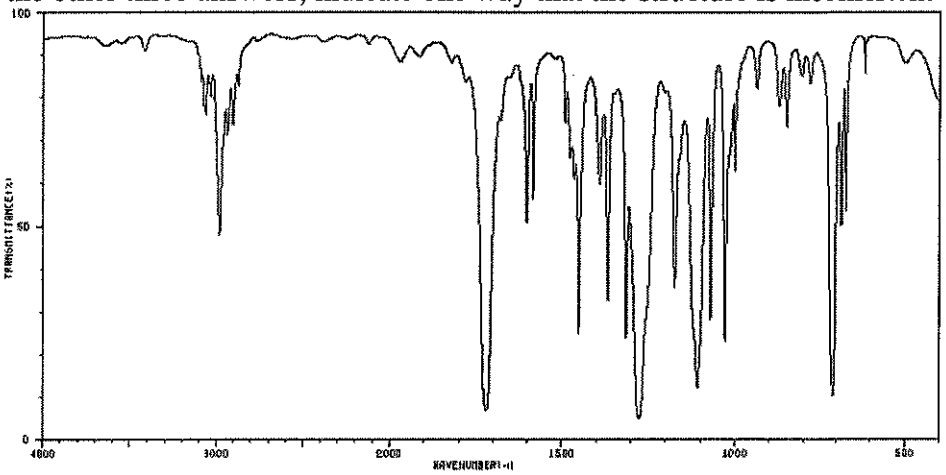
S343 Quiz 3
2/26/2015

Name Key

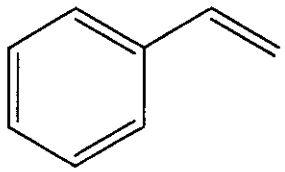
AI or Section _____

1. (8pts) Circle the structure below the spectrum which is most consistent with the spectrum. Under the other three answers, indicate one way that the structure is inconsistent with the spectrum.



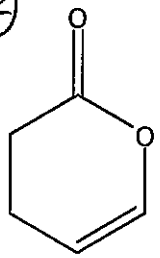
3091	81	1969	84	1466	58	1109	12	807	61
3054	72	1822	84	1452	23	1071	26	782	79
3035	77	1719	6	1392	57	1029	21	711	9
2983	46	1603	49	1368	31	1002	60	688	47
2939	68	1585	53	1315	23	937	78	675	52
2907	70	1492	72	1276	4	873	74	618	81
2874	79	1478	64	1176	34	861	70	505	84

(+2)



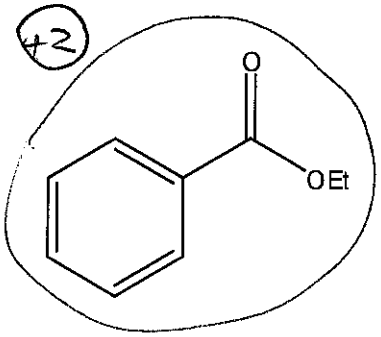
- no C=O stretch should be seen
or
- 1650 cm^{-1} C=C should be seen

(+2)

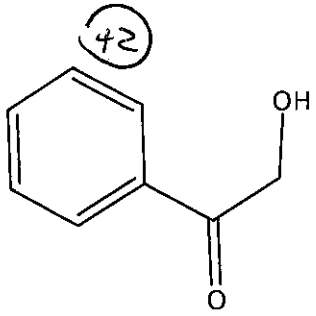


- C=C should be at 1650, not 1600 cm^{-1}
or
- C=O would be at 1745 cm^{-1}

(+2)



(+2)

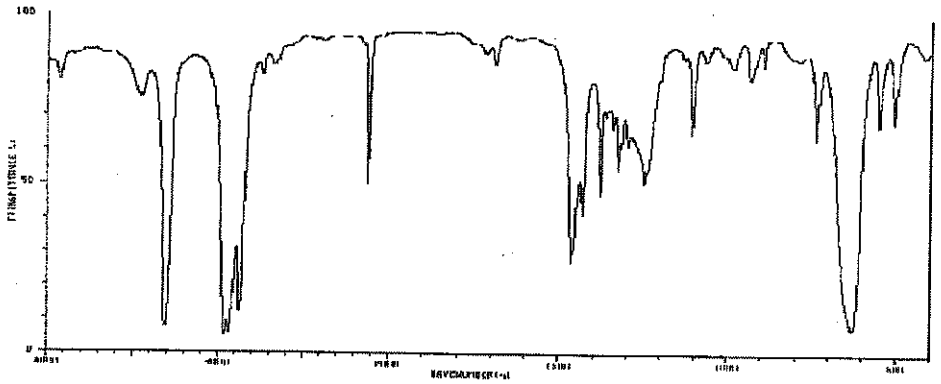


- no O-H stretch present at 3300 cm
or
- C=O should be at 1690 cm^{-1}

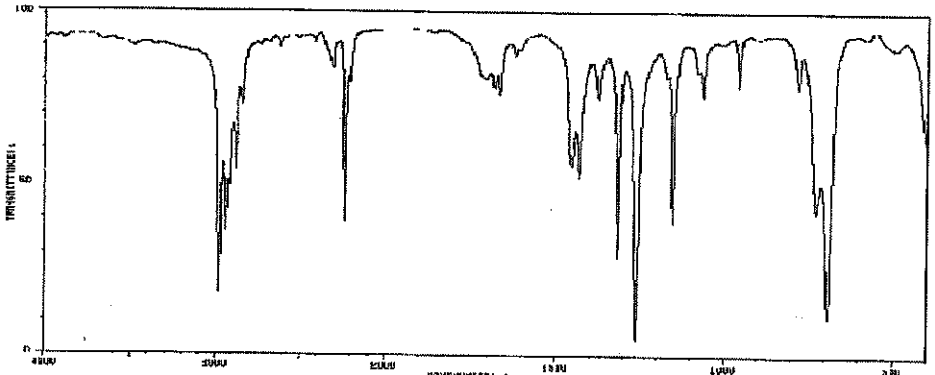
2. (2pts) If you took into account only the atomic mass, you would expect the carbon/nitrogen triple bond to have a lower frequency than the carbon/carbon triple bond, but this isn't true. Explain why the opposite is true.

(+2) Frequency also depends on bond strength. Therefore, the C≡N bond strength must be greater than C≡C.

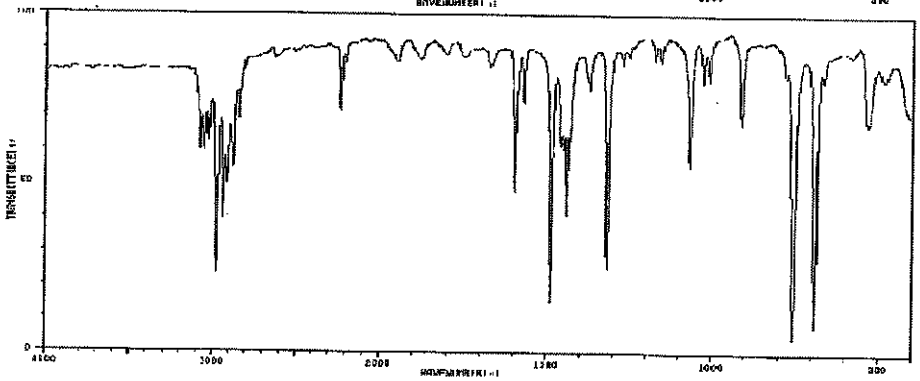
3. (4pts) Match the letter of the compounds below to the correct spectra.



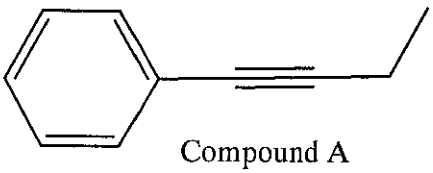
+1 compound C



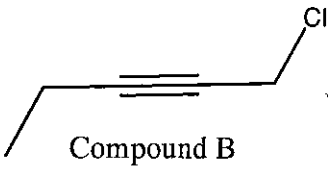
+1 compound B



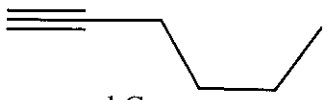
+1 compound A



Compound A



Compound B

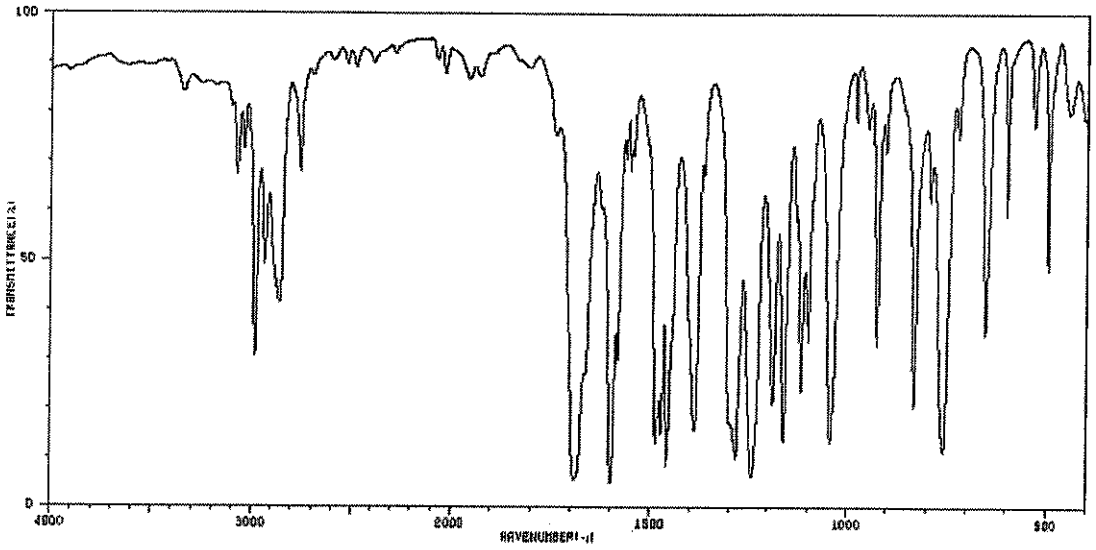


Compound C

Is the intensity of the carbon/carbon triple bond stretch consistent with the structure? Explain.

+1 The electronegative chlorine of B should polarize the C≡C bond, making the peak more intense, which is true.

4. (6pts) Propose a structure for the $C_9H_{10}O_2$ compound that is consistent with this IR spectrum. Write out your thought process clearly for partial credit. (Hint: The 2861/2760 cm^{-1} doublet is at slightly higher frequency than what is typical.)



3077	84	1600	4	1474	14	1190	28	933	19
3042	70	1584	28	1460	7	1162	12	793	60
2983	29	1564	66	1390	14	1117	22	759	10
2938	47	1562	66	1368	64	1098	32	729	72
2861	39	1546	68	1299	16	1042	12	654	33
2760	66	1466	12	1285	9	926	31	601	57
1690	6	1482	17	1243	6	906	70	497	46

+5

(+1) 5 degrees of unsaturation

(+1) aryl group (1600 cm^{-1} / above 3000)

(+1) aldehyde (2700/2800 doublet)

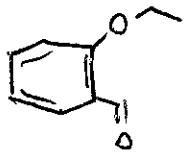
(+1) conjugated carbonyl (1690 cm^{-1})

(+1) ether / not O-H because no stretch at 3300 cm^{-1}

(+1)

final structure

Any consistent with above



Bonus: Explain the strong intensity of the 1600cm^{-1} peak:

(+1) The C=C of benzene is very polar, with EDG and EWG