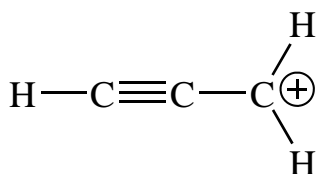


## Ex 22 - Pi delocalized systems

### Question One



The propargyl cation is shown. This molecule has five pi MOs. They are best described as two separate sets of pi MOs.

Which MO sets, and why separate?

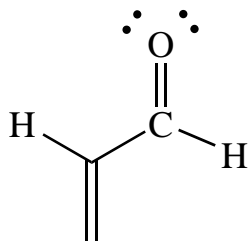
Understanding this will help with the next question.

You can think of this species as having a set of 3 pi MOs of the allyl system and a non-interacting set of 2 pi MOs of the ethylene system. The two MO sets are mutually perpendicular and that's why they are separate.

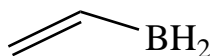
### Question Two

In class, we looked at the pi MOs for 2, 3 and 4 contiguous trigonal planar atoms corresponding to ethene, allyl and butadiene respectively. For each of the following species, determine

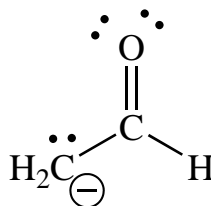
- the number of pi electrons
- whether its pi MOs will be like the ethene, allyl or butadiene system.
- which orbitals are the HOMO and the LUMO



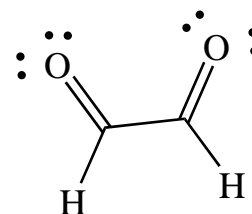
4 pi e  
butadiene  
HOMO is  $2\pi$   
LUMO is  $3\pi$



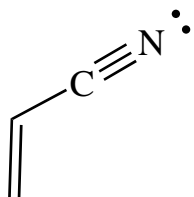
2 pi e  
allyl  
HOMO is  $1\pi$   
LUMO is  $2\pi$



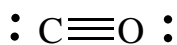
4  $\pi$  e  
allyl  
HOMO is  $2\pi$   
LUMO is  $3\pi$



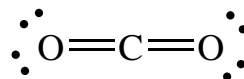
4 pi e  
butadiene  
HOMO is  $2\pi$   
LUMO is  $3\pi$



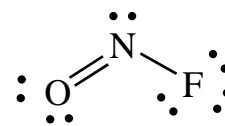
6 pi e  
4 e butadiene +  
non-interacting  
2 e ethene system



2 non-interacting  
ethene pi systems,  
4 pi e.  
HOMO are the  $1\pi$   
LUMO are the  $2\pi$



2 non-interacting  
allyl pi systems,  
8 pi e.  
HOMO are the  $2\pi$   
LUMO are the  $3\pi$



4  $\pi$  e  
allyl  
HOMO is  $2\pi$   
LUMO is  $3\pi$