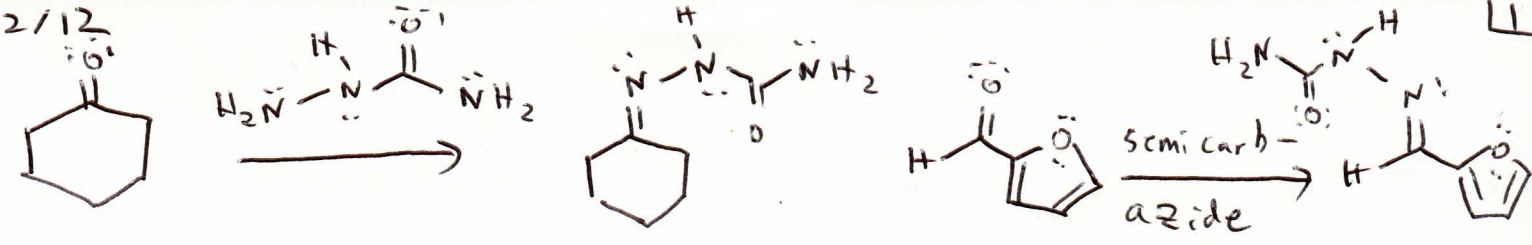
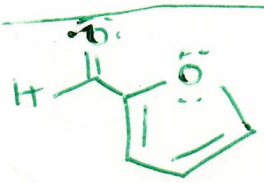
3/12/12



A A' B B'



aromatic

- Since the C=O is outside the ring, it does not affect whether the compound is aromatic
- One of the oxygen e⁻ pairs becomes part of the π system (making it aromatic), which forces the other pair to be ⊥ to the system.

Part A: A ⟶ A' 166°C

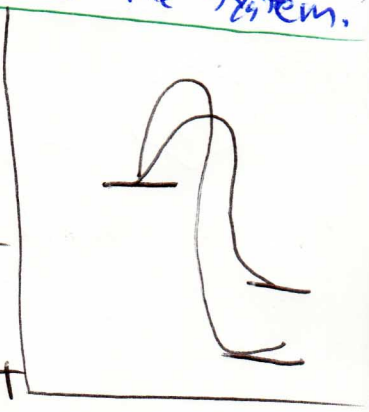
Part B: B ⟶ B' 202°C

Part C: A + B ⟶ A' + B'

Below RT ⟶ kinetic product

@ RT ⟶ mix

Above RT ⟶ thermodynamic product



* There is not necessarily any connection between thermodynamic stability + melting point. Melting point is determined by the way a compound packs with itself to form a crystal, not on the energy involved to make the molecule.

In this case, since the product formed in part C at below RT had a MP close to A', A' is the kinetic product, and since the product formed @ high T (above RT) had a MP close to B', B' is the thermodynamic product.

The fact that the product formed @ low T had a low MP is coincidence.

Part E

A' + B ⟶ [A+B+ semicarbazide] ⟶ B' + A

If A' is the thermo. product, this rxn will not occur, since the formation of A' would be the least reversible. If, instead, A' is the kinetic product, it could decompose to form semicarbazide (and A) which could react w/ B to form B', the thermo. product. The reaction can be said to occur if the mp of the product differs (drastically) from the reactant.

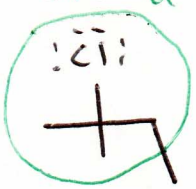
B' + A ⟶ B' + A ← In this case, since B' is the thermo. product, no rxn occurs → mp should match B'

$C_5H_{11}Cl$	δ 1.704, q, 2H δ 1.556, s, 6H δ 1.036, t, 3H
C_8H_{10}	δ 7.04, s, 4H δ 2.296, s, 6H

$C_5H_{11}Cl$ ⟶ ◯ D.O.U.

Method #1 - Chemical shift

No δ > 2, so no hydrogens on a carbon next to Cl, so there must be 3 carbons attached

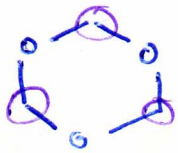


Since there are only 5 carbons total + 4 are establish using δ, the last carbon must be attached to one of the Methyl groups established initially

Method #2 – Symmetry

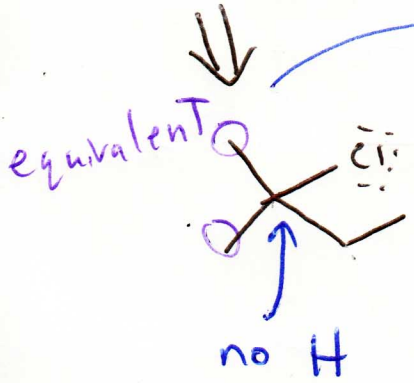
Given an integration of 6, there must be at least two chemically equivalent groups; either two methyl groups or 3 methylene ($-CH_2-$).

equal



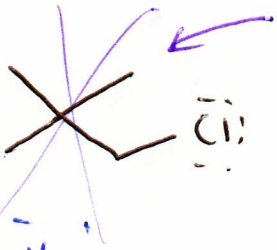
equal

Based on the small size of the molecule, it is much more likely that it has 2 equivalent methyl groups.



The peak that integrates to 6 is a singlet, which means there cannot be any hydrogen neighbors, which means there must only be C or Cl at that point.

or

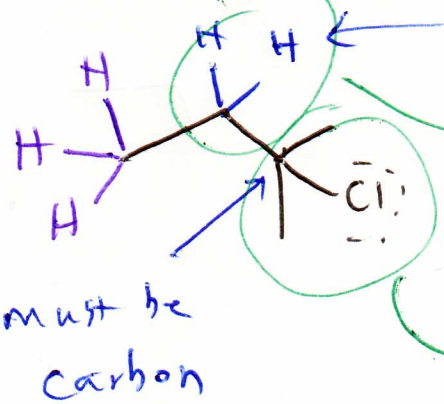


would be three equivalent methyl groups

Method #3: Splitting

An integration of 3 usually corresponds to a methyl group, which is useful since it is an "end" of the molecule.

In ~~this~~ molecule, there is a triplet w/ integration 3.

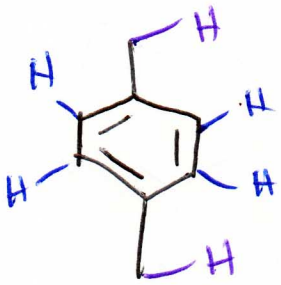


only two neighbors

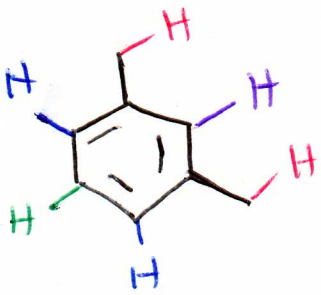
The only peak that integrates to 2 is a quarter, which means it only has hydrogen neighbors on one side.

C_8H_{10} ⟶ 4 D.O.U.

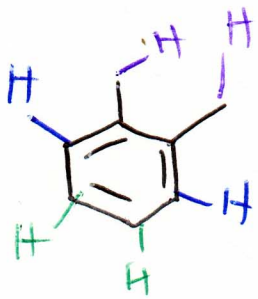
 ⟶ Has 4 D.O.U. and $7 \leq \delta \leq 8$



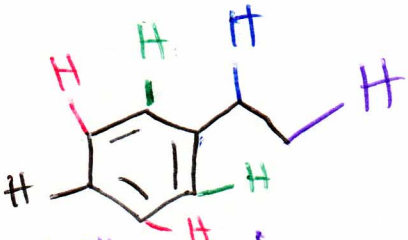
2 absorbances



4 absorbances



3 absorbances



Will not have integration of 6.

5 absorbances