

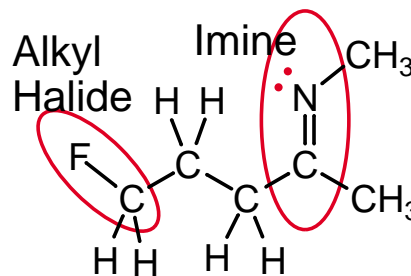
Note that only 200 of 600 semester points have gone by so far

[Comments in square brackets are for your interest and were not expected in the answer.]

1. The molecule shown to the right includes two functional groups from Table 3.1 of the course textbook.

A. (2 minutes) **Circle** and **name** the **two** functional groups.

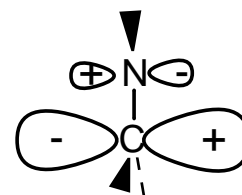
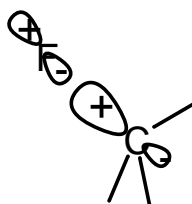
B. (7.5 minutes) In the space below **draw the shape** (not the energy) of **two** reasonable candidates for the **LUMO** of this molecule and of **three** reasonable candidates for its **HOMO**. Don't lavish too much artistic care on the drawings, but be sure to show relative sizes and signs of component AOs unambiguously. Give the conventional **name** for each of the five orbitals.



LUMO? I name σ_{CF}^*

LUMO? II name $\pi_{C=N}^*$

large on C, small on F
node between atoms



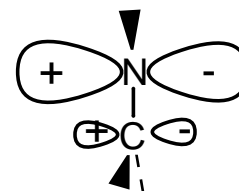
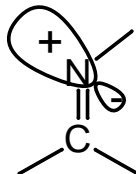
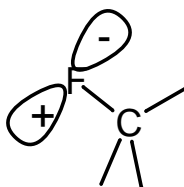
[Note the difference between σ (end-on) overlap on the left and π (side-by-side) overlap on the right.]

HOMO? I name n_F

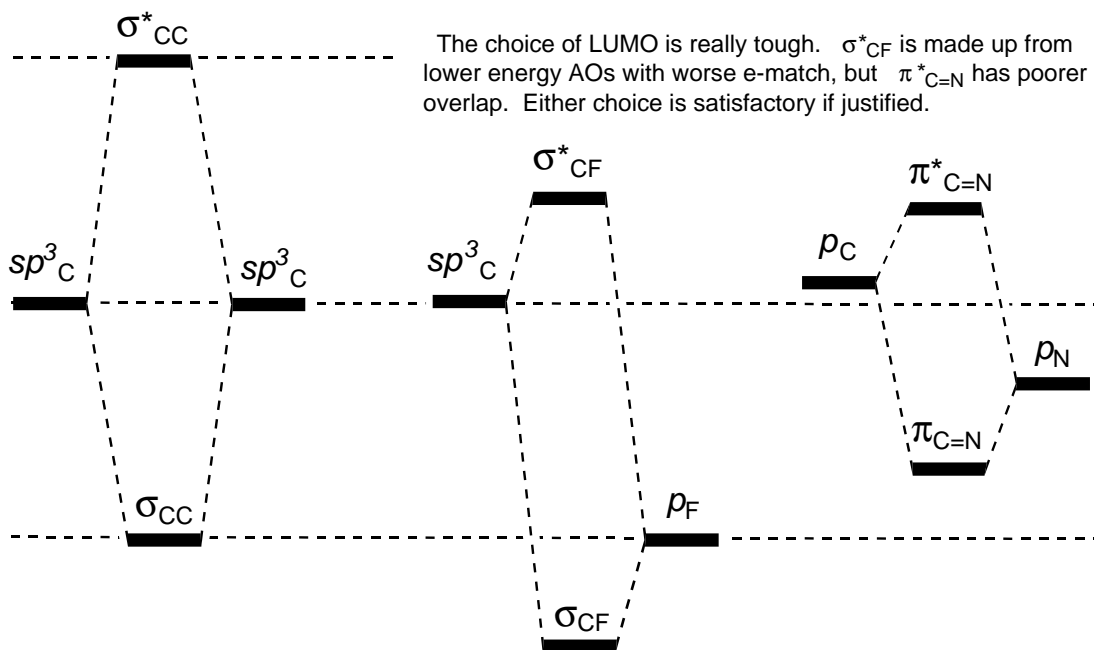
HOMO? II name n_N

HOMO? III name $\pi_{C=N}$

n = unshared pair



- C. (3 min) Use **lines** on the energy diagram below and **words** to **explain** which of your candidates should be **THE** LUMO.



[Note that the energy difference between differently hybridized orbitals on the same atom (p vs sp^3) is minor compared to the difference between orbitals on atoms with different nuclear charges (p_C vs p_N).]