Chem 341-02/341-03 EXAM 2 October 21, 2015

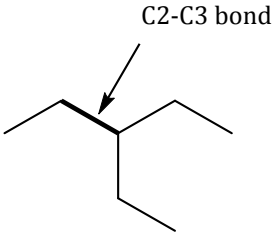
Dr. Richter

PRINT NAME_____.

SIGN NAME_____.

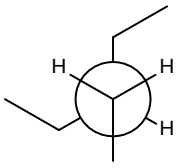
You are required to answer all questions. Please write legibly and draw clearly. Points will be deducted for illegible and unclear answers. Please answer in the space provided after each question. Use the reverse side if you need more space. There are a total of 100 points possible for this exam and the value of each section is shown in parenthesis beside that question. Note that some of the questions may give you a choice. Do only the number of choices asked for. Extra answers will not be graded. ***READ ALL QUESTIONS CAREFULLY AND APPORTION YOUR TIME APPROPRIATELY.***

1. Consider the rotation about the C2-C3 bond of 3-ethylpentane (see below) and answer **A-D**. **(20)**



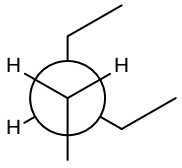
3-ethylpentane

Below are the Newman projections for 3 staggered conformations of 3-ethylpentane with respect to the C2-C3 bond.



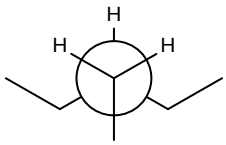
1

2



3

4



5

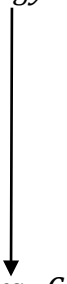
6

A. Draw the three missing eclipsed conformers (**2**, **4**, and **6**). *Please draw your answers in the boxes below.* **(6)**

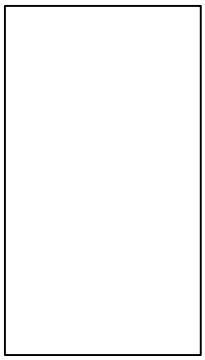
Conformer 2	**Conformer 4**	**Conformer 6**

B. In the box below, list conformers **1-6** *from highest in energy to lowest in energy*. <u>If two conformers are energetically equivalent then list them ***next*** to one another</u>. **(6)**

Highest Energy Conformer(s)



Lowest Energy Conformer(s)



C. At room temperature, in which conformation(s) (**1-6**) would you expect 3-ethylpentane to exist the majority of the time? *Circle all that apply.* **(4)**

1 **2** **3** **4** **5** **6**

D. Recall that H,H eclipsing interactions cost 4.0 kJ/mol of energy *per interaction*.

Suppose the energetic costs of a few other interactions are as shown in the table below. (*You can assume gauche interactions involving H have no energetic cost*).

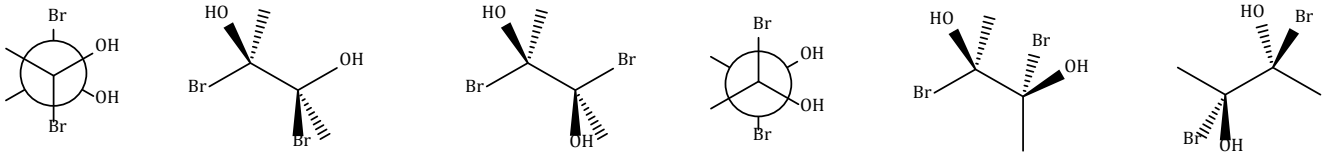
Interaction	**Energetic "Cost" (kJ/mol)**
H, CH_2CH_3 eclipsing	8.0
CH_3, CH_2CH_3 eclipsing	13.0
CH_3, CH_2CH_3 gauche	7.0
CH_3, H eclipsing	6.0

Using this information, what is the difference in energy (kJ/mol) between

i. conformer **3** and conformer **6**? **(2)**

ii. conformer **5** and conformer **2**? **(2)**

Answer questions 2 - 5 regarding the structures A-F below. (16)



A **B** **C** **D** **E** **F**

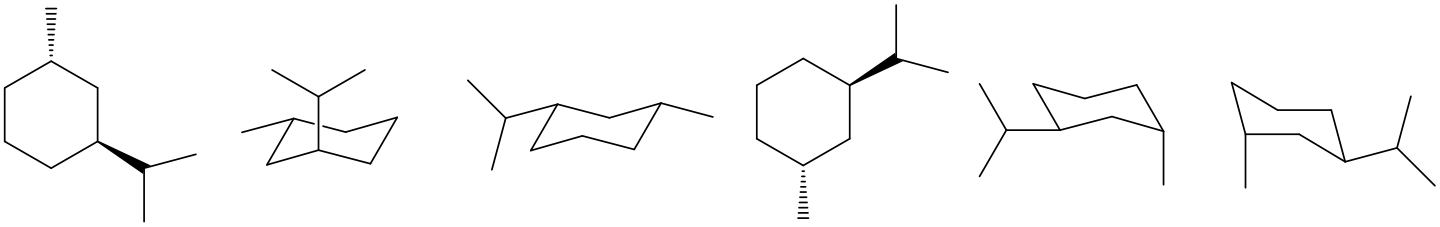
2. From the structures **A-F** above, identify any **one** (**1**) pair of enantiomers. **(4)**

3. From the structures **A-F** above, identify any **one** (**1**) pair of diastereomers. **(4)**

4. From the structures **A-F** above, identify any **one** (**1**) *meso* structure. **(4)**

5. From the structures **A-F** above, select two that, if mixed in equimolar proportions, would yield an optically active mixture. **(4)**

For questions 6-10, consider the structures A-F below and circle "True" or "False." (15)



A **B** **C** **D** **E** **F**

6. Structures **A** and **E** are identical. *True* *False*

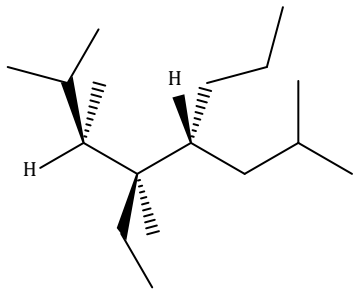
7. Structure **C** has no enantiomer. *True* *False*

8. Structures **C** and **D** are diastereomers. *True* *False*

9. Molecules **A** and **D** would have the same boiling point. *True* *False*

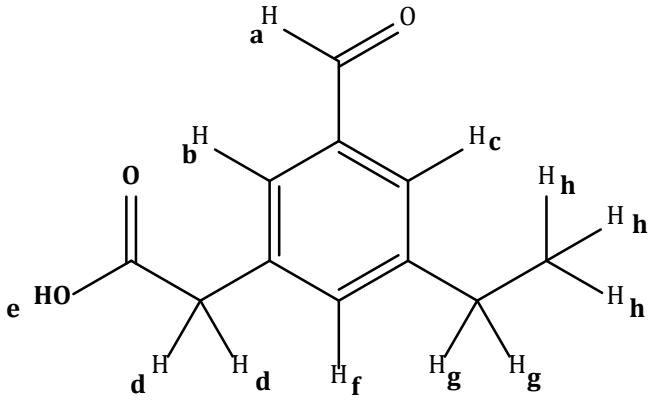
10. Molecule **B** is in its preferred chair conformation. *True* *False*

11. What is the correct IUPAC name for the following molecule? *Circle your answer*. **(6)**



a. (3S, 4R, 5R)-4-ethyl-2,3,7-trimethyl-5-propyloctane
b. (3R, 4R, 5R)-4-ethyl-2,3,7-trimethyl-5-propyloctane
c. (1R, 2R, 3R)-2-ethyl-1-isopropyl-1,2,5-trimethyl-3-propylhexane
d. (3S, 4R, 5R)-5-ethyl-2,6,7-trimethyl-4-propyloctane
e. (3R, 4R, 5R)-4-ethyl-5-isobutyl-2,3-dimethyloctane

Question 12 relates to the molecule below. **(15)**



On the drawing above, like groups of protons are labeled the alphabetically.

12. Predict and fill in the proton NMR data for the above molecule. List the data in approximate order of increasing chemical shift. Use the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sext = sextet, sept = septet, m = multiplet.

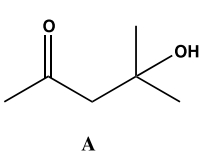
Lowest Chemical Shift

↓

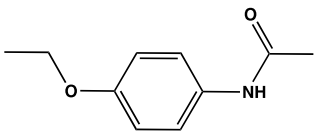
Highest Chemical Shift

Splitting Pattern	Integration Value	Assignment

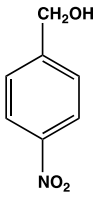
Answer questions 13-15 regarding structures **A-F** below.



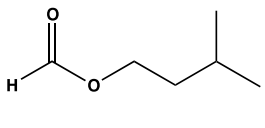
A



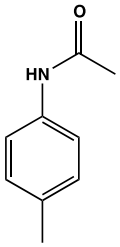
B



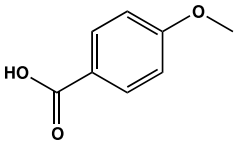
C



D



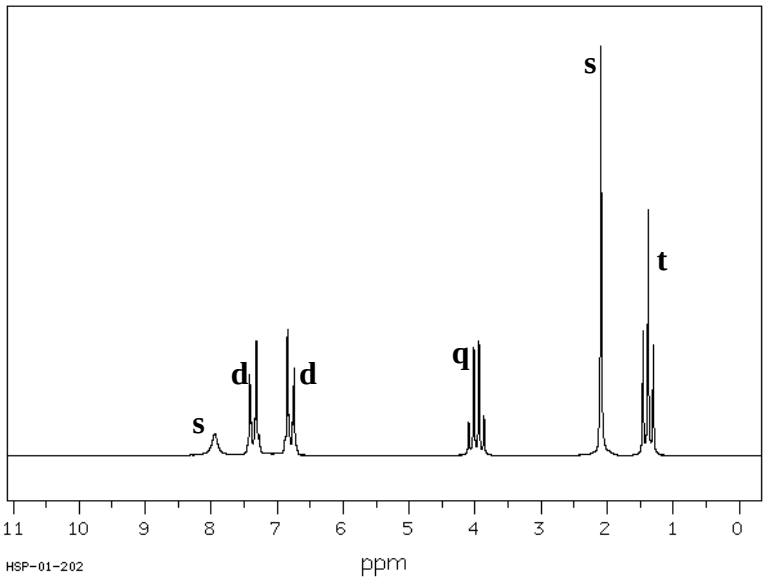
E



F

13. Which of the above structures (**A-F**) matches the ^{1}H NMR spectrum below? *Circle your answer.* **(4)**

A **B** **C** **D** **E** **F**



14. How many signals would you expect to see in the ^{1}H NMR spectrum of compound **D**? *Circle your answer.* **(4)**

3 **4** **5** **6** **7**

15. The ^{1}H NMR spectrum of one of the compounds **A-F** is found to have the following integration values: 2.1:0.7:1.4:1.4:2.1. The spectrum must be that of which compound? *Circle your answer.* **(4)**

A **B** **C** **D** **E** **F**

16. Four unique stereoisomers exist for the molecule 1-ethyl-2,3-dimethylcyclopropane.

A. Draw a stereoisomer of 1-ethyl-2,3-dimethylcyclopropane that is **achiral**. **(4)**

B. Draw a stereoisomer of 1-ethyl-2,3-dimethylcyclopropane that would give 7 signals in an ^{1}H NMR experiment. **(4)**

17. Indicate if each the following statements **A-D** regarding NMR spectroscopy is true or false. *Circle your answer.* **(8)**

A. During an NMR spectroscopy experiment, electromagnetic radiation in the radiofrequency range is used to cause nuclear spin excitations. *True* *False*

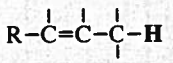
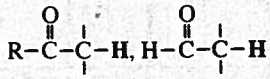
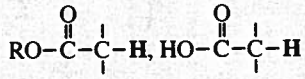
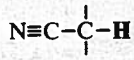
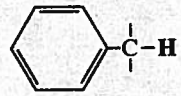
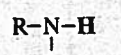
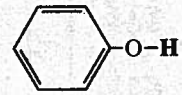
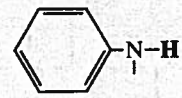
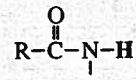
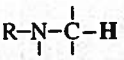
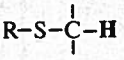
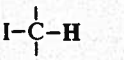
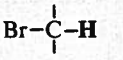
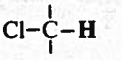
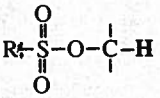
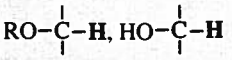
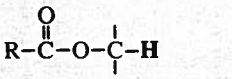
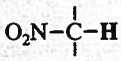
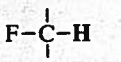
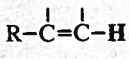
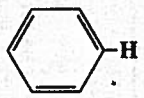
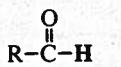
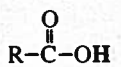
B. An NMR signal that appears at higher ppm value is said to be upfield from a signal that appears at a lower ppm value. *True* *False*

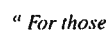
C. In an NMR spectrum, nuclei that are shielded appear at lower ppm values than nuclei that are deshielded. *True* *False*

D. The amount of energy required to cause "resonance" during an NMR experiment is directly proportional to the strength of the external magnetic field. *True* *False*

APPENDIX 2

Approximate ^{1}H Chemical Shift Ranges (ppm) for Selected Types of Protons[a]

$R-CH_3$		0.7 – 1.3
$R-CH_2-R$		1.2 – 1.4
R_3CH		1.4 – 1.7
		1.6 – 2.6
		2.1 – 2.4
		2.1 – 2.5
		2.1 – 3.0
		2.3 – 2.7
$R-C\equiv C-H$		1.7 – 2.7
$R-S-H$	var	1.0 – 4.0[b]
	var	0.5 – 4.0[b]
$R-O-H$	var	0.5 – 5.0[b]
	var	4.0 – 7.0[b]
	var	3.0 – 5.0[b]
	var	5.0 – 9.0[b]
		2.2 – 2.9
		2.0 – 3.0
		2.0 – 4.0
		2.7 – 4.1
		3.1 – 4.1
		ca. 3.0
		3.2 – 3.8
		3.5 – 4.8
		4.1 – 4.3
		4.2 – 4.8
		4.5 – 6.5
		6.5 – 8.0
		9.0 – 10.0
		11.0 – 12.0

[a] *For those hydrogens shown as*  *if that hydrogen is part of a methyl group (CH_3) the shift is generally at the low end of the range given, if the hydrogen is in a methylene group ($-CH_2-$) the shift is intermediate, and if the hydrogen is in a methine group (*  *) the shift is typically at the high end of the range given.*

[b] *The chemical shift of these groups is variable, depending not only on the chemical environment in the molecule, but also on concentration, temperature, and solvent.*

THE PERIODIC TABLE

	1	2											13	14	15	16	17	18
1	1 H 1.008																	2 He 4.003
2	3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
3	11 Na 22.99	12 Mg 24.31	3	4	5	6	7	8	9	10	11	12	13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
4	19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.87	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.38	31 Ga 69.72	32 Ge 72.63	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
5	37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.96	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
6	55 Cs 132.9	56 Ba 137.3	57 La 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209)	85 At (210)	86 Rn (222)
7	87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (265)	105 Db (268)	106 Sg (271)	107 Bh (270)	108 Hs (277)	109 Mt (276)	110 Ds (281)	111 Rg (280)	112 Cn (285)	113 Uut (284)	114 Uuq (289)	115 Uup (288)	116 Uuh (293)	117 Uus (294)	118 Uuo (294)

58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (145)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.1	71 Lu 175.0
90 Th 232.0	91 Pa 231.0	92 U 238.0	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

Based on IUPAC 2009, 2007 (publ 2011, 2009).