mathrm{C}_{6} \mathrm{H}_{8} \mathrm{O}$ |  |
| $\mathrm{C}_{10} \mathrm{H}_{22} \mathrm{NCl}$ |  |

3. For the following molecules, how many different signals (peaks) would you expect to see in the ${ }^{1} \mathrm{H}$ NMR spectrum?
\# of 1H NMR peaks
4. What should be the multiplicity of the 1H NMR peaks of each of the following groups of protons:

5. Which group of protons of the following molecule corresponds to which peak on the NMR spectrum shown?



| Type of proton | Approximate chemical shift (ppm) | Type of proton | Approximate chemical shift (ppm) |
| :---: | :---: | :---: | :---: |
| $\left(\mathrm{CH}_{3}\right)_{4} \mathrm{Si}$ | 0 |  | 6.5-8 |
| $-\mathrm{CH}_{3}$ | 0.9 | 0 |  |
| $-\mathrm{CH}_{2}-$ | 1.3 | $-\mathrm{C}-\mathrm{H}$ | 9.0-10 |
| $\stackrel{1}{-\mathrm{C}} \mathrm{H}-$ | 1.4 |  | 2.5-4 |
|  | 1.7 |  | 2.5-4 |
| $-\mathrm{C}-\mathrm{CH}_{3}$ | 2.1 |  | 3-4 |
|  | 2.3 |  | 4-4.5 |
| $-\mathrm{C} \equiv \mathrm{C}-\mathrm{H}$ | 2.4 | RNH2 | variable, 1.5-4 |
| $\mathrm{R}-\mathrm{O}-\mathrm{CH}_{3}$ | 3.3 | ROH | variable, 2-5 |
|  | 4.7 | ArOH | variable, 4-7 |
|  | 5.3 |  | variable, 10-12 |

Table of IR Absorptions

| Functional Group | Characteristic Absorption(s) $\left(\mathrm{cm}^{-1}\right)$ |
| :---: | :---: |
| Alkyl C-H Stretch | $2950-2850(\mathrm{~m}$ or s) |
| Alkenyl C-H Stretch | $3100-3010(\mathrm{~m})$ |
| Alkenyl C=C Stretch | $1680-1620(\mathrm{v})$ |
| Alkynyl C-H Stretch | $\sim 3300(\mathrm{~s})$ |
| Alkynyl C=C Stretch | $2260-2100(\mathrm{v})$ |
| Aromatic C-H Stretch | $\sim 3030(\mathrm{v})$ |
| Aromatic C-H Bending | $860-680(\mathrm{~s})$ |
| Aromatic C=C Bending | $1700-1500(\mathrm{~m}, \mathrm{~m})$ |
| Alcohol/Phenol O-H Stretch | $3550-3200(\mathrm{broad}, \mathrm{s})$ |
| Carboxylic Acid O-H Stretch | $3000-2500(\mathrm{broad}, \mathrm{v})$ |
| Amine N-H Stretch | $3500-3300(\mathrm{~m})$ |
| Nitrile C=N Stretch | $2260-2220(\mathrm{~m})$ |
| Aldehyde C=O Stretch | $1740-1690(\mathrm{~s})$ |
| Ketone C=O Stretch | $1750-1680(\mathrm{~s})$ |
| Ester C=O Stretch | $1750-1735(\mathrm{~s})$ |
| Carboxylic Acid C=O Stretch | $1780-1710(\mathrm{~s})$ |
| Amide C=O Stretch | $1690-1630(\mathrm{~s})$ |
| Amide N-H Stretch | $3700-3500(\mathrm{~m})$ |

