Chemistry 3351: Organic Chemistry/3rd Exam/HLMS 252
Tuesday: Nov. 13th from **7:00pm → 9:00pm**

Name:_____ (please print, 1 points)

Note: See Pages 11 and 12 for IR/NMR references

Page	Possible Points	Score
1	1	_____
2	12	_____
3	12	_____
4	10	_____
5	15	_____
6	10	_____
7	10	_____
8	10	_____
9	10	_____
10	10	_____
TOTAL	100	_____

1. Clickers in Action (3 pts each):

1) Which compound has the highest boiling point?

A) Dimethylamine
B) Dimethyl ether
C) Ethanol
D) Ethyl fluoride
E) Propane

2) Order these nucleophiles from strongest to weakest under S_N2 reaction conditions.

A) $I^- > Br^- > H_2O > NH_3$
B) $I^- > Br^- > NH_3 > H_2O$
C) $Br^- > I^- > H_2O > NH_3$
D) $Br^- > I^- > NH_3 > H_2O$

3) The rate law for S_N2 reaction of $CH_3CH_2CH_2Cl$ with NaCN in DMSO is:

A) rate = k $[CH_3CH_2CH_2Cl]$
B) rate = k $[CH_3CH_2CH_2Cl][CN^-]$
C) rate = k $[CH_3CH_2CH_2Cl]^2[CN^-]$
D) rate = k $[CH_3CH_2CH_2Cl][CN^-]^2$

4) Which nucleophile would react at the fastest rate in this reaction?

A) Nucleophile = CH_3OH
B) Nucleophile = CH_3O^-
C) Nucleophile = CH_3S^-
D) Nucleophile = $CH_3CO_2^-$

5) Which alcohol is the relatively strongest acid?

A) CH_3CH_2OH
B) CF_3CH_2OH
C) $CF_3CH_2CH_2OH$
D) $CF_3CH_2CH_2CH_2OH$

6) Predict which alcohol is the relatively strongest acid in aqueous solution.

A) CH_3OH
B) CH_3CH_2OH
C) $(CH_3)_2CHOH$
D) $(CH_3)_3COH$

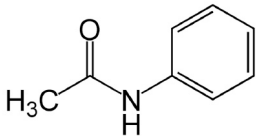
7) How many constitutional isomers of C_4H_9Br are possible? How many of these are primary alkyl bromides?

A) 3, 1
B) 4, 1
C) 4, 2
D) 5, 1
E) 5, 2

8) Which type of intermolecular forces account for the decreasing solubility of alcohols such as methanol, ethanol, propanol, etc. in water and their increasing solubility in hexane as the solvent?

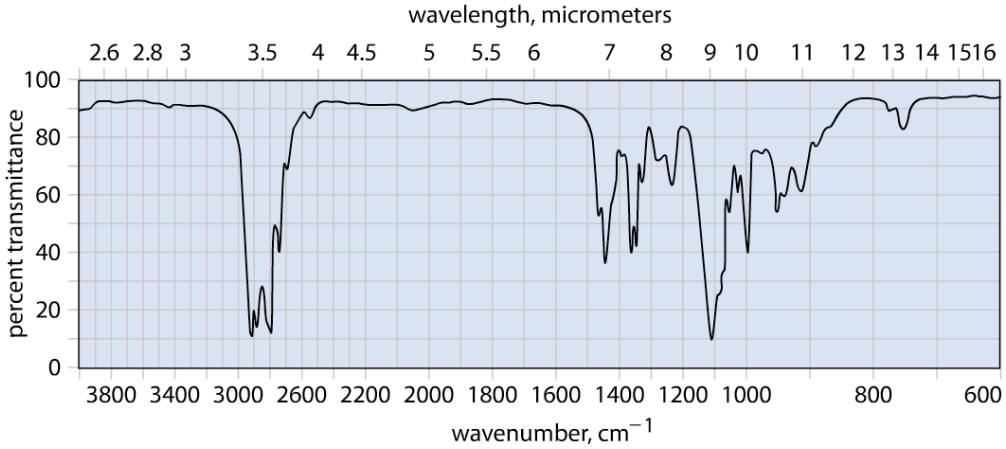
A) van der Waals forces
B) Hydrogen bonding
C) Dipole-dipole forces
D) Ion-dipole forces

2. (5 pts). A widely used undergraduate experiment is the recrystallization of acetanilide from water. Acetanilide (structure shown below) is moderately soluble in hot water, but much less soluble in cold water. Identify one structural feature of the acetanilide molecule that would be expected to contribute positively to its solubility in water and one that would be expected to contribute negatively.



Acetanilide

3. (5 pts).



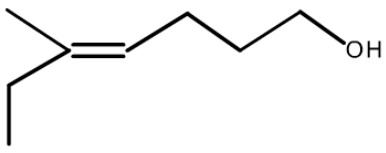
Which compound matches the IR spectrum?

- 1,5-hexadiene
- *trans*-4-octene
- cyclohexane
- 1-methylcyclopentene
- dipropyl ether
- 1-hexen-3-ol
- 3-hexanol

4. (9 pts). Three alkyl halides, each with the formula $C_7H_{15}Br$, have different boiling points. One of the compounds is optically active. Following reaction with Mg in ether, then with water, each compound gives 2, 4-dimethylpentane. After the same reaction with D_2O instead of water, a different product is obtained from each compound. Suggest a structure for each of the three alkyl halides.

5. (6 pts)

Select the correct name for the following compound, including the correct (E) or (Z) designation where appropriate.



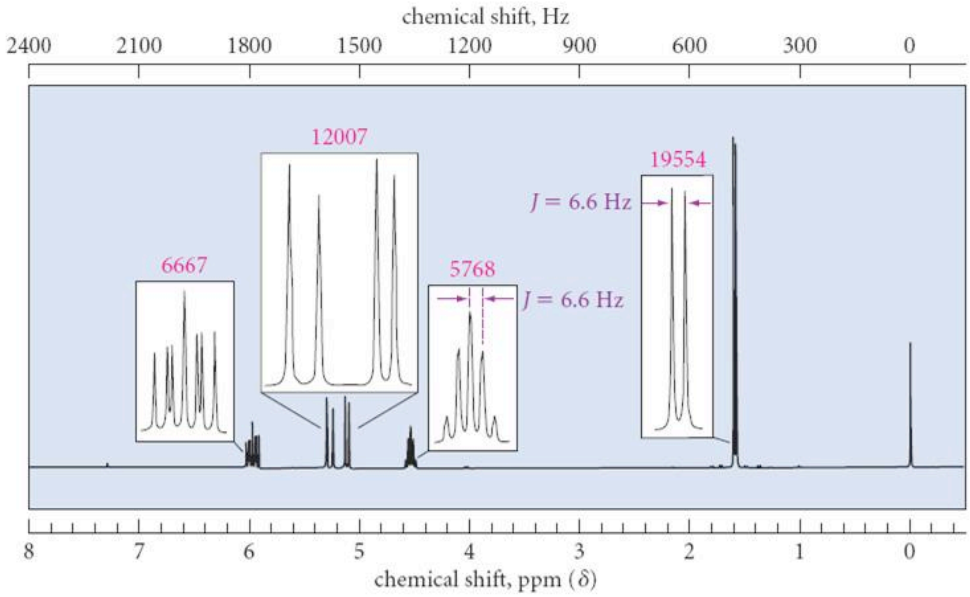
- (Z)-5-methyl-4-hepten-1-ol
- (Z)-2-ethyl-2-hexen-1-ol
- (E)-5-ethyl-4-hexen-1-ol
- (E)-5-methyl-4-hepten-1-ol

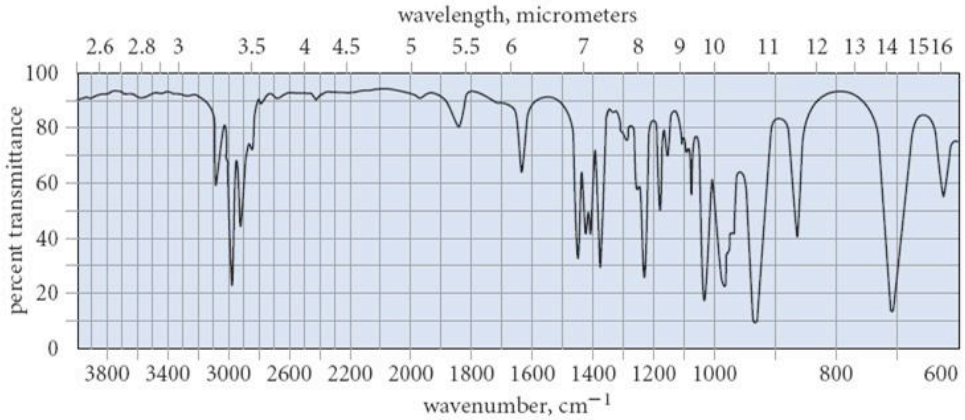
6. (10 pts). Rank the following compounds in order of increasing S_N2 reaction rate with KI in acetone.
   A: $(CH_3)_3CCl$
   B: $(CH_3)_2CHCl$
   C: $(CH_3)_2CHCH_2Cl$
   D: $CH_3CH_2CH_2CH_2Br$
   E: $CH_3CH_2CH_2CH_2Cl$

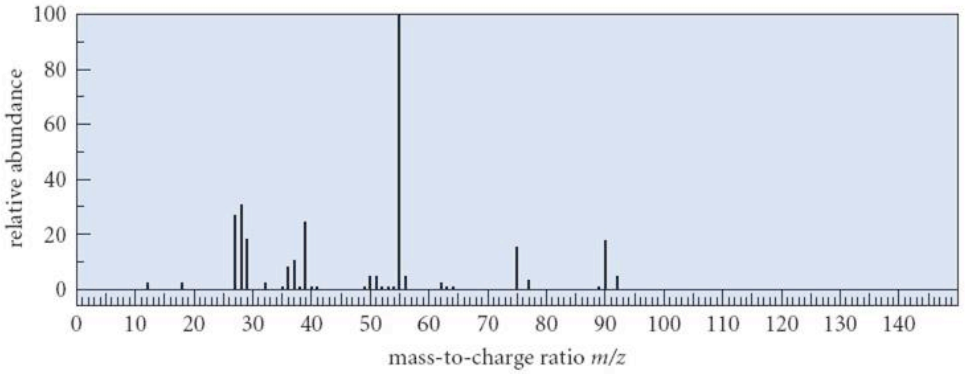
7. (10 pts). The mass spectrum of an organic compound shows the relative abundances of M to be 49.96% and M+1 to be 2.702%. Assuming the peaks are caused by ^{12}C and ^{13}C isotopes, determine the number of carbon atoms in the compound (Natural abundances: ^{12}C is 98.93% and ^{13}C is 1.07%).

8. (10 pts). Give the structure that corresponds to the following molecular formula and ^{1}H NMR spectrum: $C_7H_{16}O_4$: δ=1.93 (t, *J*=6 Hz); δ= 3.35 (s); δ= 4.49 (t, *J*=6 Hz); relative integral 1:6:1

9. (10 pts). Propose a structure for the compound with IR, NMR, and EI mass spectra shown below. See appendix for the common reference values.







10. (10 pts) Tell whether each of the following reactions favors reactants or products at equilibrium (assume that all reactants and products are soluble).

a)

$CH_3Cl + F^- \rightarrow CH_3F + Cl^-$

b)

$CH_3Cl + I^- \rightarrow CH_3I + Cl^-$

c)

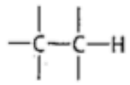
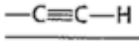
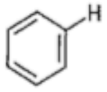
$CH_3Cl + N_3^- \rightarrow CH_3N_3 + Cl^-$

(Hint: the pKa of HN_2 is 4.72)

d)

$CH_3Cl + {}^-OCH_3 \rightarrow CH_3)CH_3 + Cl^-$

hydrogen 1 H 1.0079																	helium 2 He 4.0026
lithium 3 Li 6.941	beryllium 4 Be 9.0122											boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305											aluminium 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078		scandium 21 Sc 44.956	titanium 22 Ti 47.867	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selenium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80
rubidium 37 Rb 85.468	strontium 38 Sr 87.62		yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.60	iodine 53 I 126.90	xenon 54 Xe 131.29
caesium 55 Cs 132.91	barium 56 Ba 137.33	57-70 *	lutetium 71 Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	tungsten 74 W 183.84	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]
francium 87 Fr [223]	radium 88 Ra [226]	89-102 **	lawrencium 103 Lr [262]	rutherfordium 104 Rf [261]	dubnium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [269]	meitnerium 109 Mt [268]	ununnilium 110 Uun [271]	unununium 111 Uuu [272]	ununbium 112 Uub [277]		ununquadium 114 Uuq [289]				

Group	Chemical shift, ppm
	0.7–1.5
	4.6–5.7
	varies with solvent and with acidity of O—H
	1.7–2.5
	6.5–8.5

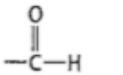
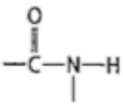
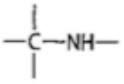
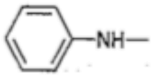
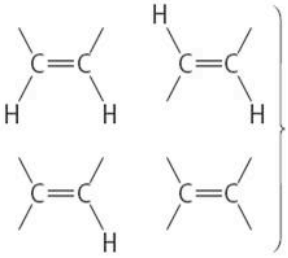
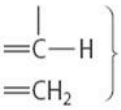
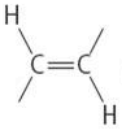
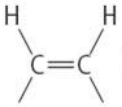
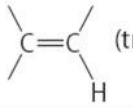
Group	Chemical shift, ppm
	9–11
	7.5–9.5
	0.5–1.5
	2.5–3.5

TABLE 12.1 Regions of the Infrared Spectrum

Wavenumber range, cm^{-1}	Type of absorptions	Name of region
3400–2800	O—H, N—H, C—H stretching	Functional group
2250–2100	C≡N, C≡C stretching	
1850–1600	C=O, C=N, C=C stretching	
1600–1000	C—C, C—O, C—N stretching; various bending absorptions	Fingerprint
1000–600	C—H bending	C—H bending

TABLE 12.2 Important Infrared Absorptions of Alkenes

Functional group	Absorption*
C=C stretching absorptions	
—CH=CH_2 (terminal vinyl)	1640 cm^{-1} (m, sh)
C=CH_2 (terminal methylene)	1655 cm^{-1} (m, sh)
	1660–1675 cm^{-1} (w) (absent in some compounds)
=C—H stretching absorptions	
	3000–3100 cm^{-1} (m)
=C—H bending absorptions	
—CH=CH_2 (terminal vinyl)	910, 990 cm^{-1} (s) two absorptions
C=CH_2 (terminal methylene)	890 cm^{-1} (s)
 (*trans*-alkene)	960–980 cm^{-1} (s)
 (*cis*-alkene)	675–730 cm^{-1} (br) (ambiguous and variable for different compounds)
 (trisubstituted)	800–840 cm^{-1} (s)

**Intensity designations:* s = strong; m = moderate; w = weak
Shape designations: sh = sharp (narrow); br = broad (wide)