Return to Index: http://valhalla.chem.udel.edu/SpecBook.pdf

Chapter One, Problem C

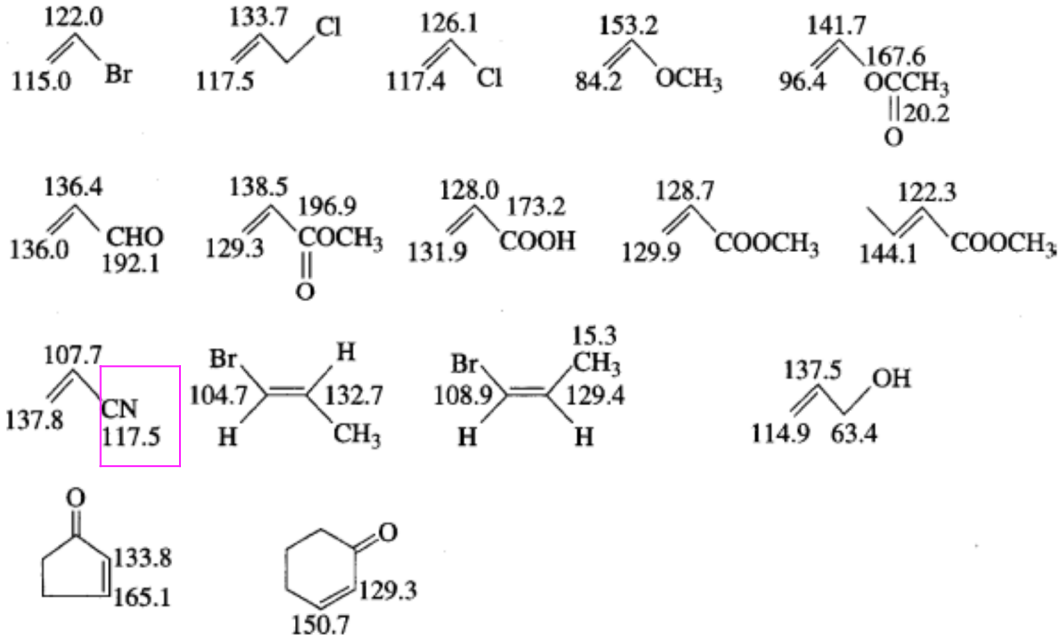
Worksheet, step one: The formula contains N, so we need to remember that each N brings with it an extra H. For calculating IHD, the H count is 4, and the IHD = 4. All of the H's are attached to carbon.

$C_5H_6N_2$

16, t (2)
22, t
119, s (2)

Worksheet, step two: With so much unsaturation and N in the formula, we should suspect a nitrile. This is confirmed when we find a nitrile in Table C4, at 117.5. We have two nitriles, at 119, s. Each nitrile has a triple bond, so an IHD = 2. We have two nitriles, so this accounts for the IHD = 4.

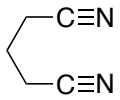
Table C.4 Chemical Shifts of Substituted Alkenes (ppm from TMS)



Worksheet, step three: There are no more heteroatoms.

Worksheet, step four: There is only one more carbon, a $-CH_2-$.

Worksheet, step five: There is only one way to assemble the structure.



Return to Index: http://valhalla.chem.udel.edu/SpecBook.pdf