Name _____ Test 2 (3/28)[1]
CHEM 0203 (Organic) Spring 2025

1. The molar mass of chlorocyclohexane is 118.60 g/mol. The mass spectrum of chlorocyclohexane contains peaks at m/z of 118.05 and 120.05, but there is no peak at m/z of 118.60. (**a. 6 pts.**) Explain why there is no peak at 118.60 and (**b. 6 pts.**) why there are peaks at 118.05 and 120.05.

1. _____

2. _____

3. _____

4. _____

5. _____

6. _____

2. (10 pts.) Determine the formula of a molecular ion that contains only C and H atoms and has a m/z of 68.06.

7. _____

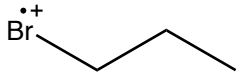
8. _____

9. _____

3. In a mass spectrometer, radical, cationic alkyl halides fragment using homolytic and heterolytic mechanisms. (**a. 12 pts.**) Draw the fragments that would form from the most likely heterolytic and homolytic cleavage reactions, and (**b. 6 pts.**) circle the fragments that would be observed in the mass spectrum.

10. _____

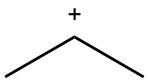
homolytic cleavage



heterolytic cleavage

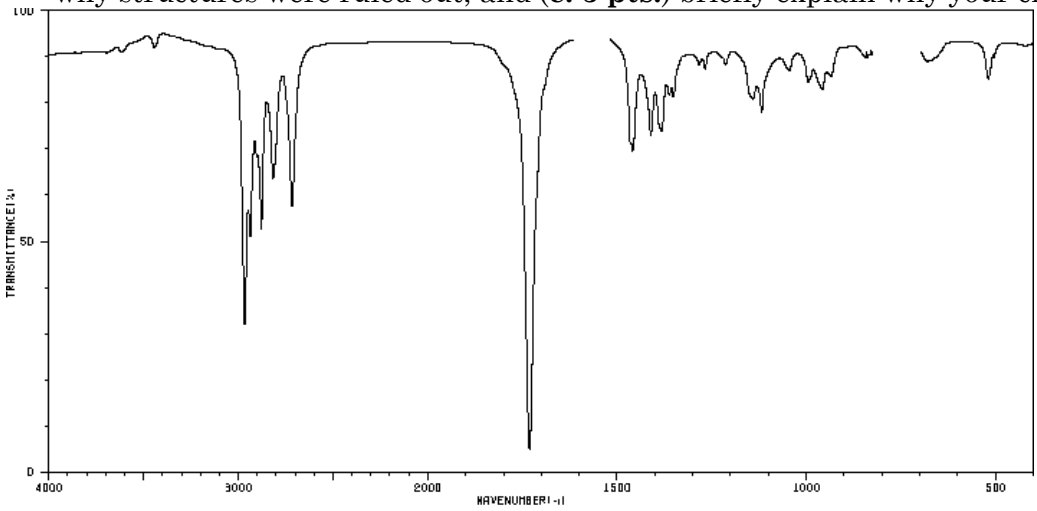
[1] Spectral Data from SDBS : https://sdbs.db.aist.go.jp/, National Institute of Advanced Industrial Science and Technology, 2025-3-25 and 2003-4-23

4. (6 pts.) A common fragment that appears in many mass spectra appears below. Determine the mass-to-charge ratio (the m/z where the peak would be seen) for the fragment.

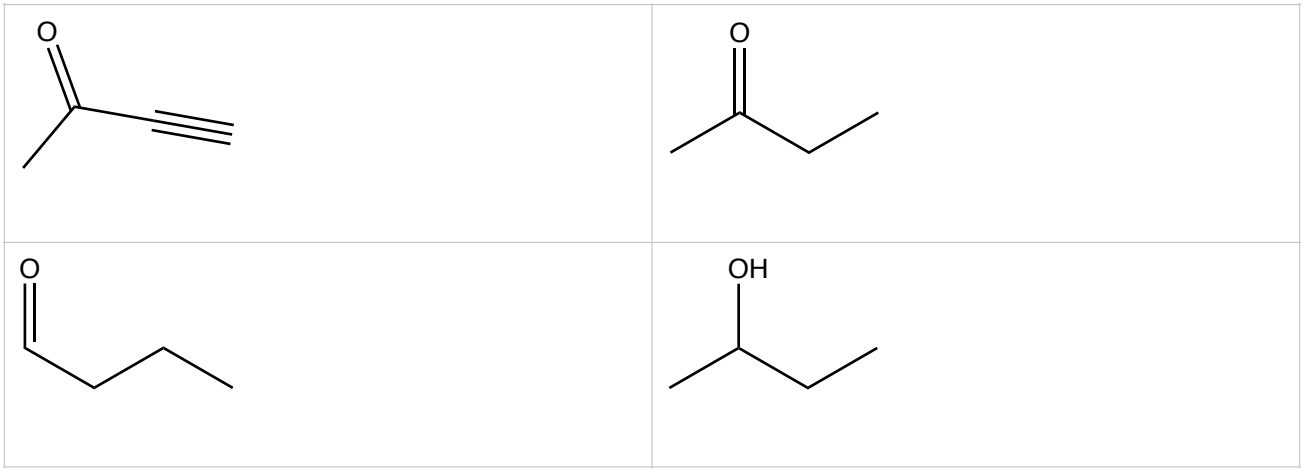


5. (10 pts.) Briefly explain why C to N triple bonds absorb higher frequency IR light than C to N double bonds.

6. (**a. 4 pts.**) Circle the molecule that produced the following spectrum, (**b. 9 pts.**) briefly explain why structures were ruled out, and (**c. 3 pts.**) briefly explain why your choice is the correct one.

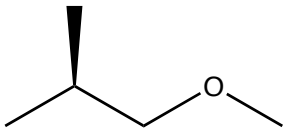


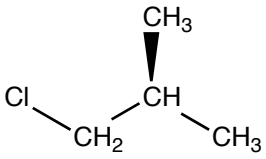
2966	31	1268	84
2937	49	1222	86
2878	50	1214	84
2817	62	1141	77
2716	55	1118	74
1731	4	1056	84
1464	68	1046	84
1459	66	994	81
1411	70	958	79
1388	72	934	81
1382	70	843	86
1362	79	677	86
1351	79	672	86
1284	84	620	81

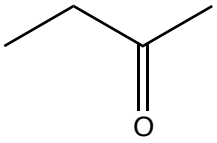


7. a. (9 pts.) Determine the number of peaks that are expected in the ^{1}H NMR spectra of the following molecules, and

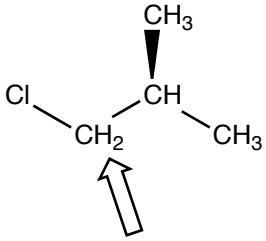
b. (9 pts.) determine the relative positions of the peaks in the ^{1}H NMR spectrum and label the protons alphabetically starting with the proton(s) that resonate at the highest frequency (appear farthest to the left in the NMR spectrum).

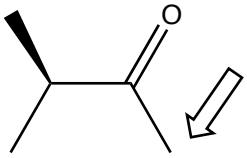


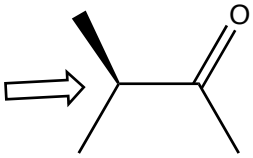




8. (12 pts.) Determine the multiplicity of the peaks attributed to the indicated H atoms.

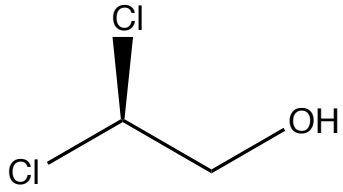


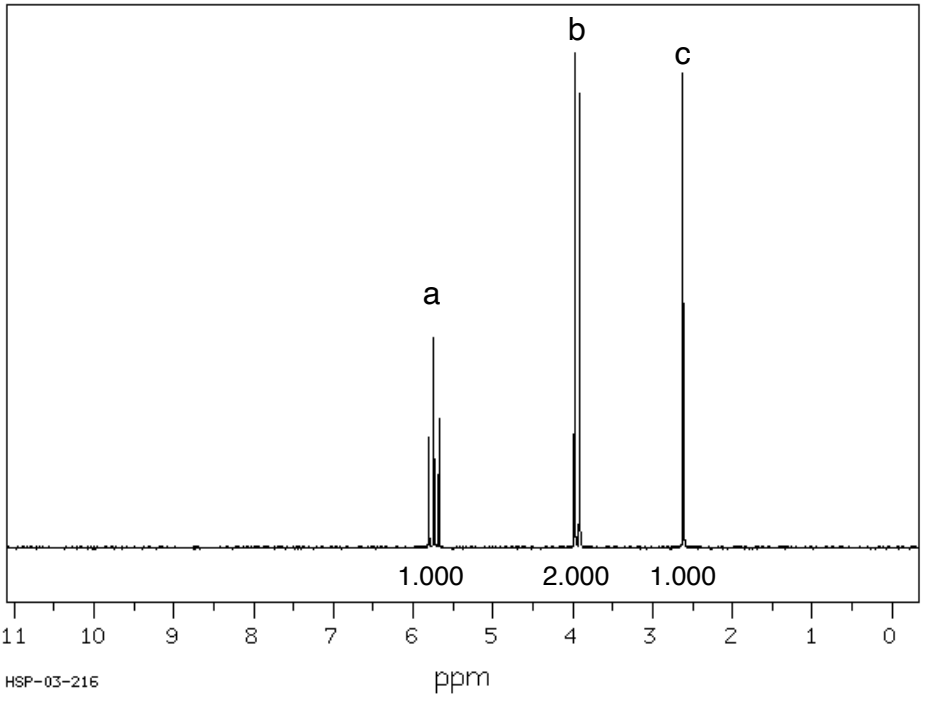




9. (12 pts.) Assign the peaks in the ^{1}H NMR spectrum of 2,2-dichloroethanol shown below. The peaks in the NMR spectrum below have been labeled with the letters “a”, “b”, and “c”. Place the appropriate letter next to the H atom(s) in the structure that gives rise to the peak labeled with the letter.

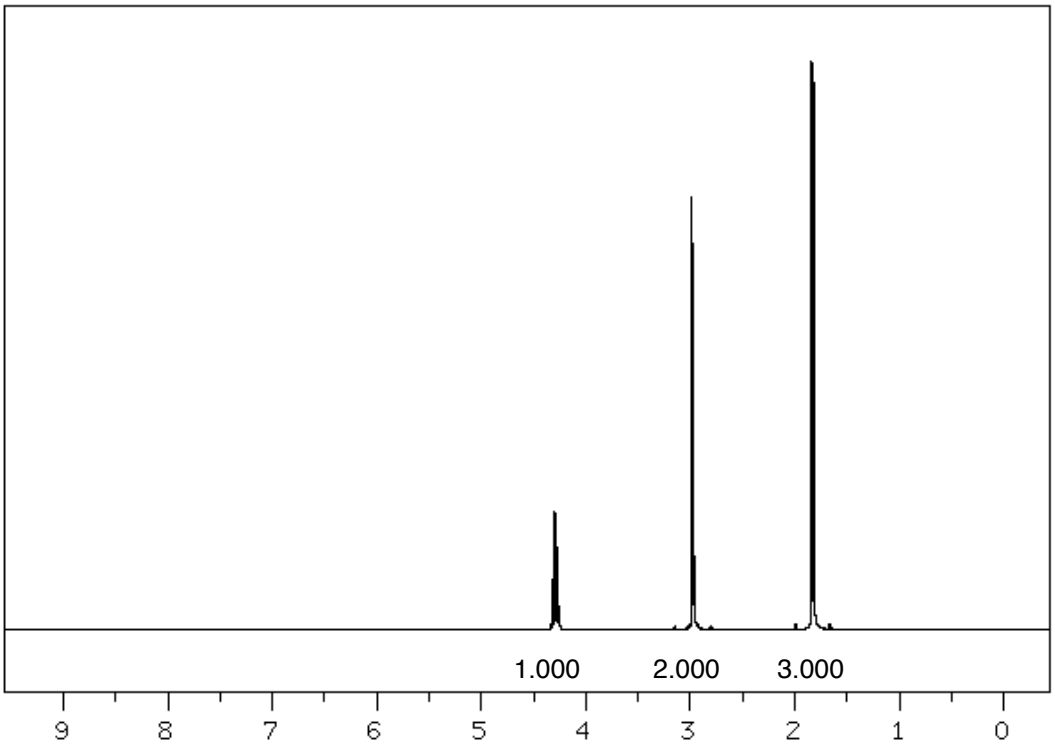
ppm	Intensity
5.804	223
5.740	425
5.678	260
3.979	1000
3.916	919
2.619	960

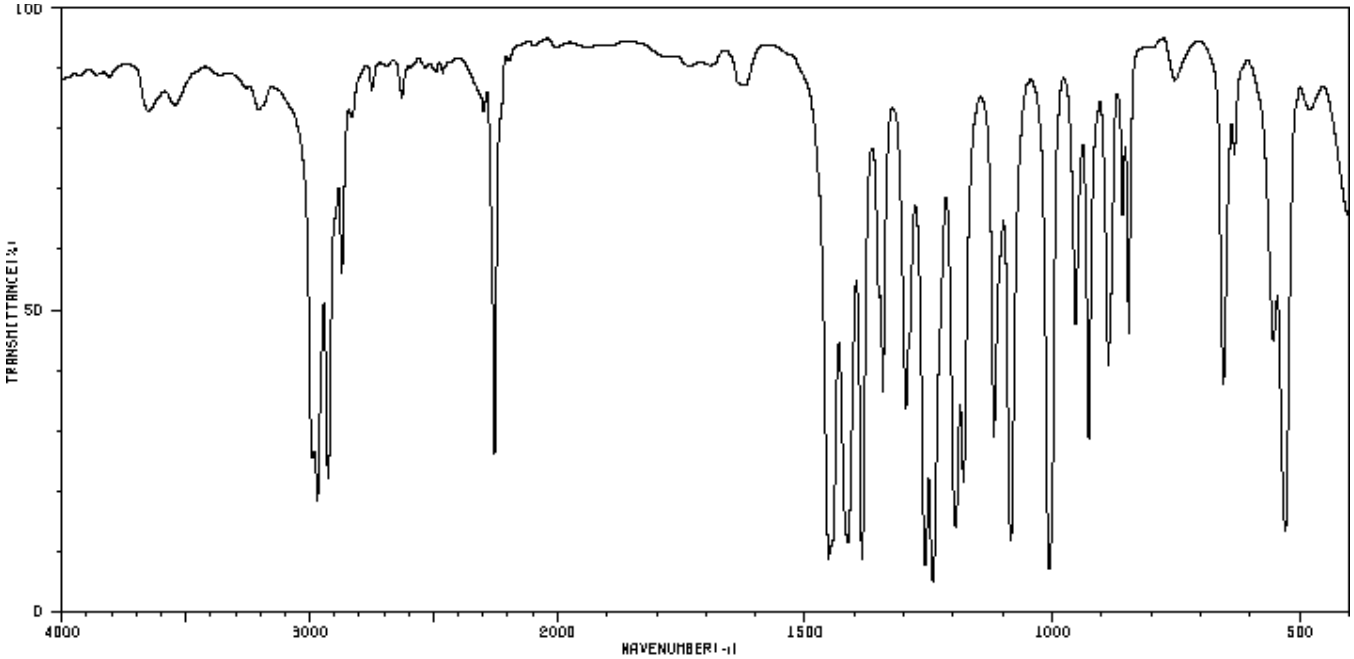




10. A molecule with the formula C_4H_6BrN produced the following IR and NMR spectra. Based on the spectral data provided below (**a. 10 pts.**) determine the structure of the unknown C_4H_6BrN, (**b. 4 pts.**) identify/label two peaks in the IR spectrum, and (**c. 4 pts.**) unambiguously assign the peaks in the 1H NMR spectrum. That is, label each peak in the 1H NMR spectrum alphabetically starting with an "a" at the left end of the spectrum and label the protons on your structure with the corresponding letter. (Remember, you can earn partial credit for identifying parts of the molecule.)

ppm	Intensity
4.328	32
4.311	107
4.296	209
4.279	203
4.264	122
4.248	36
2.982	762
2.968	681
1.837	1000
1.820	963





3660	79	2828	79	1386	8	1180	20	868	62
3542	81	2627	81	1350	50	1118	27	846	44
3208	79	2297	79	1343	35	1084	11	655	36
2988	24	2266	26	1296	32	1007	6	632	72
2969	17	1453	8	1257	7	953	46	554	43
2926	21	1447	10	1242	4	927	27	530	12
2870	63	1414	10	1196	13	887	38	480	79