

1. (6 pts.) What property of the proton allows the proton to be investigated using NMR? 1. _____

2. _____

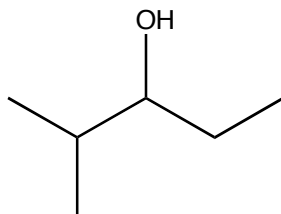
2. (4 pts) What does NMR stand for? 3. _____

4. _____

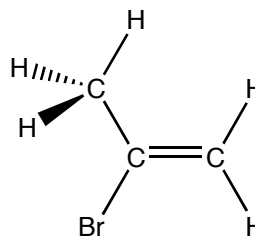
3. (4 pts. each) Identify the chemically inequivalent protons on the following molecules (label them with letters. It is not necessary to correlate lettering with chemical shift). 5. _____

6. _____

a.



b.

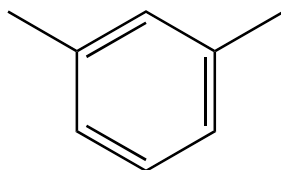


7. _____

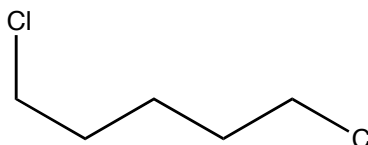
8. _____

9. _____

c.



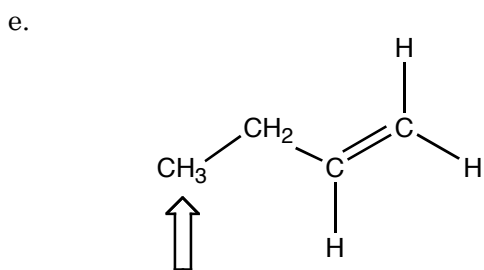
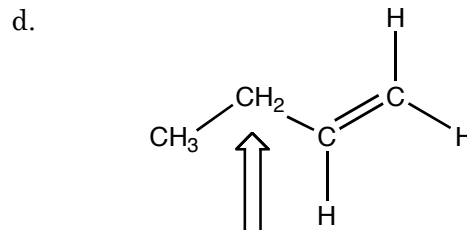
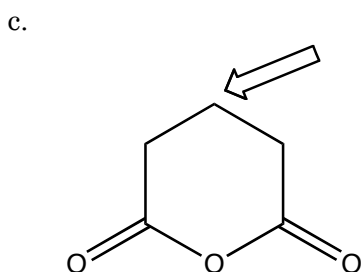
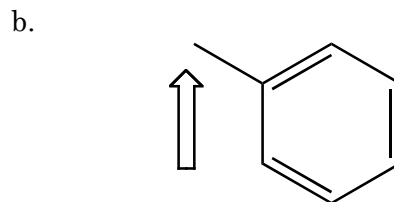
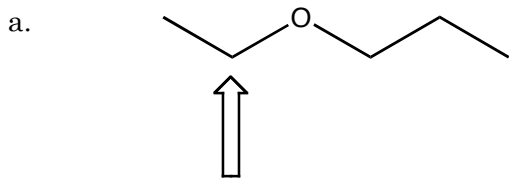
d.



4. (4 pts. each) Using the labeling scheme from question 3, determine the relative area of the peaks that you expect to find in the NMR spectra of the molecules.

a.	b.
c.	d.

5. (4 pts. each) For each of the indicated hydrogen atoms, determine the multiplicity (the splitting pattern) observed.



6. On the following page, you will find an IR spectrum and an NMR spectrum for a compound with the following formula C_4H_9Br .

a. (6 pts.) What does the formula tell you about the structure of the molecule? That is, are there any π bonds or rings? Explain.

b. (6 pts.) How does the IR spectrum support your response to part a.

c. (12 pts.) Determine the structure of the molecule, and assign the peaks in the NMR spectrum to the appropriate H atoms.

¹H NMR

ppm Int.

3.308 604

3.293 608

2.007 47

2.006 50

1.991 99

1.974 127

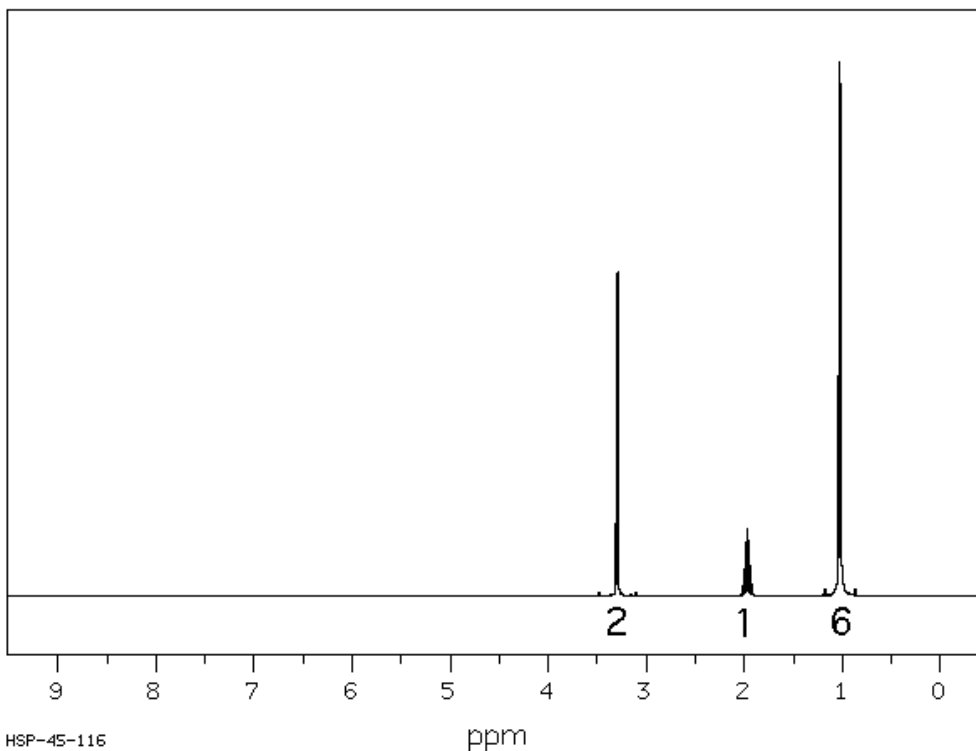
1.957 102

1.942 56

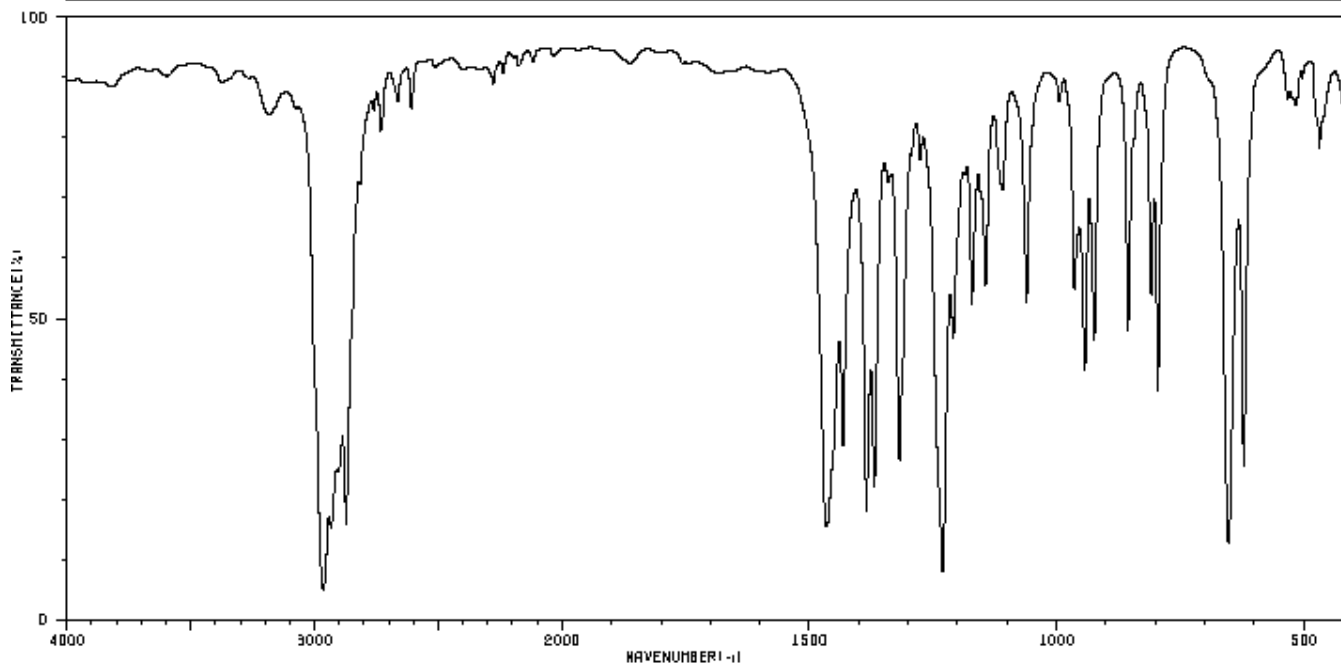
1.941 51

1.037 1000

1.02 959

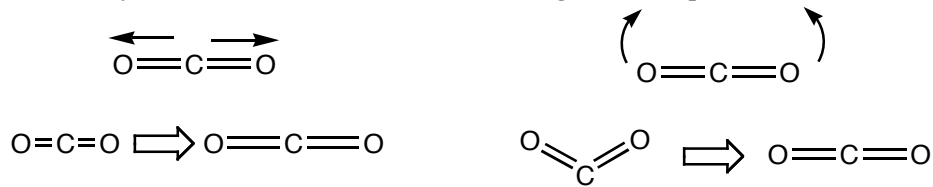


C₄H₉BR



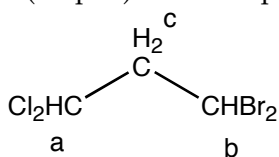
3369	86	2662	81	1318	25	1061	60	796	36
3184	81	2609	81	1276	74	994	81	653	12
2964	4	1466	14	1231	7	964	52	622	24
2933	14	1432	27	1209	44	943	39	633	84
2872	15	1385	17	1171	50	924	44	523	84
2760	81	1369	21	1144	53	855	46	516	61
2733	79	1340	70	1109	68	809	52	470	74

7. (10 pts.) Drawn below are representations of two vibrational modes for CO₂. To the left is a representation of a symmetrical stretch, and to the right is a representation of a bending mode.



- Are either of these vibrational modes IR active (can they be seen in an IR spectrum)? Explain, briefly.

8. (10 pts.) Draw a splitting tree for the protons labeled “c” in the following molecule.



$$J_{ac} = 10 \text{ Hz}$$

$$J_{bc} = 10 \text{ Hz}$$

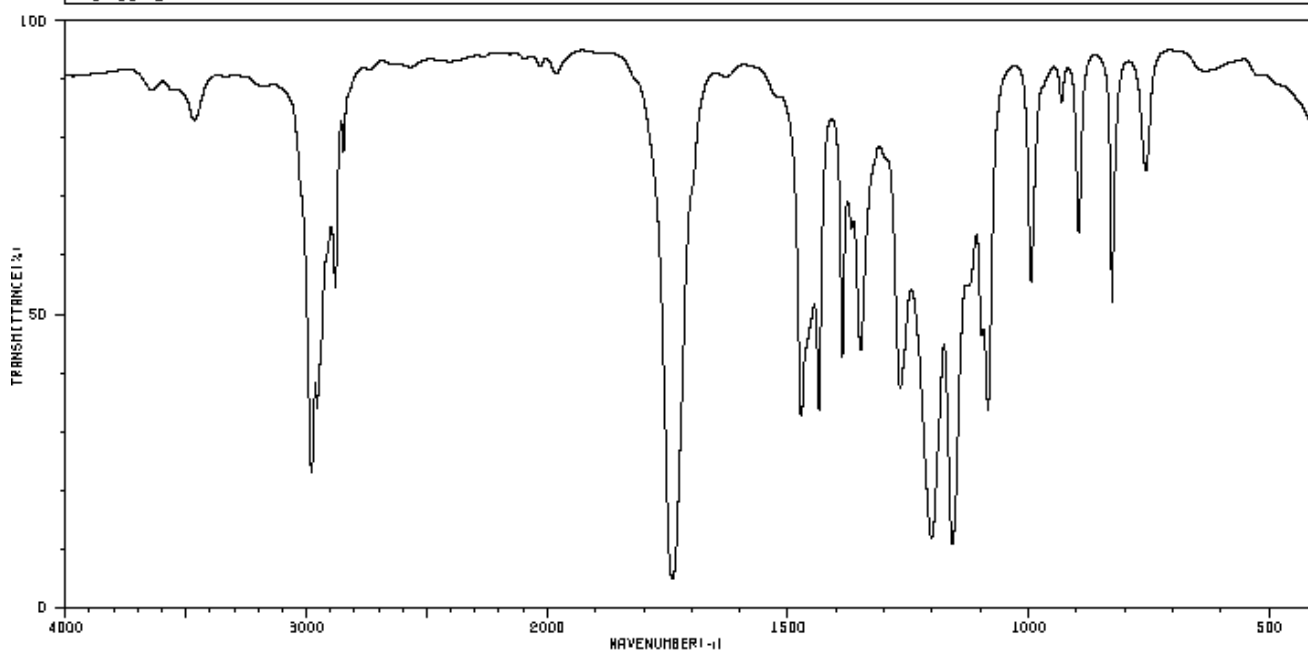
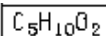
9. On the following page, you will find an IR spectrum and an NMR spectrum for a compound with the following formula C₅H₁₀O₂.

a. (6 pts.) What does the formula tell you about the structure of the molecule? That is, are there any π bonds or rings? Explain.

b. (6 pts.) The IR spectrum reveals the presence of what functional groups (label the peak(s) on the spectrum)?

c. (12 pts.) Determine the structure of the molecule, and assign the peaks in the NMR spectrum to the appropriate H atoms.

IR



3636	84	1473	31	1168	10	826	60
3465	79	1436	32	1097	44	756	72
2977	21	1387	41	1064	32		
2956	32	1368	62	994	63		
2880	52	1350	42	937	86		
2846	74	1267	36	931	84		
1740	4	1202	11	896	60		



¹H NMR

ppm Int.

3.669 1000

2.627 5

2.604 28

2.581 68

2.557 92

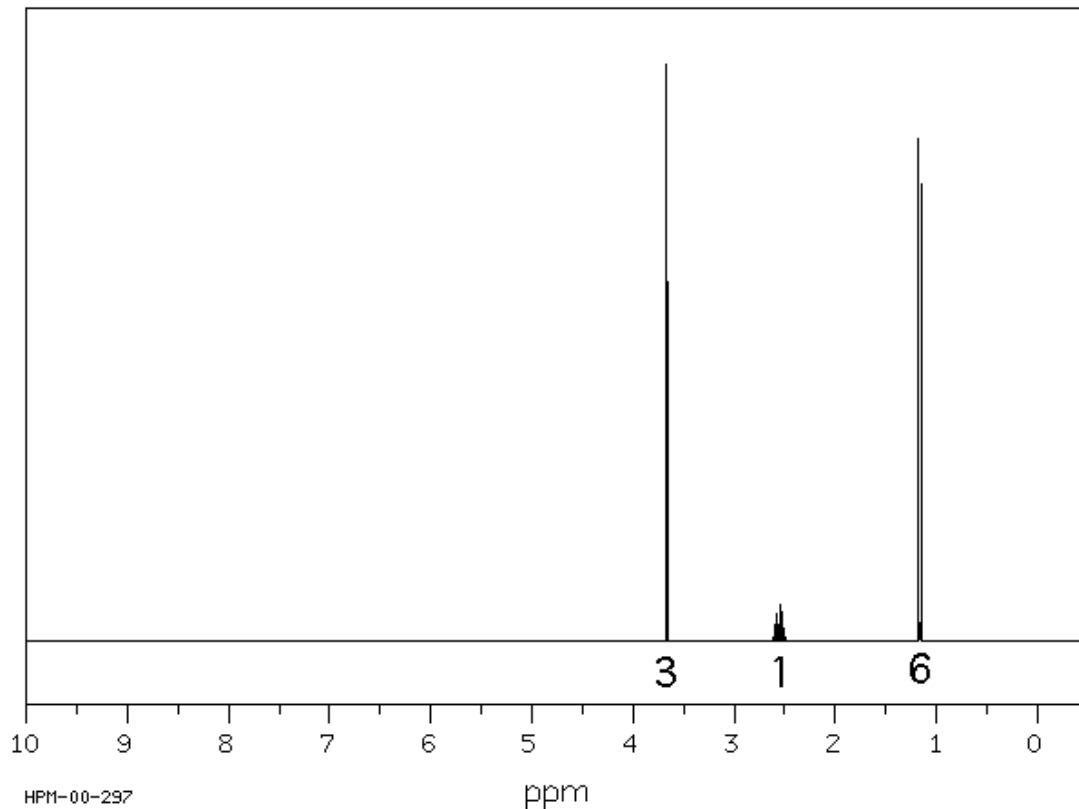
2.534 72

2.511 31

2.488 5

1.182 994

1.158 957



HPM-00-297