Chem 22 HW set 12 non-graded

1. a-g in no particular order —

All have $\pi \rightarrow \pi^*$ transitions only —

Naphthalene is colorless, so it absorbs only in the UV;

Tetracene is the same type of chromophore, but extended so it absorbs in the visible —

appears orange ⇒ abs blue, $\lambda \approx 450-500$ nm

Azulene is very different — 7- + 5-membered rings produces a very different π-MO $\bar{e}$-level pattern than ≥ 6-membered rings — appears blue ⇒ abs orange, $\lambda \approx 600-650$ nm — (actually this abs is very broad, but centered in the orange, so we perceive blue.

Azulene has the smallest HOMO-LUMO gap since it absorbs at the longest λ

(h) Naph — 1,24 β ; Tetracene — 0,59 β ; Azulene — 0,477 + 0,400 → 0,88 β

↑ wow — that's not consistent with the observed λs. Keep in mind that these calcs are very approximate — but this chromophore clearly has a π-MO pattern much different than the others.

2. π-Systems ONLY


⇒

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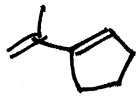
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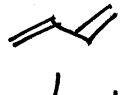
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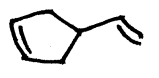
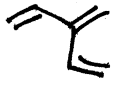
└ both 1,24 β


2 isolated π-bonds (2 $H_2C=CH_2$) ∴ 2,0 β

4 π


1,04 β

5 π


NBMO is HOMO 1,0 β

(b) (c)