First Three Letters of Last Name:

CHEM 14C-1
Final- Spring 2018

Name:_____

Student ID:_____

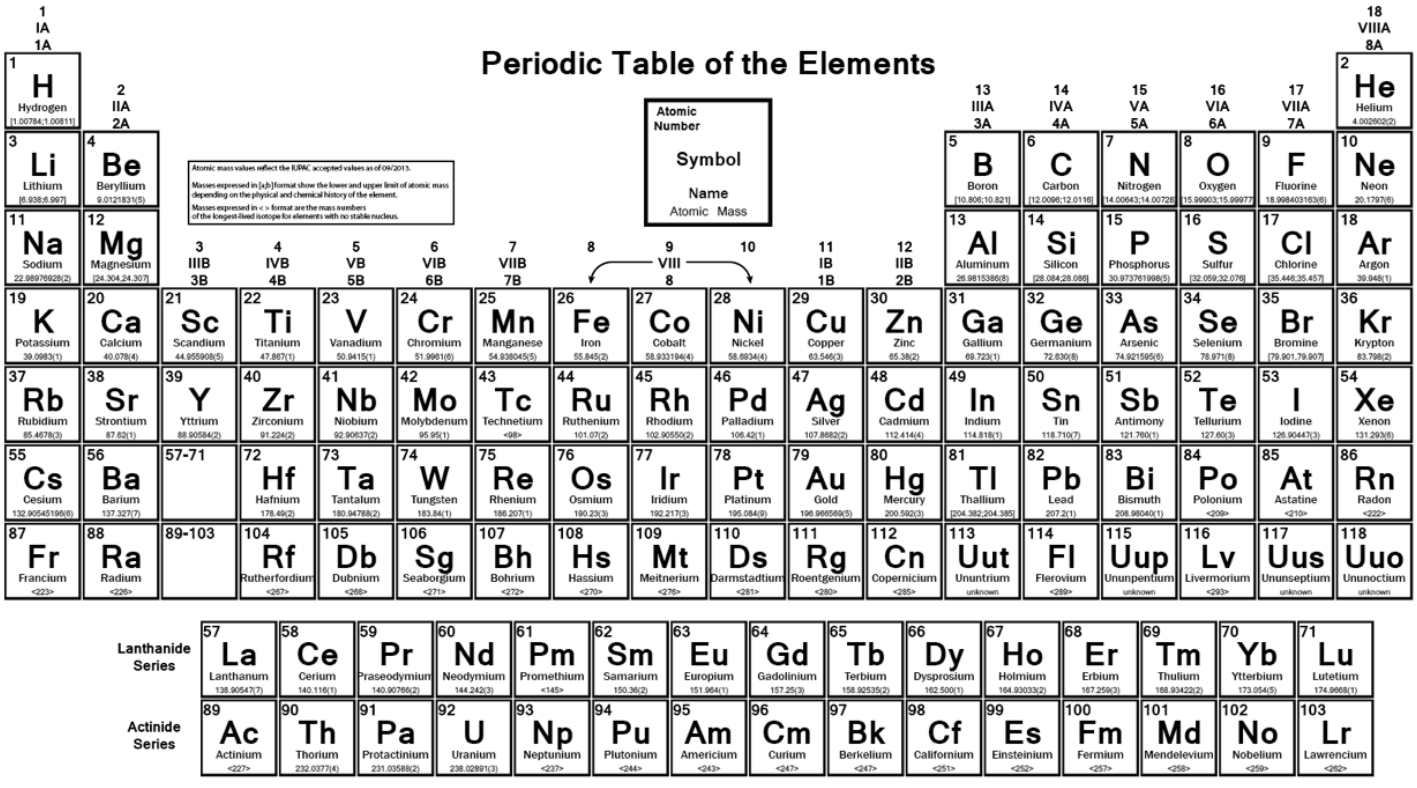
TA Name and Section:_____

Key

Instructions:

1. **Write your full name on every page.**
2. **This is a closed book exam. The use of notes, cell phones, or other devices will not be allowed during exam.**
3. **You may use model sets brought in a clear ziplock bag.**
4. **Answer questions as concisely as possible. Nothing over the word in limit will be graded.**
5. **For full credit show your work, partial credit will be awarded.**
6. **Turn in your test to your TA's folder.**

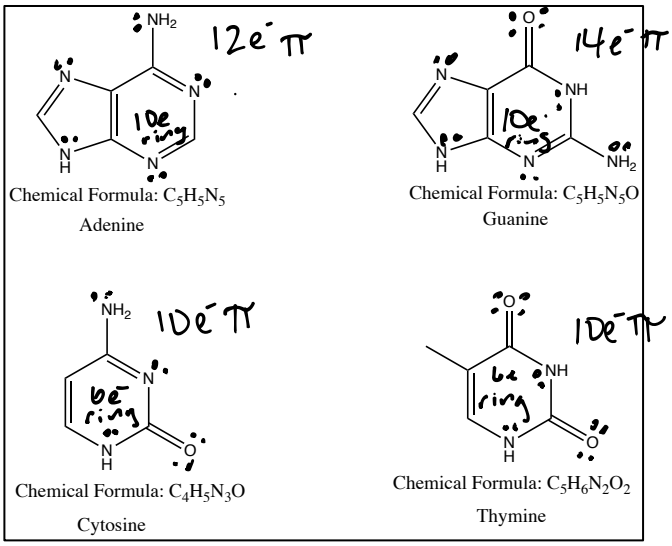
Section	When?	TA
1A	Mon. 1:00–1:50 pm	Shanlin
1B	Mon. 2:00–2:50 pm	Ruxi
1C	Tues. 9:00–9:50 am	Shanlin
1D	Tues. 1:00–1:50 am	Zeeshan
1E	Wed. 9:00–9:50 am	Ruxi
1F	Wed. 2:00–2:50 pm	Ruxi
1G	Wed. 4:00–4:50 pm	Shanlin
1H	Thurs. 9:00–9:50 am	Zeeshan
1I	Thurs. 12:00–12:50 pm	Zeeshan
1J	Fri. 9:00–9:50 am	Dayanni
1K	Fri. 12:00–12:50 pm	Dayanni
1L	Fri. 2:00–2:50 pm	Dayanni



BLANK for scratch work

Name:_____ Student ID:_____

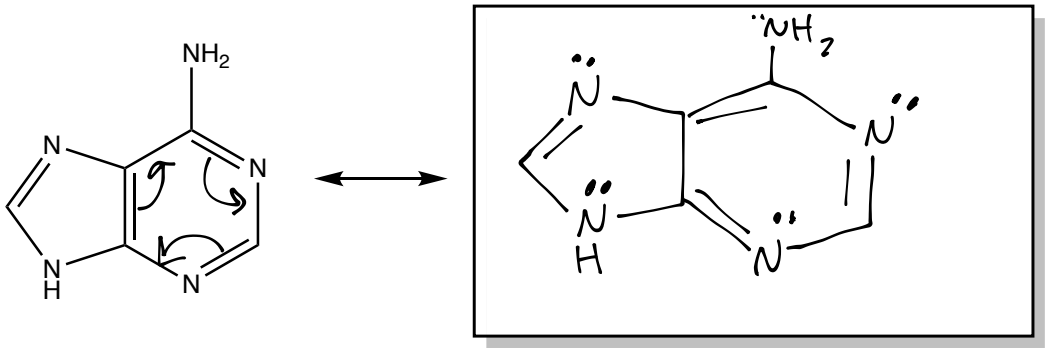
This quarter we did not cover nucleic acids in lecture. Let's combine everything we have learned in 14C to determine structural characteristics of nucleic acids and their derivatives. Four nucleic acids incorporated in DNA are given in the box.



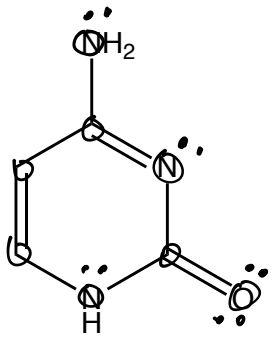
1. (12 pts) Circle the first letter of the nucleic acid (A, G, C, or T) that correctly answers the statement. If none of nucleic acids answer the question, circle none. If there is a tie, circle as many of the nucleic acids that meet the requirement.

   a. Nucleic acid(s) with the most delocalized pi electrons: A T C (G) none
   b. Nucleic acid(s) that is/are aromatic: (A) (T) (C) (G) none
   c. Nucleic acid(s) capable of being a hydrogen bond donor and acceptor: (A) (T) (C) (G) none
   d. Nucleic acid(s) which has/have chiral carbons: A T C G (none)
   e. Nucleic acid(s) with the least delocalized pi electrons: A (T) (C) G none
   f. Nucleic acid(s) with the lowest M+1 intensity: A T (C) G none

2. (4 pts) Draw a resonance structure of adenine that is **significant as possible**; include all lone pairs and formal charges.



3. (10 pts) For cytosine, answer the questions (a-e).



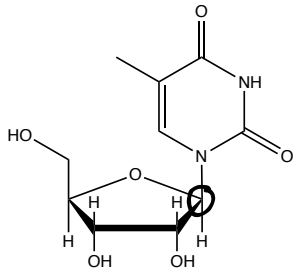
   a. Circle all the conjugated atoms in the structure.
   b. Name three functional groups in the molecule:

      alkene, amine, amide

   c. How many lone pairs are in the molecule? 5
   d. How many sp^3 N atom(s) is/are in the structure? 0
   e. How many N atom(s) have a nonzero formal charge? 0

Page 1 score

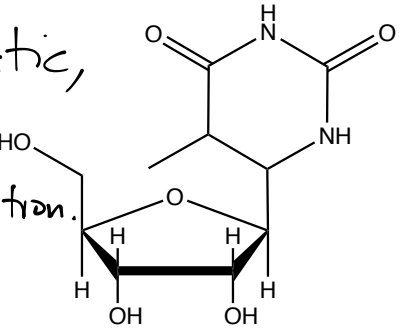
4. (18 pts) Before being incorporated into DNA, nucleic acids are bonded to a sugar molecule to become nucleosides. Answer the following questions (a-g) for ribothymidine given below:



a. Circle the anomeric carbon in the sugar portion of ribothymidine.
b. Is the nucleic acid bonded through an α or β glycosidic linkage? Circle α or (β)
c. Give the full name of the sugar molecule incorporated in ribothymidine (note: this should have three pieces of information in the name): D-ribofuranose
d. What is the strongest noncovalent force in ribothymidine? H-bonding
e. How many chiral carbons does ribothymidine have? 4

f. A fellow student proposes the following structure for ribothymidine. How would you convince this student, using structural characteristics learned this quarter, that the structure is incorrect? ***Answer in 30 words or less***.

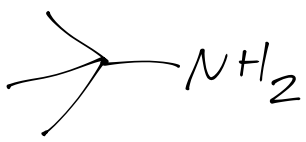
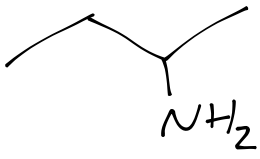
This structure is not aromatic, thus has a higher energy and is an unlikely connection.



g. Using our zone analysis, what stretches in the IR could you use to determine the difference between ribothymidine and thymine? Explain your reasoning in ***20 words or less***.

Zone 1 OH stretching

5. (8 pts) Draw two isomers in the boxes below for $C_4H_{11}N$; one isomer with two signals in a NMR spectrum and one with five signals in a NMR spectrum. Your molecule should have zero formal charge.

Two signals in NMR	5 signals in NMR
	

other answers accepted

Page 2 score

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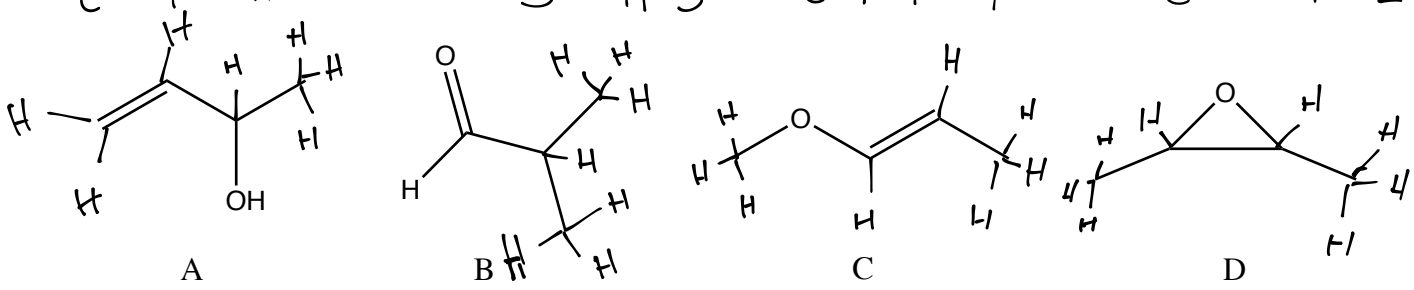
Using the following molecules (A-D) to answer questions 6-8.

^{13}C-4 ^{1}H-6 ^{13}C-3 ^{1}H-3 ^{13}C-4 ^{1}H-4 ^{13}C-2 ^{1}H-2



A B C D

Zone 1,2,5 Zone 2,4 Zone 2,5 Zone 2

6. (2 pts) Which type of isomers are these compounds? constitutional

7. (16 pts) Put a check mark in the box that answers the statement correctly. If there is a tie, check as many boxes as needed. If none of the molecules fit, check 'none'.

	Molecule A	**Molecule B**	**Molecule C**	**Molecule D**	**None**
Molecule with the highest boiling point.	✓				
The molecule(s) having proton(s) whose ^{1}H-NMR chemical shift(s) is/are influenced by magnetic induction.	✓	✓	✓		
The molecule(s) having fewest number of ^{1}H-NMR signals in its spectrum.				✓	
The molecule(s) whose IR spectrum has peaks appear only in zone 2 (excluding fingerprint region).				✓	
The molecule(s) having highest number of ^{1}H-NMR signals in its spectrum.	✓				
The molecule(s) having highest number of ^{13}C-NMR signals in spectrum.	✓		✓		
The molecule(s) whose IR spectrum has peaks appearing in 4 zones (excluding fingerprint region).					✓
The molecule(s) having equal number signals in ^{13}C-NMR and ^{1}H-NMR spectra.		✓	✓	✓	

8. (4 pts) If you only had a limited sample of molecules A-D, which spectroscopy technique would you **not** use to gain information about the sample. Answer choices: mass spectrometry, infrared spectroscopy, ^{1}H-NMR, and ^{13}C-NMR. ***Explain your reasoning in 20 words or less.***

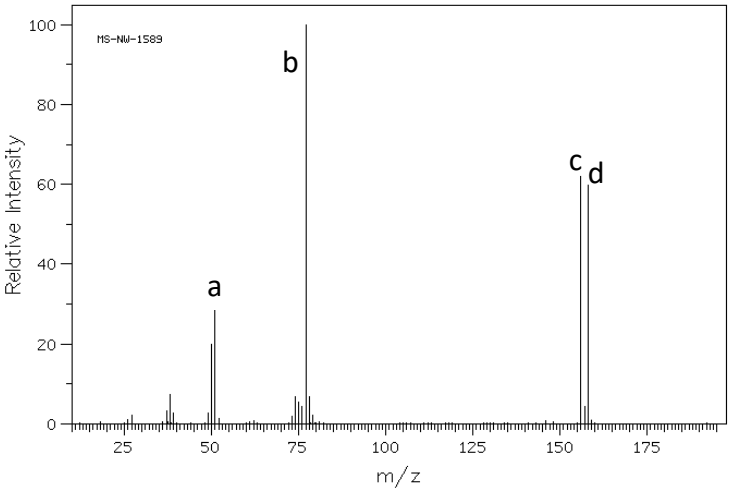
Mass spec - destroys the sample

9. (4 pts) In which of the following methods does a magnetic field play a role in acquiring data about a sample? Circle all of the answer choices that apply.

mass spectrometry infrared spectroscopy ^{1}H-NMR ^{13}C-NMR

Page 3 score

10. (10 pts) Name the peaks (a-d) for the mass spectrum below.



Identity of peak

a. fragment ion

b. base peak

c. molecular ion peak

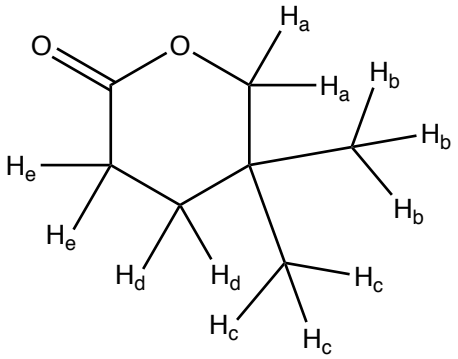
d. M+2 peak

e. Circle the atom this compound contains:

S Cl (Br) cannot determine

M+2 ≈ 100% of M

11. (10 pts) For the following molecule, predict the NMR splitting and integral for each H_{a-e} in the box below. Example for an equivalent H set: H_x & H_y = doublet, 2.0.



Splitting and Integration:

H_a: singlet, 1.0

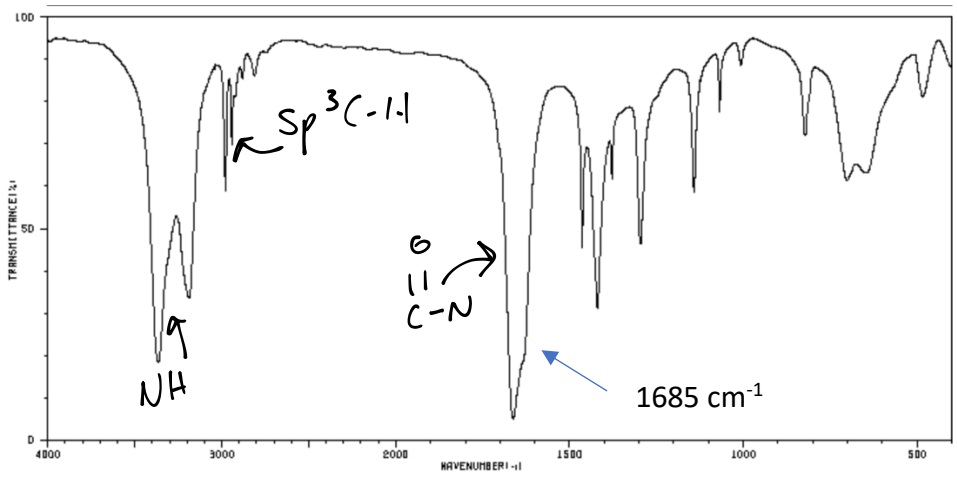
H_b & H_c: singlet, 3.0

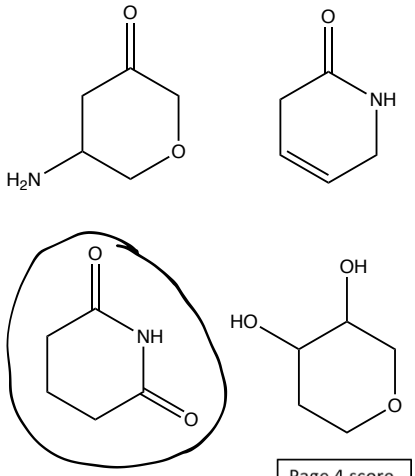
H_d: triplet, 1.0

H_e: triplet, 1.0

a. Which is the most deshielded H? Circle (H_a) H_b H_c H_d H_e cannot determine

12. (10 pts) For the IR spectrum below, circle the compound that correct matches the spectrum and **label stretches on the IR spectrum present** in zones 1-5 you used to make the determination.





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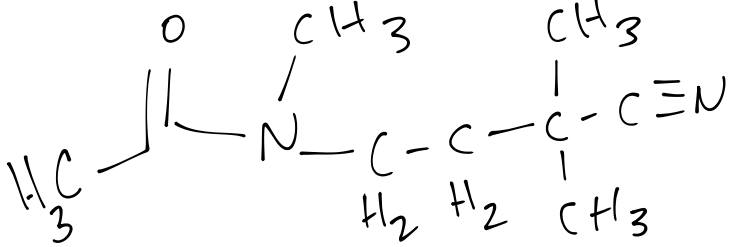
13. (42 pts) Deduce the structure that corresponds to the spectral data on the following pages. Write your final answer in the box. A correct answer is worth full credit. If the answer is incorrect, your analysis of the spectra can be worth significant partial credit, so show your work clearly in the space below each set of data only. **Answers outside of these places will be ignored**.

Final Structure Box



(5 pts) Mass Spectrum: m/z = 168 (M; 100%) m/z = 169 (9.7%), and m/z = 170 (0.3%). No F or I.

even N = 0, 2, 4 M+1 : $\frac{9.7\%}{1.1\%} = 8.8 \rightarrow 9C$ M+2 < 4% no S, Cl, Br

168 amu - (9 x 12 amu) = 60 amu N, O, H

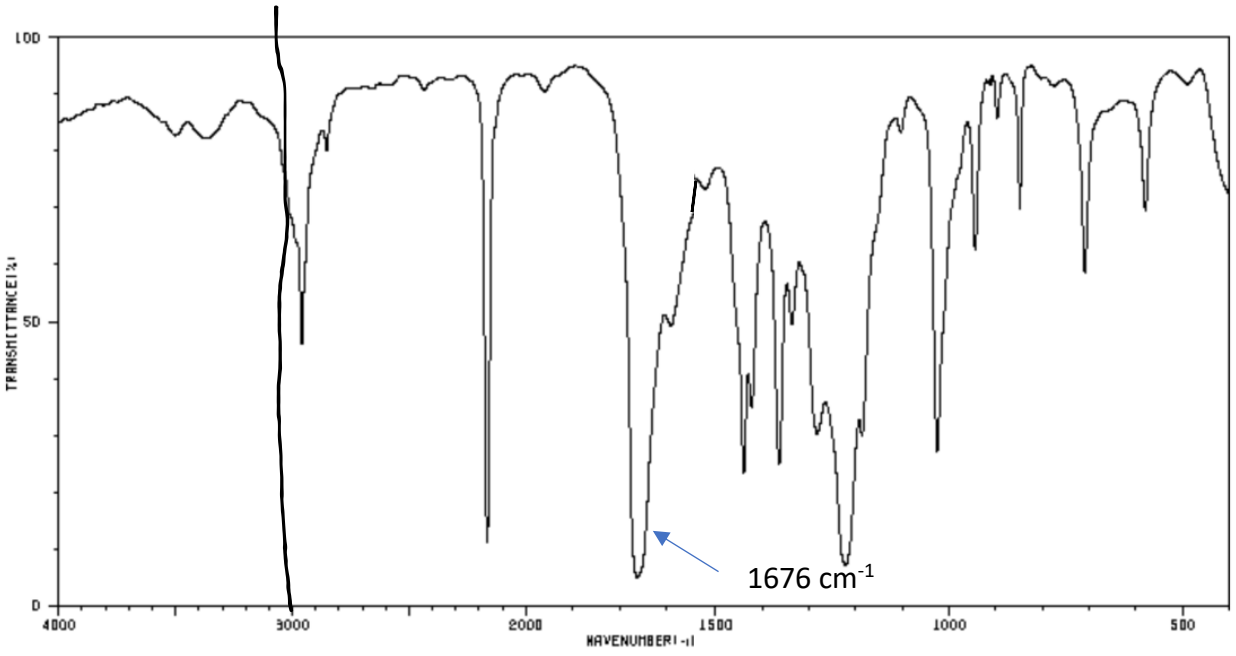
D	N	60 - O - N = H	formula	notes
0	0	60 - 0 - 0 = 60	C_9H_{60}	violates H rule
1	0	61 - 16 - 0 = 44	$C_9H_{44}O$	"
2	0	61 - 32 - 0 = 28	$C_9H_{28}O_2$	"
3	0	61 - 48 - 0 = 12	$C_9H_{12}O_3$	possible
0	2	61 - 0 - 28 = 32	$C_9H_{32}N_2$	violates H rule
1	2	61 - 16 - 28 = 16	$C_9H_{16}N_2O$	fits NMR
2	2	61 - 32 - 28 = 0	$C_9N_2O_2$	NMR shows H
0	4	61 - 0 - 56 = 5	$C_9H_5N_4$	possible

$C_9H_{16}N_2O$

Write in the box **one** formula that is consistent with the MS and is not rejected due to other reasons.

DoU: $9 - \frac{16}{2} + \frac{2}{2} + 1 = 3$

(10 pts) IR:



IR workspace:

OH - absent

NH - absent

C≡C-H - absent

sp^2 C-H - absent

sp^3 C-H - present


C-H - absent


C-OH - absent

C≡C - possible

C≡N - possible


C-O - only one O


C-H - no peak in zone 2

ketone - too low for ketone


C-OH - only one O


C-N - fits

(note no NH stretching)

alkene - absent

benzene - absent

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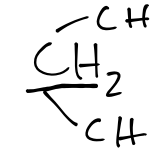
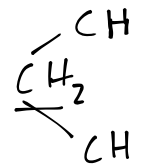
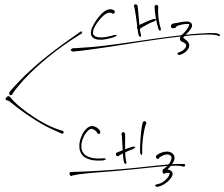
Anything written outside the boxes on this page will be ignored. Write only ^{1}H-NMR implications in the ^{1}H-NMR boxes.

(15) ^{1}H-NMR:

Chemical Shift	Splitting	Integral	#H	Implications
2.9 ppm	Singlet n = 0	3.0		$-CH_3$
2.7 ppm	Triplet n = 2	2.0		CH_2CH_2 or  or 2x $CHCH_2$
2.3 ppm	Singlet n = 0	3.0		$-CH_3$
1.8 ppm	Triplet n = 2	2.0		CH_2CH_2 or  or 2x $CHCH_2$
1.4 ppm	Singlet n = 0	6.0		

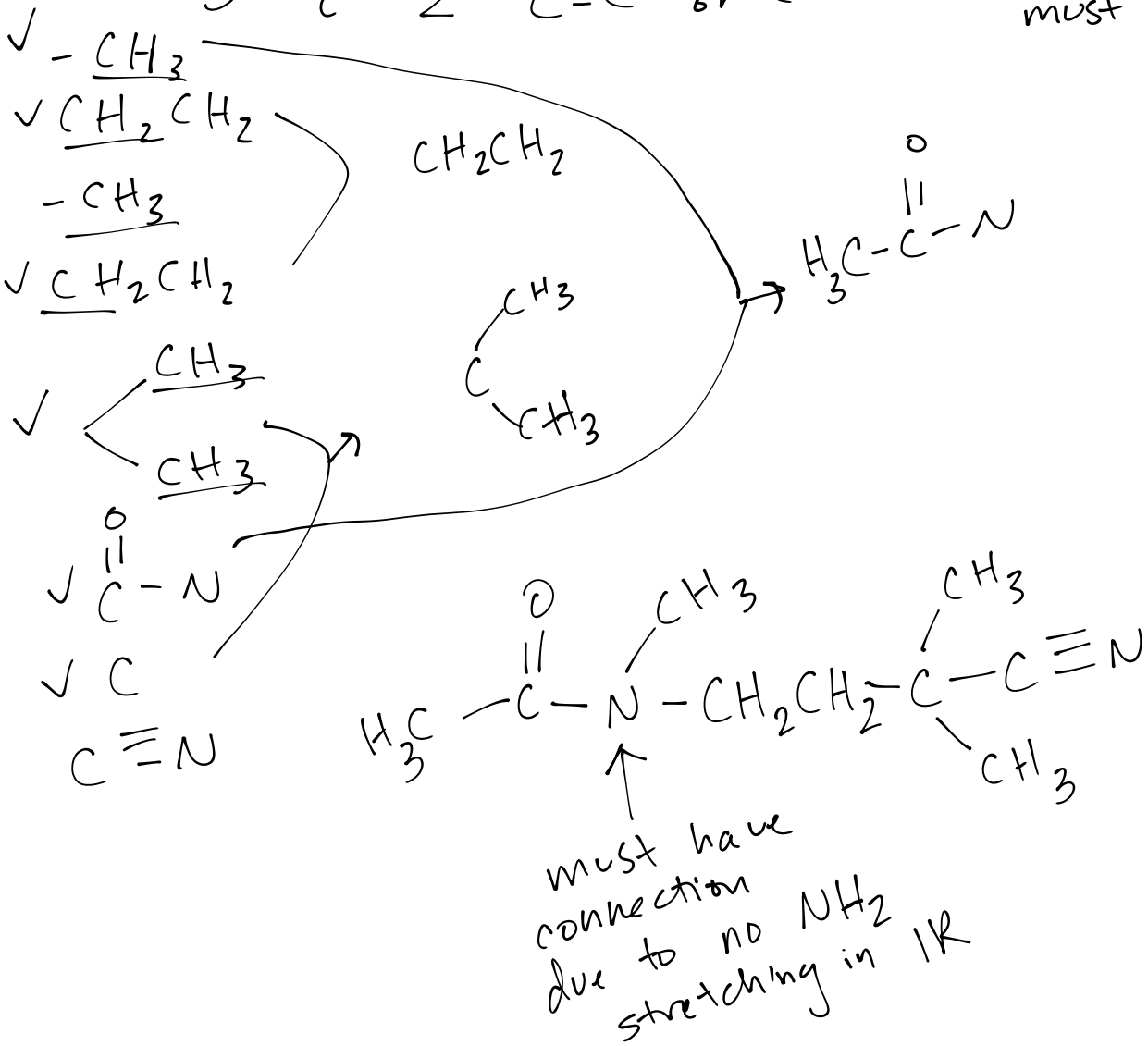
$CH_3 + CH_2 + CH_3 + CH_2 + 2xCH_3$

$= C_6H_{16}$

Blank space for assembling molecule:

Atoms check: $C_9H_{16}N_2O - C_6H_{16} - \overset{O}{\overset{\|}{C}} - N = 2C + N$

DoU check: $3 - \overset{O}{\overset{\|}{C}} = 2 \quad C\equiv C \text{ or } C\equiv N$ ← only 2 C leftover must be $C\equiv N$



must have connection due to no NH_2 stretching in IR

* cannot swap $C\equiv N$ & CH_3 then NMR would have Singlet with integral of 9.0

Name:_____ Student ID:_____

Page	Points
1	
2	
3	
4	
Combo Spectra	
Discussion Section Bonus	
Total	