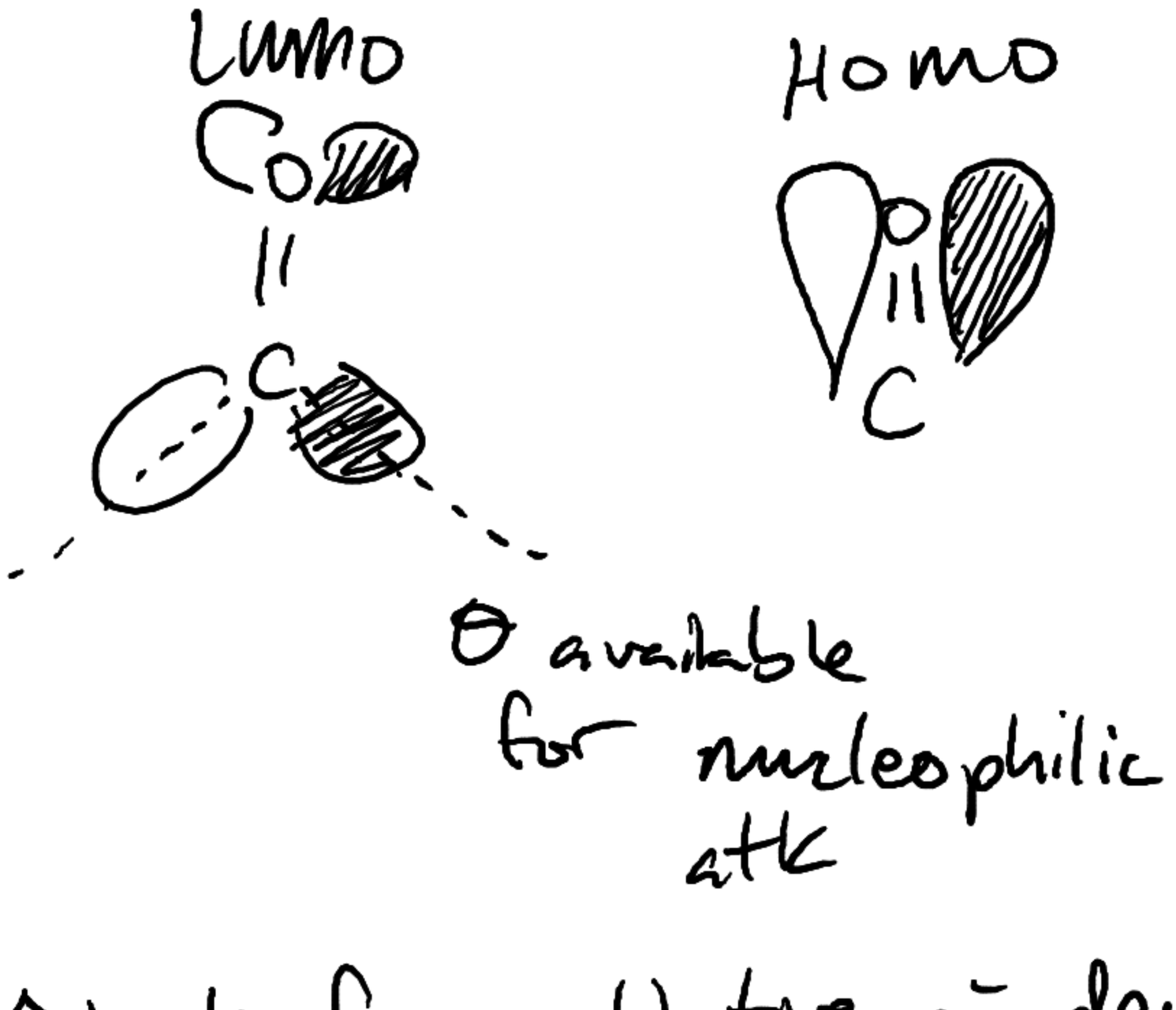
△ Identify the HOMO & LUMO & more importantly, the MOs @ play



△ look for qualitative e^- densities

more localized = more ionic
= greater splitting
= "harder"

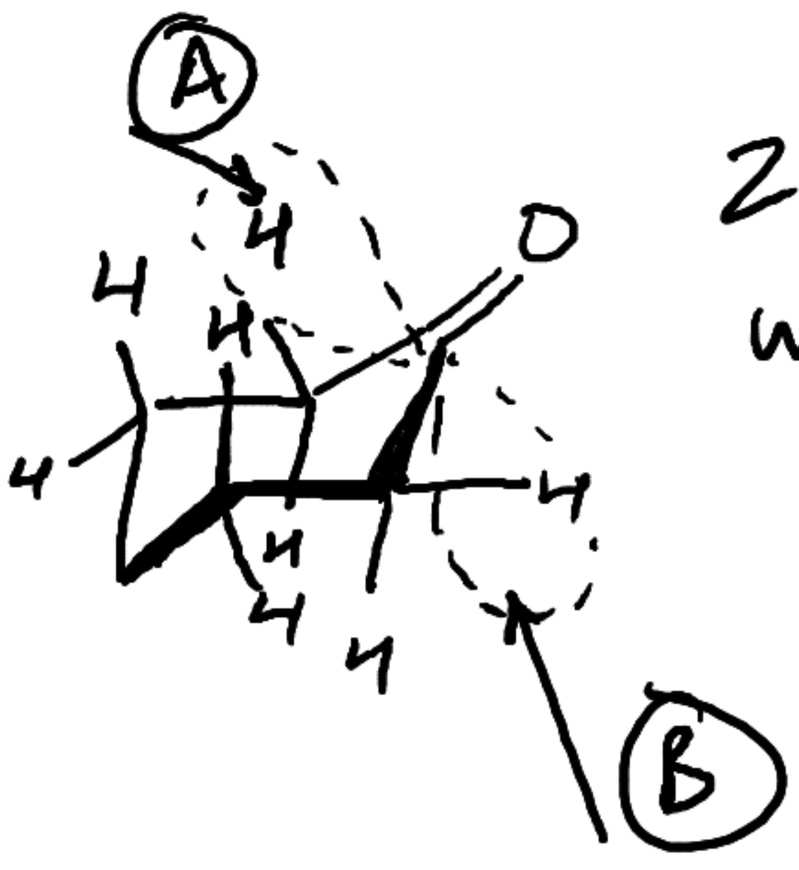
more likely the interaction between MOs if energy is similar between the two

△ intramolecular more likely than intermolecular interactions

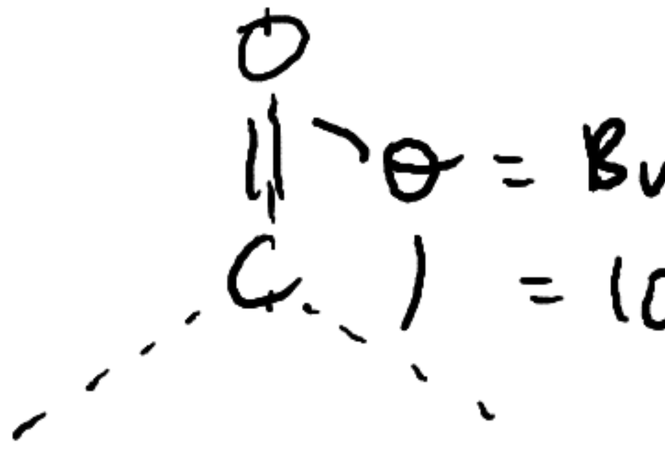
Δ e^- going into LUMO "activates" group
(Ex: carbonyl) → increases bond length
& opens HOMO for
atk

Δ relative energy can be inferred from
structural results → think in 3D
for better rxn
pathways

ex:



2 directions for
nucleophilic atk
however (A) is
more favorable
due to sterics

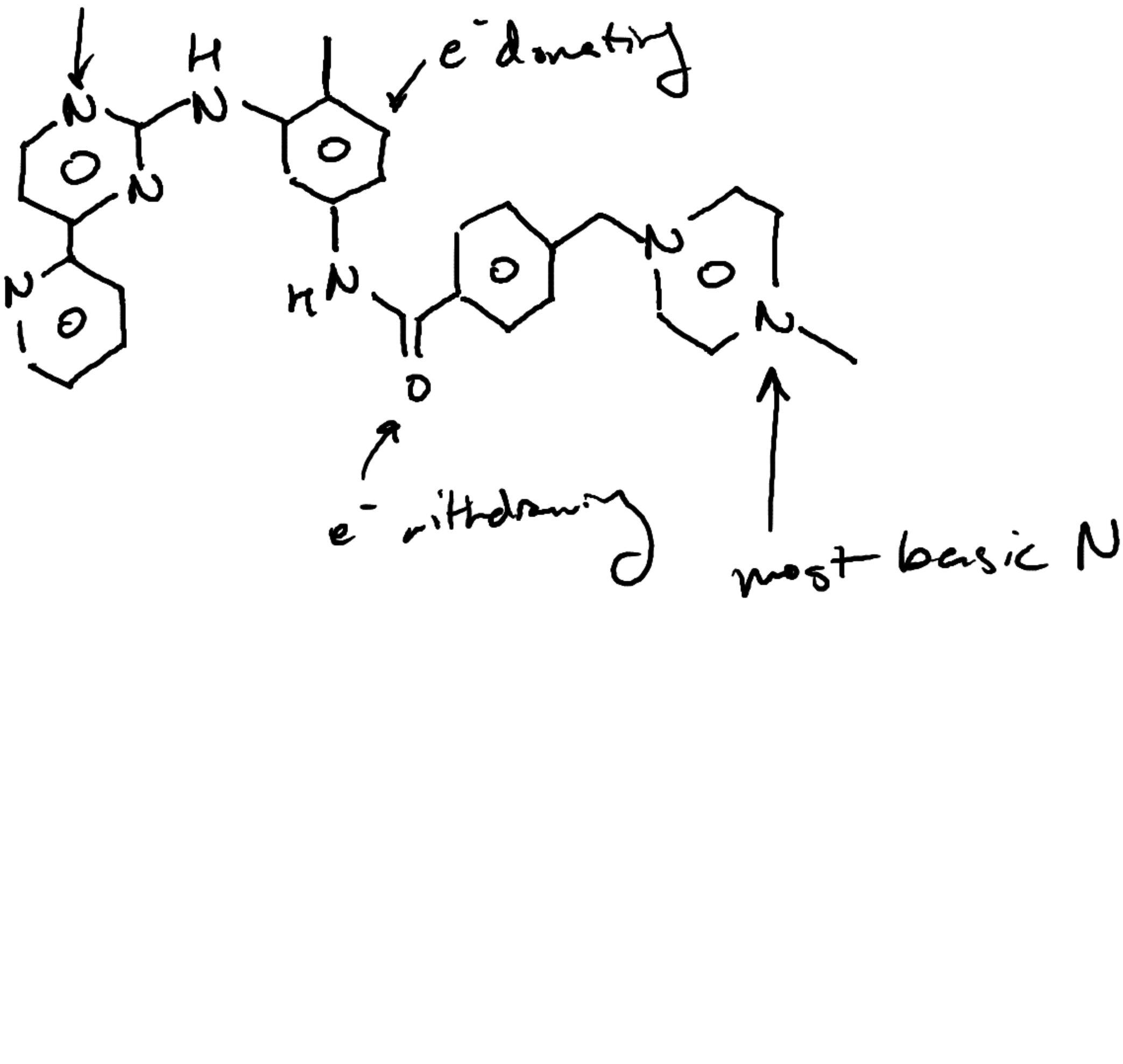


△ understanding energetics leads to better qualitative comparisons of pKa

↳ visualize e⁻ density

↳ consider the solvent as well when determining choice of acid or base

Ex:



- rearrangements are products of overlapping π systems
  - ↳ rearrange molecules to check for "opportunity"