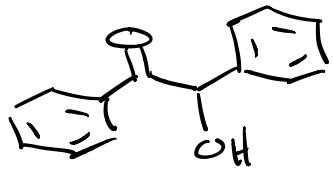
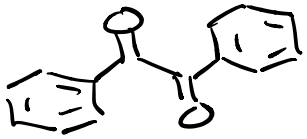
Benzoin → Benzil



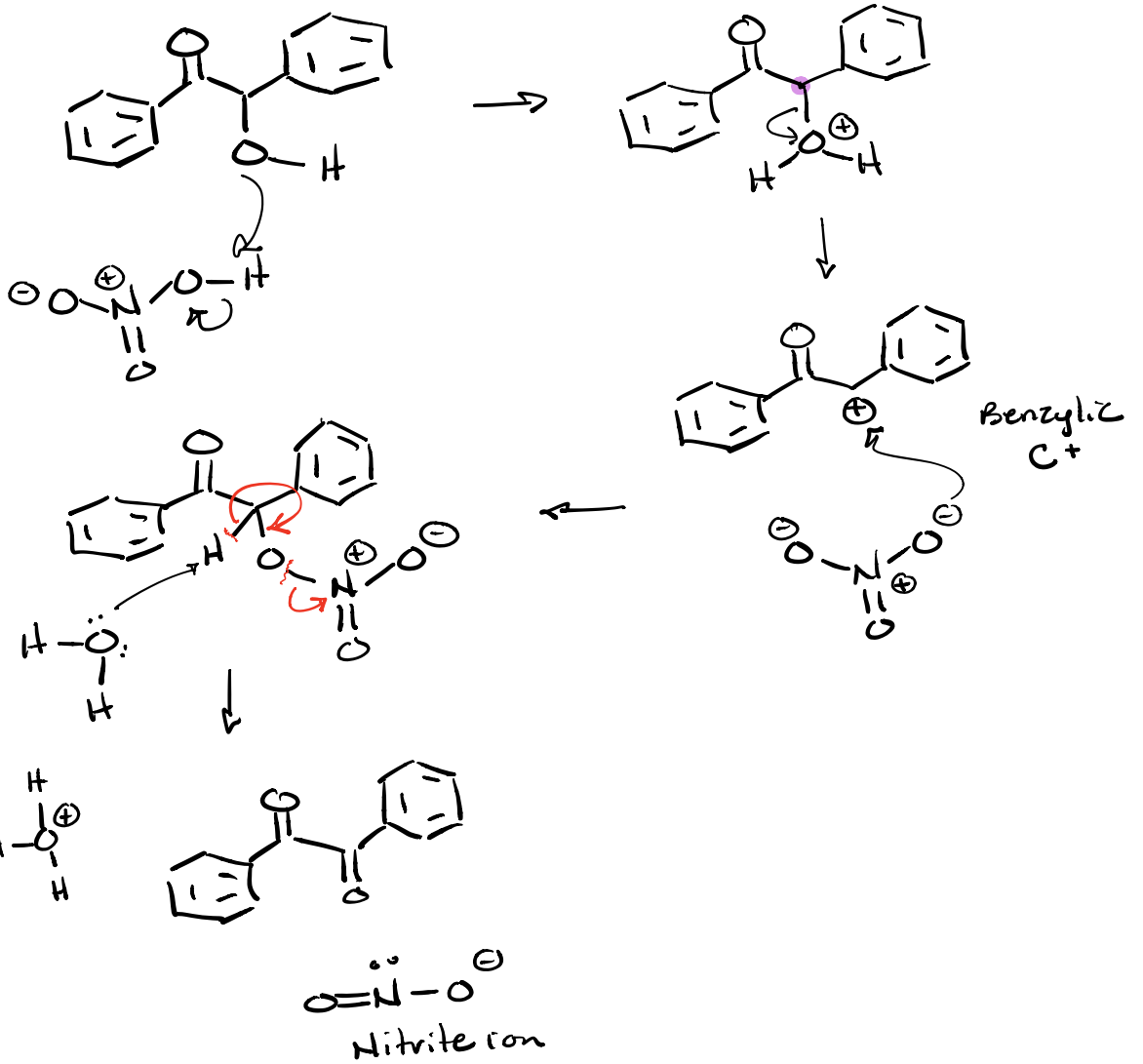
Benzoin

HNO_3

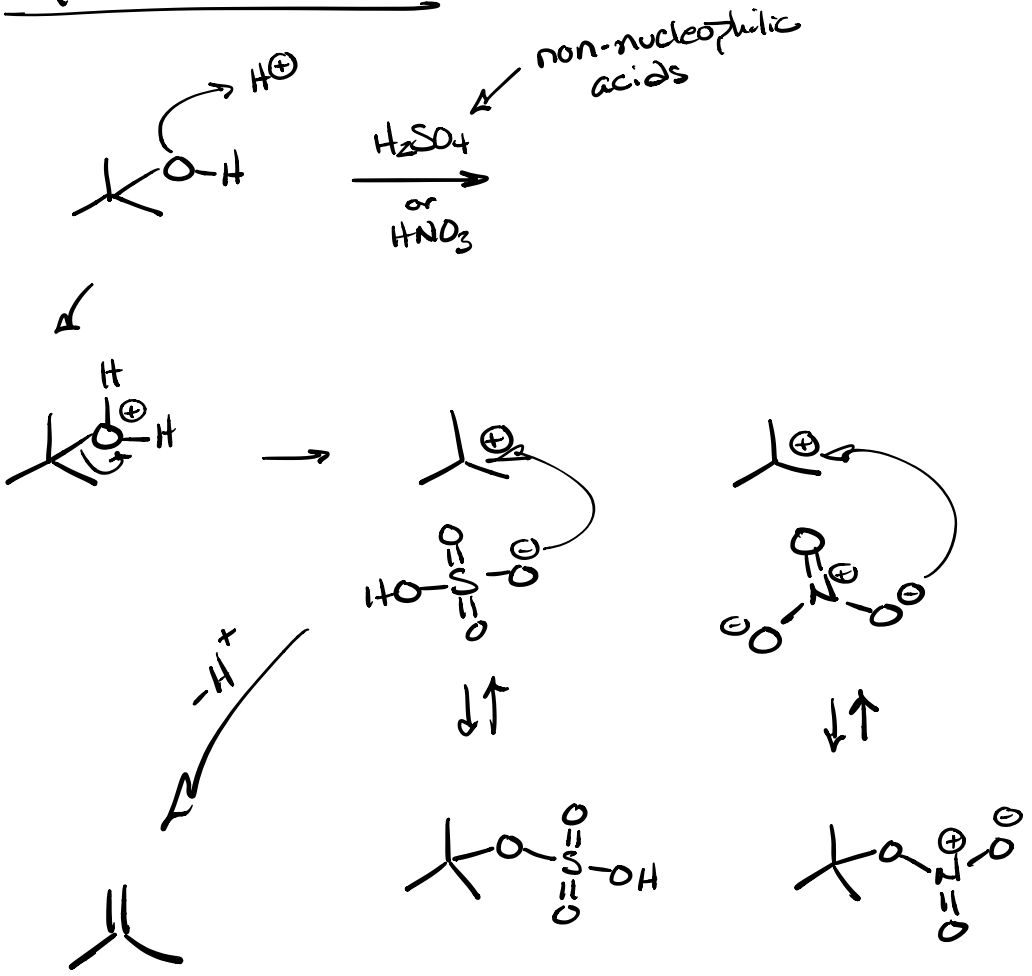


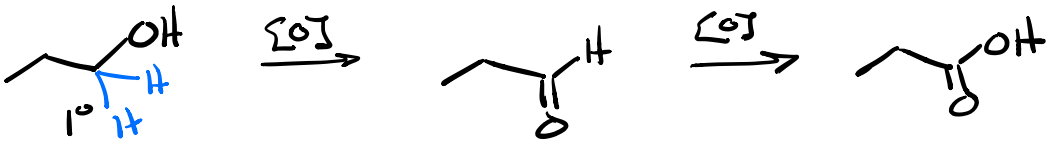
Benzil

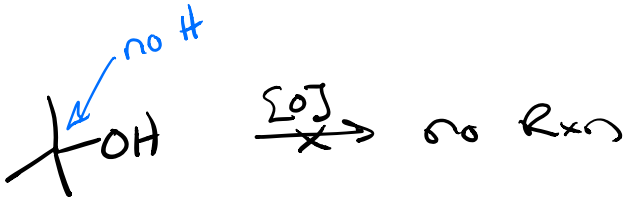
Benzylic leaving group



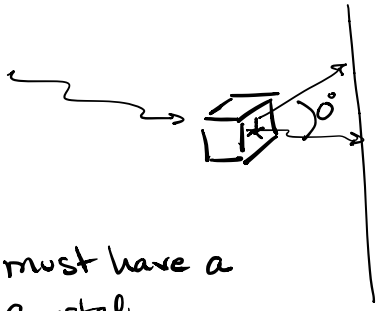
E_1 mechanism

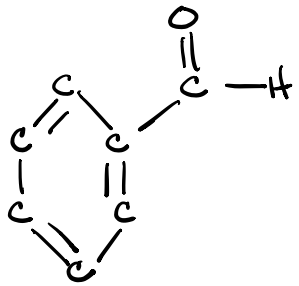






X-Ray Crystallography



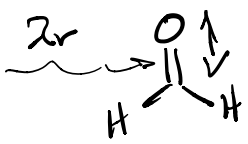


① must have a crystal

② must also a good crystal → pure & good repeat pattern

③ Expensive & difficult

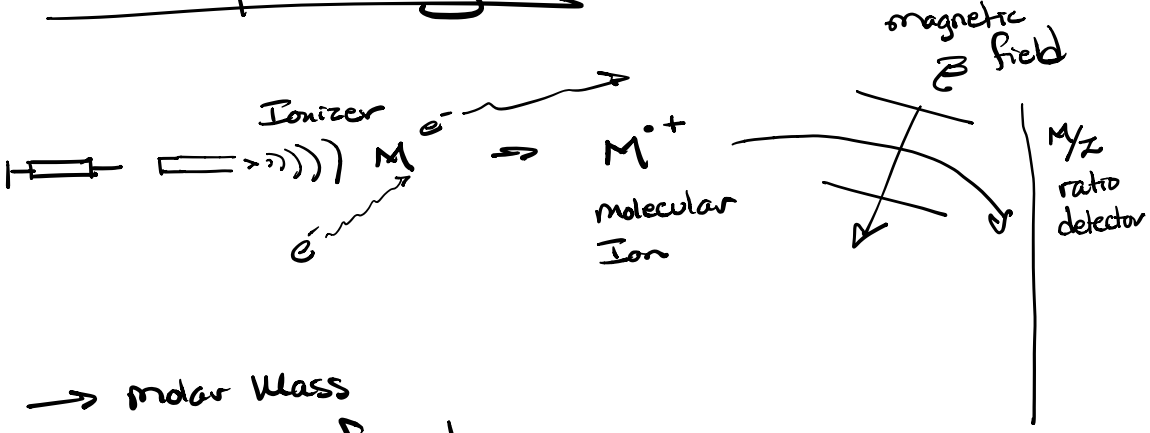
IR Vibrational frequencies



λ_r - harmonic frequency

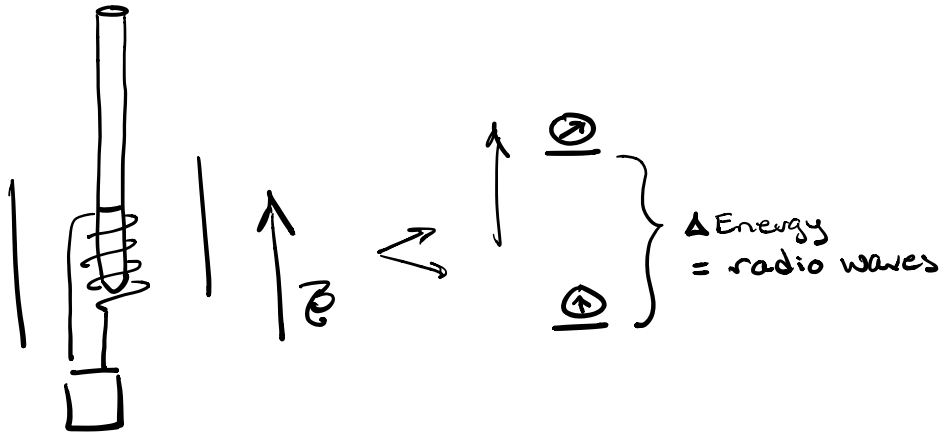
Cheap
fast
easy
⇒ But no Connectivity
⇒ Part of picture
but can't
rebuild molecule
from just IR

Mass Spetrometry

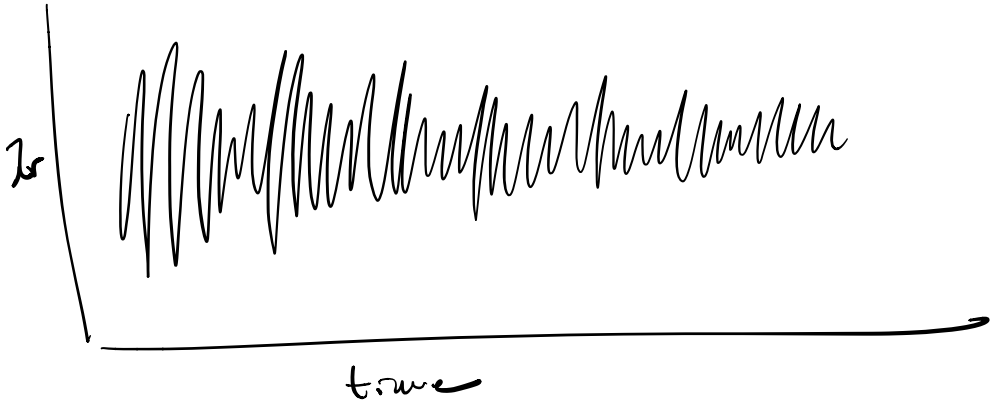


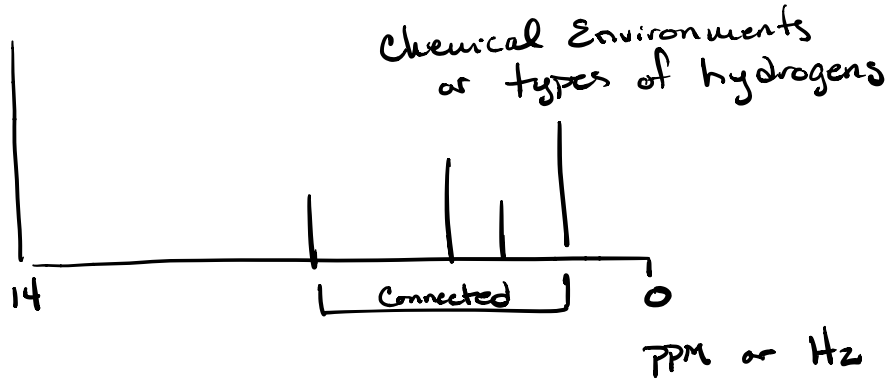
→ molar Mass
⇒ molecular formula

NMR → nuclear transitions



Pulse with radio frequency



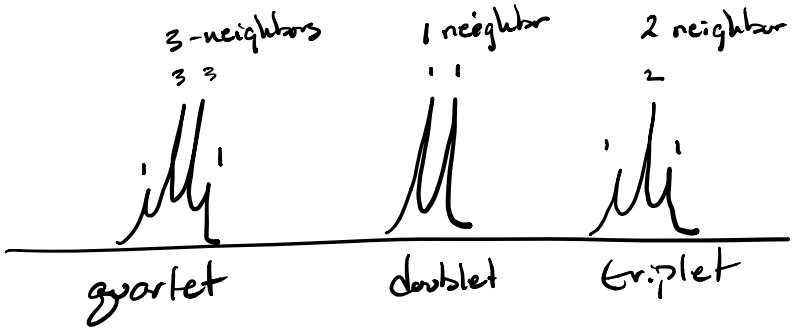


$$ppm = \frac{\nu_{sample} - \nu_{ref}}{\nu_{applied}} \times 10^6$$

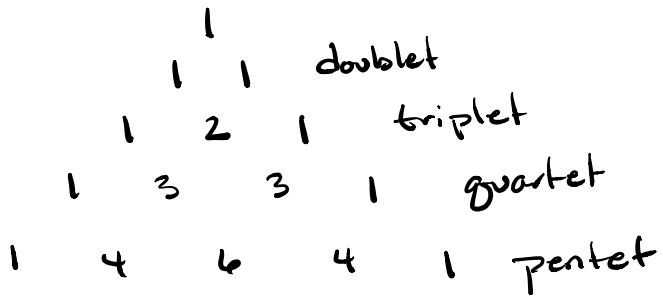
- we can tell neighbors
- Rebuild atom connectivity
- fast
- Relatively cheap

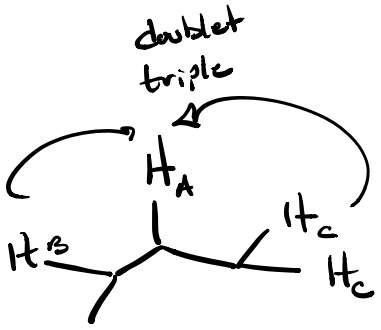
- IR functional Groups
- Mass Spec molecular formula
- NMR ^{13}CNMR, ^{1}HNMR } atom connectivity

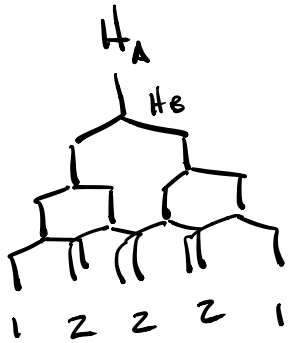
Rebuild Molecular Structure

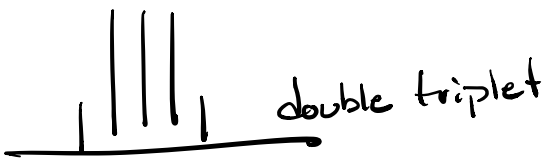

3-neighbors
3 3
1 neighbor
1 1
2 neighbor
2
quartet
doublet
triplet

n+1 rule


1
1 1 doublet
1 2 1 triplet
1 3 3 1 quartet
1 4 6 4 1 pentet


doublet
triple
H_A
H_B
H_C
H_C


H_A
H_B
1 2 2 2 1


double triplet