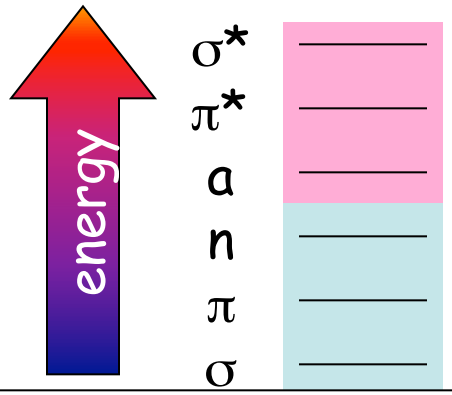
Recognizing Nucleophiles and Bases

Nucleophiles donate electrons from their highest occupied MO

The signatures of a nucleophile

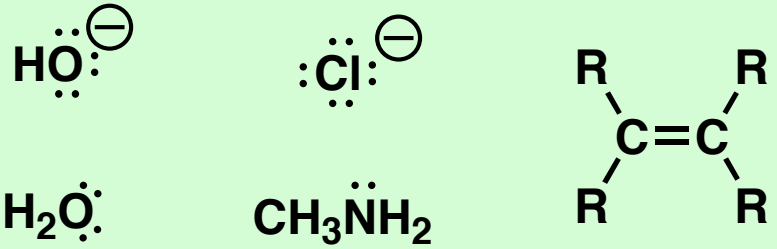
- an electron rich atom, especially as revealed by negative formal charge
- a nonbonded pair of electrons (a lone pair)
- an electron pair in a pi bond
- a partial negative charge revealed via resonance contributor(s)
- strong bases tend to be strong nucleophiles
- any species with a high-lying HOMO

The usual order of energy levels



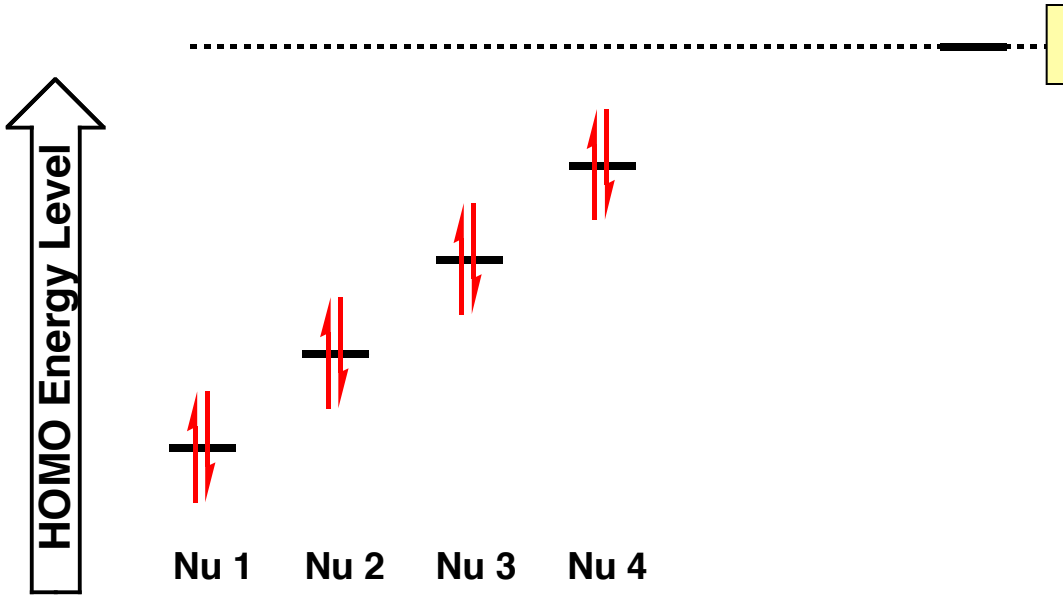
empty / filled	σ*	a	π*
σ	σ→σ*	σ→a	σ→π*
n	n→σ*	n→a	n→π*
π	π→σ*	π→a	π→π*

Typical nucleophiles



Nucleophilicity and HOMO Energy Level

There's a good analogy between nucleophiles and bases. Just as some bases are stronger than others, some nucleophiles are stronger than others. Whereas we speak of basicity to describe the strength of bases, we speak of **nucleophilicity** to describe the strength of nucleophiles.



Consider the series of nucleophiles **Nu 1** to **Nu 4** with HOMO energies as shown above

Given the LUMO energy of E+ as indicated above:

Which frontier orbital interaction will be the strongest?

Which electron pair is the most "energized"?

Which nucleophile has the highest nucleophilicity ?