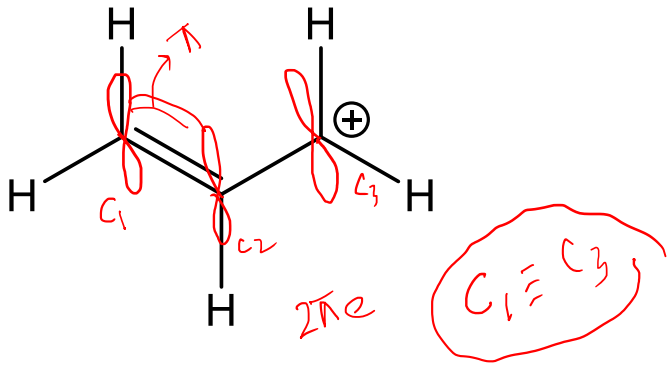
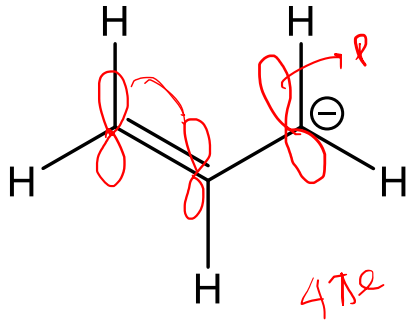
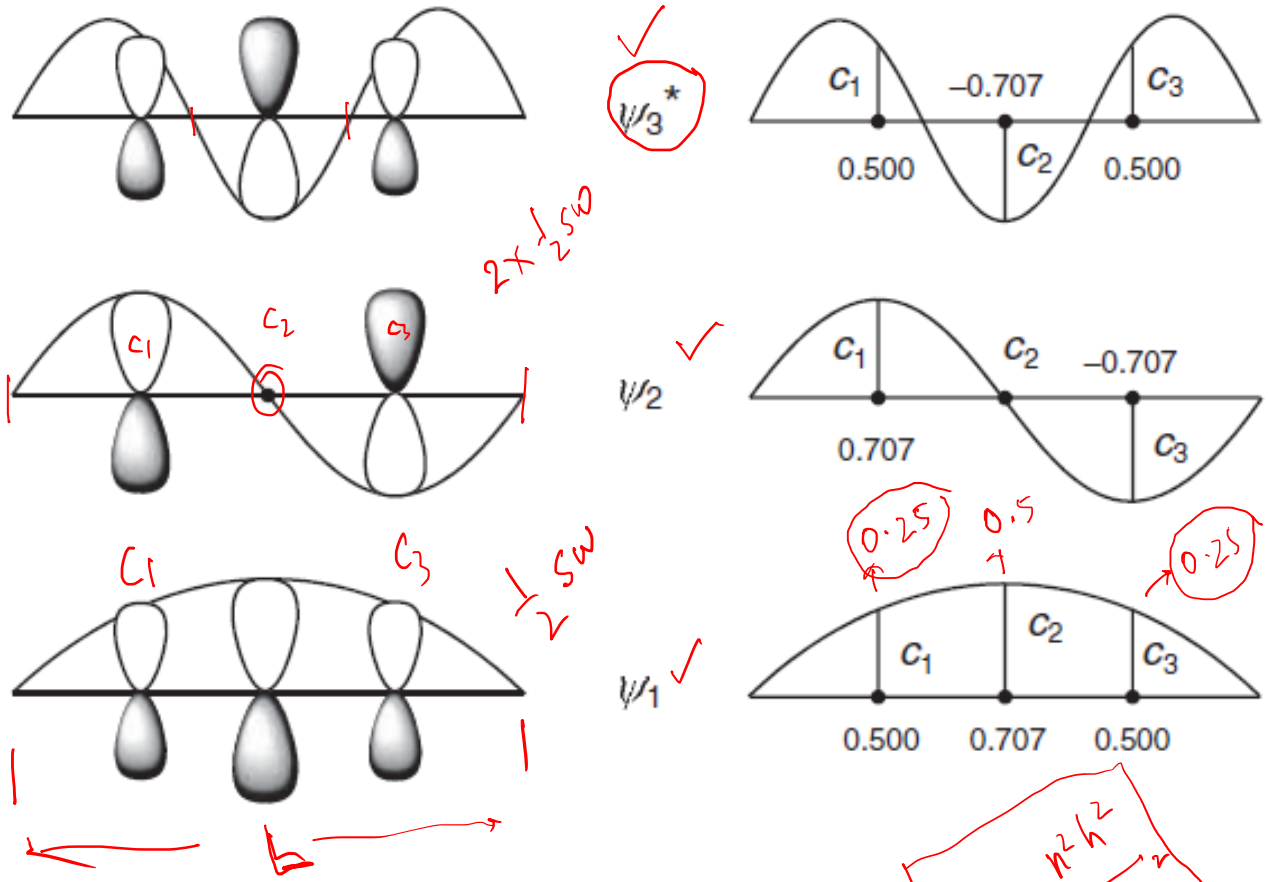
π-Molecular orbitals of allyl cation/anion



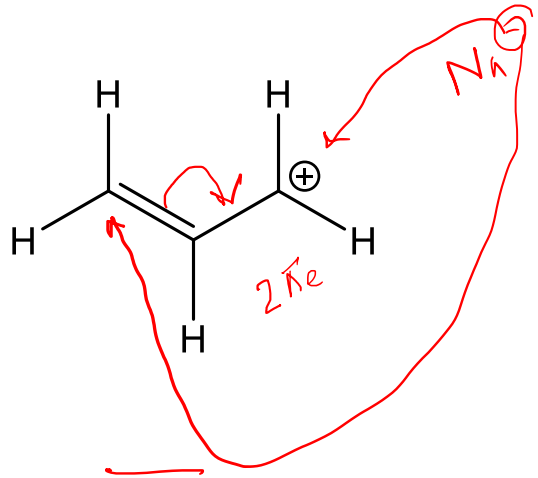


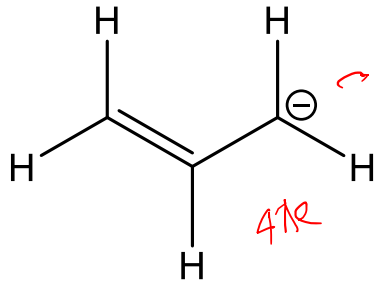
- ✓ *Both the allyl cation and anion are planar and symmetrical*
- ✓ *Two end carbons are same*

$\sum c_i^2 = 1$



$E_n = \frac{n^2 h^2}{8 m L^2}$

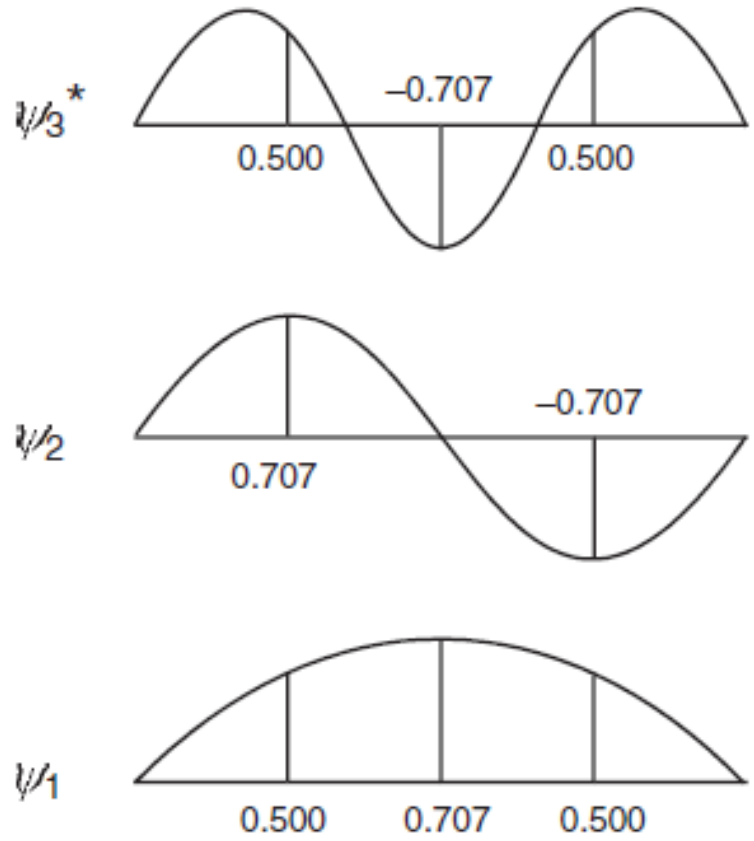




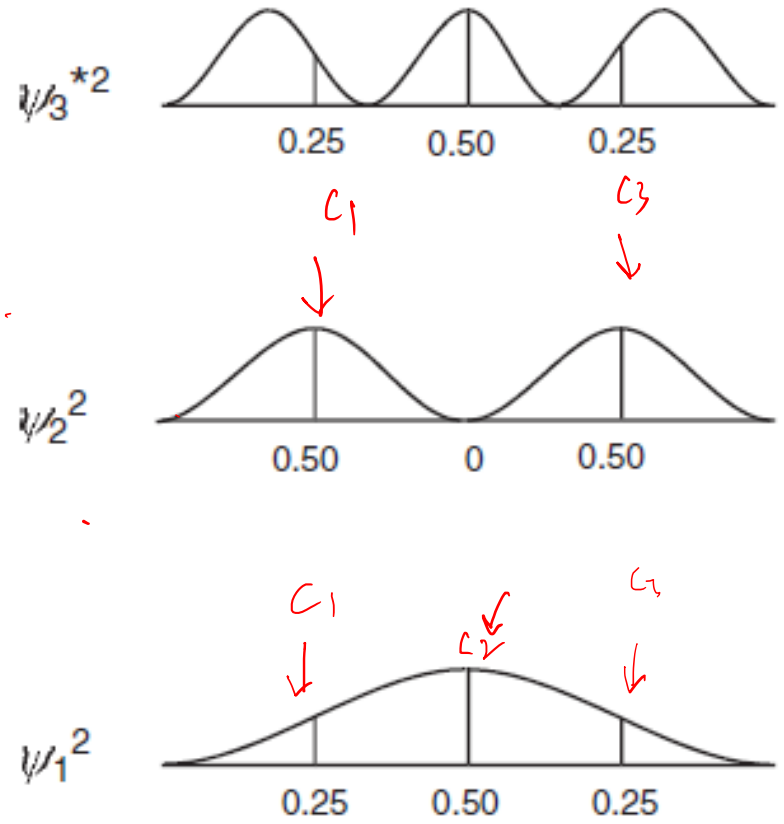
HOMO

LUMO

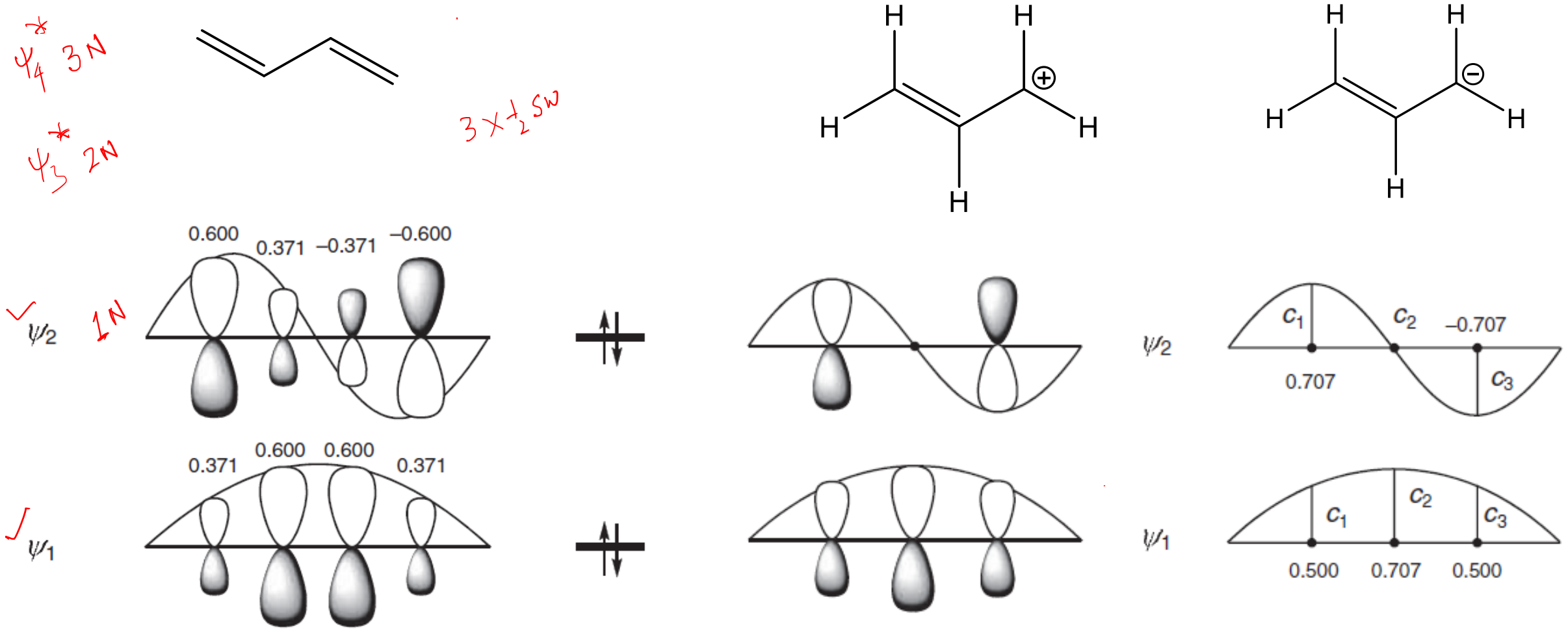
$c_1 = c_3$



(a) Wave functions



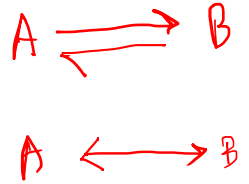
(b) Electron populations for one electron



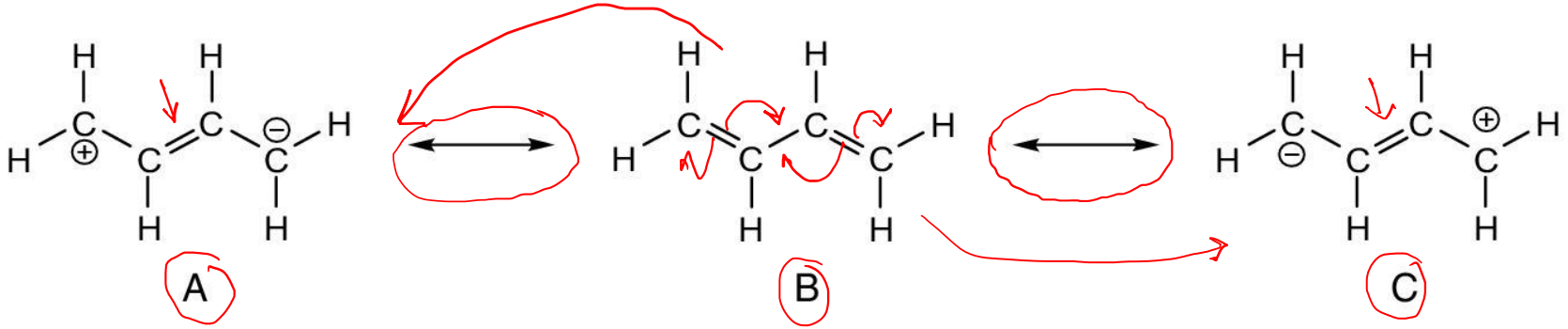
MO approach can explain: a) partial double bond character in the C2-C3 bond in butadiene

b) the equivalence of C1 and C3 carbons in allyl cation and anion

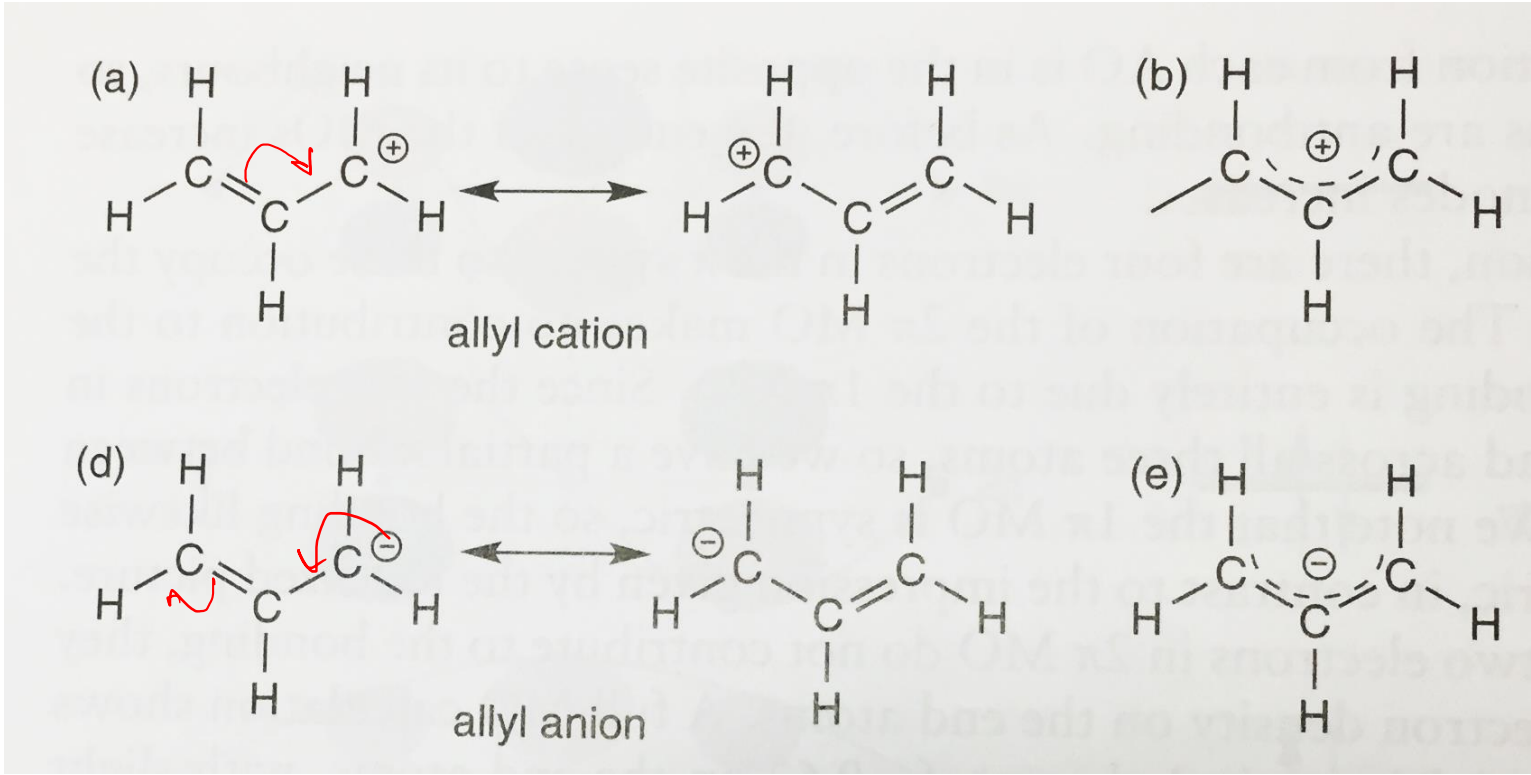
How do we explain these observations from hybridization approach (localized bonding)?



Resonance Structures

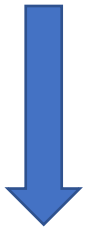


- *Resonance*: More than one possible Lewis structures for a molecule
- **A, B** and **C** are resonance structures; *they don't exist in reality*
- Butadiene is a combination of all the resonating structures-Resonance Hybrid


(a)
(b)
allyl cation
(d)
(e)
allyl anion

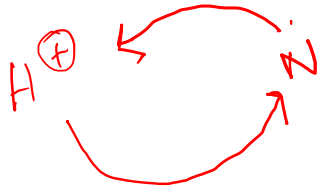
Formal Charge

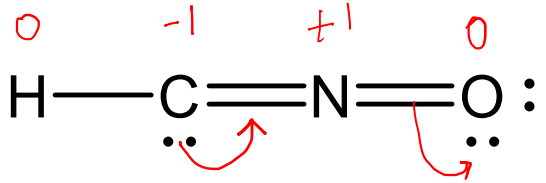
Formal charge: (Number of valence electrons in the neutral atom) – (number of valence electrons around the atom in molecule)



(Number of valence electrons in the neutral atom) – ½ (number of electrons in covalent bonds) - (number of electrons in lone pairs)

1. Calculate the formal charges on each atom in each structure.
2. Which are resonance structures?

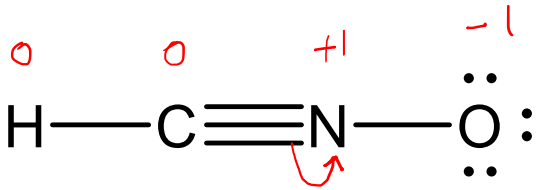


A) 

C = 4 − ½×6 − 2 = −1

N = 5 − ½×8 = +1

O = 6 − ½×4 − 4 = 0

B) 

C = 4 − ½×8 = 0

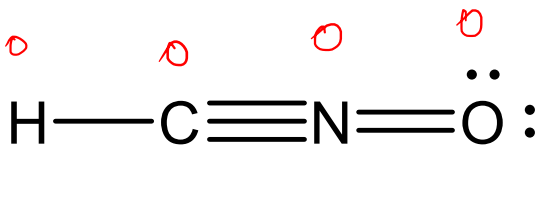
N = 5 − ½×8 = +1

O = 6 − ½×2 − 6 = −1

A, B, D

Res stm

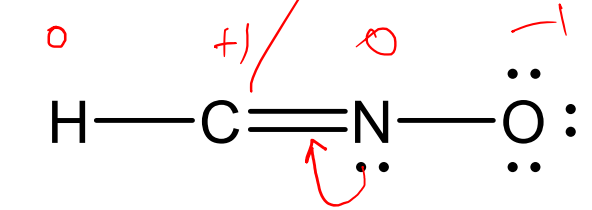
D less rxnt

C) 

C = 4 − ½×8 = 0

N = 5 − ½×10 = 0

O = 6 − ½×4 − 4 = 0

D) 

C = 4 − ½×6 = +1

N = 5 − ½×6 − 2 = 0

O = 6 − ½×2 − 6 = −1