CHEM 3201 Fall 2010 Midterm Examination I open textbook
100 TOTAL MARKS. SHOW YOUR THOUGHTS BECAUSE PART MARKS ARE AVAILABLE!
Budget your time wisely. Look at question 6 last.

NAME: _____
STUDENT #: _____

YOU MUST HAND IN YOUR QUESTION SHEET WITH YOUR EXAM BOOKLET!

1. Indicate how many signals you would expect to see in the ^{1}H decoupled ^{13}C NMR spectrum of each of the following molecules. **12 marks**
a. 1,1-dibromocyclohexane b. *p*-methylphenol c. *N,N*-dimethylpropionamide d. 2-methoxybenzoic acid

2. From the possible compounds with the formula $C_5H_{10}O$ identify the isomers with the following characteristics. **20 marks**

a. 1.08 (s, 9H), 9.48 (s, 1H)
b. 1.11 (d, 6H), 2.14 (s, 3H), 2.58 (septet, 1H)
c. 0.93 (t, 3H), 1.60 (sextet, 2H), 2.13 (s, 3H), 2.40 (t, 3H)
d. 1.25 (s, 6H), 4.3 (s, 4H) (Hint: the second peak is more deshielded than you might expect. You would probably expect it to be closer to 3.6 ppm)

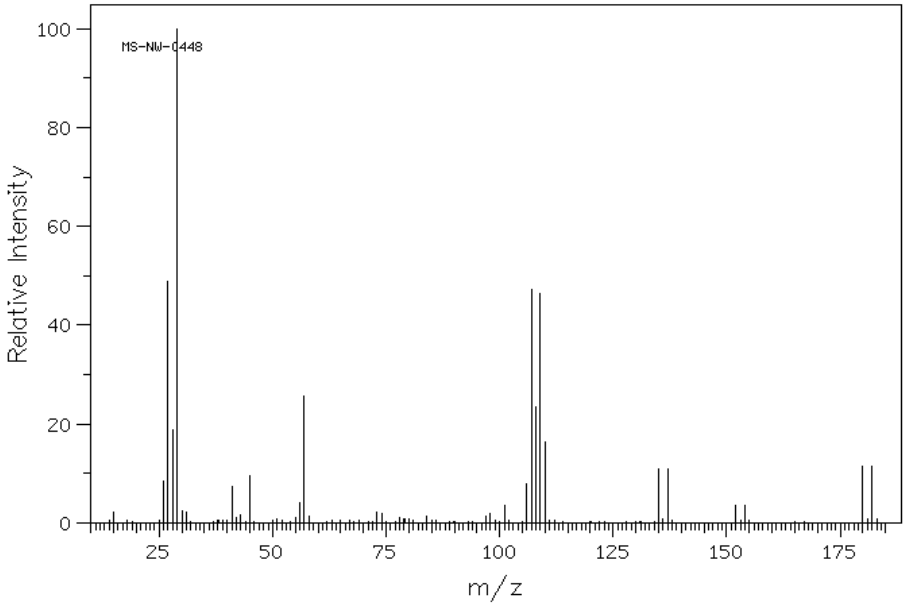
3. Compound "X" gives the following elemental analysis data (by weight): C, 66.60; H, 9.62; N, 11.18, O, 12.63%. The largest ion in the mass spectrum (except isotope peaks) has a mass to charge ratio of 252. **12 marks**
a. Calculate the empirical formula of X.
b. Calculate the molecular formula of X.
c. Determine the index of hydrogen deficiency of X.

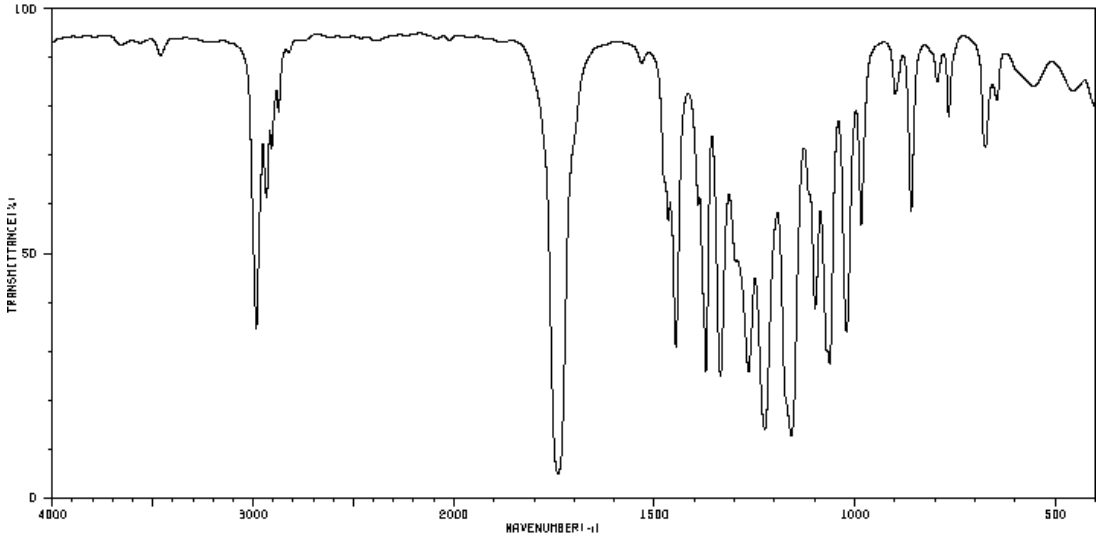
4. The mass spectrum of ethyl benzoate contains *fragment* peaks at m/z = 122 (31%), 106 (9%), 105 (100%), 77 (41%). Provide likely structures for these ions and indicate via arrow pushing how they might arise. **16 marks**

5. Identify each of the following isomers with the molecular formula C_4H_8O, based on ^{13}C NMR and DEPT-135 data (in brackets). For some there may be more than one possible answer. **20 marks**

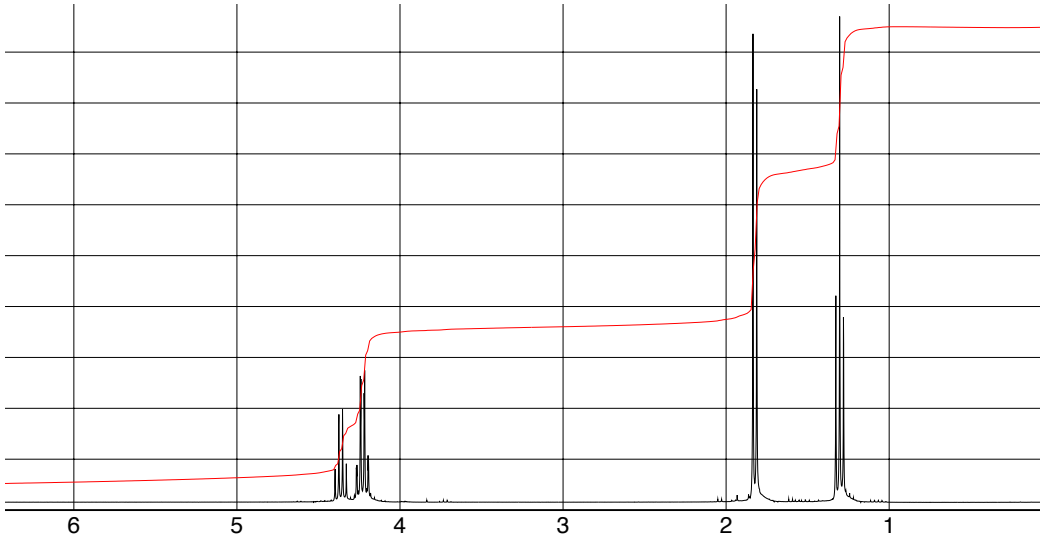
a. 209.3 (no peak), 36.9 (-), 29.4 (+), 7.9 (+)
b. 204.9 (+), 41.1 (+), 15.5 (+)
c.145.0 (no peak), 109.9 (-), 66.5 (-), 19.1 (+)
d. 67.0 (+), 33.5 (-), 12.1 (-)

6. Use the following spectral data to determine the structure of the compound. Part marks are available so write down your thoughts and reasoning. Assign the ^{1}H and ^{13}C NMR peaks. **20 marks**





2983	33	1446	29	1099	37	795	81
2933	58	1391	57	1070	28	766	74
2908	66	1372	24	1063	26	674	68
2873	77	1336	23	1020	32	646	79
1740	4	1268	24	984	53	554	81
1532	86	1225	15	899	79	457	79
1466	66	1168	12	860	67		



peak list (DEPT-135 data in brackets)
170.2 (no peak)
62.0 (–)
40.2 (+)
21.7 (+)
14.0 (+)